Lecture notes

Advanced Quantum Mechanics

Master Degree in Physics

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Contents

Introduction

The aim is to provide the basic tools for working with open quantum systems, those systems whose interaction with the surrounding environment cannot be neglected. The general formalism will be revised, and the most important master equations will be introduced.

The main points of the course are:

- Matrix density formalism in analogy with the wavefunction
- Dynamics for the density matrix in two different approaches:

  axiomatic approach $\rightarrow$ Lindblad equation,
  microscopic approach $\rightarrow$ quantum brownian motion.

In parallel to this part of the course will be made a second part whose main points will be:

- Path Integral Theory
- Feynman-Vernon Theory
- Caldeira-Leggett Model

0.1 Suggested Books

H.P. Breuer and F. Petruccione, *The theory of open quantum systems*, Oxford University Press, Oxford, 2002.

E. Joos, H.D. Zeh, C. Kiefer, D.J.W. Giulini, J. Kupsch, I.-O. Stamatescu, *Decoherence and the Appearance of a Classical World in Quantum Theory*, Springer, 2nd ed. 2003, XII

Chapter 1

Standard Quantum Mechanics

In this first part of the course we recap the basic instruments of standard quantum mechanics, i.e. closed systems. Then we wisll consider this systems in statistical operator formalism.

A closed quantum system is assumed to be decoupled from the rest of the "universe" and fully described by its hamiltonian H.

1.1 The Axioms of the Quantum Mechanics

Quantum mechanics is based on the following axioms:

1. **States** To every physical system is associated an Hilbert space $\mathcal{H}$. The possible states of the system are represented by vectors $\psi \in \mathcal{H}$, with $||\psi|| = 1$.

2. **Evolution** The vector representing the state of a system evolve according to the Schrödinger equation

$$i\hbar \frac{d}{dt}\psi_t = H\psi_t$$

with initial condition $\psi_0 = \psi$, where H is the hamiltonian operator associated to the system.

3. **Observable Quantities** Observable quantities are represented by self-adjoint operators: The classical observable A will be mapped into a self-adjoint operator $\hat{A}$

$$A \longrightarrow \hat{A} : \hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$$

where $\{\,|a_n\rangle\,\}$ are eigenstates of the operator $\hat{A}$. They form an orthonormal basis. $\{\,a_n\,\}$ are eigenvalues, they are real numbers.

Since $\{\,|a_n\rangle\,\}$ is an orthonormal basis, the decomposition on this basis of a whatever state of the system is unique:

$$|\psi\rangle = \sum_n C_n\,|a_n\rangle \qquad \text{where} \quad \begin{cases} Cn = \langle a_n|\psi\rangle \\ \\ \sum_n |C_n|^2 = 1 \end{cases}$$

4. **Outcomes of measurements** The possible outcome of a measurement of the observable A are the eigenvalues a_n of the corresponding operator $\hat{A}$. The outcomes are randomly distributed, and the probability of obtaining the outcome a_n, when the system is described by the state vector ψ, is

$$P[a_n] = |\langle a_n|\psi\rangle|^2$$

5. **Collapse of the wave function** At the end of the measurement process, the system collapse to the eigenstate corresponding to the eigenvalue which has been observed:

$$|\psi\rangle \xrightarrow[\text{MEASUREMENT}]{} |a_n\rangle \qquad \text{if } a_n \text{ is the measured outcome}$$

NOTES:

- The Schrödinger equation is linear and deterministic. The collapse of the wave function is non-linear and stocastic. They are two incompatible dynamical principle.
- It is not clear when a system evolves according to the Schrödinger equation and when according to the collapse $\rightarrow$ measurement problem.
- If the collapse is so problematic, why was introduced in the first place?

The requiring to have an evolution due to two different dynamics is one of the open problems in quantum mechanics. Let's consider a system which have probability of 50% to be in $x = a$ and 50% to be in $x = b$. We measure the position and we find the system in $x = a$. Immediately after, if the evolution it was only due to deterministic dynamics of the Schrödinger equation, we'll have again probability 50% and 50% to find the system in $x = a$ or in $x = b$. Instead if we do again a measure of position we will find the system in $x = a$. For this reason we hate to introduce the concept of the wave function collapse and the measurement postulate.

1.1.1 Entanglement

A subject in quantum mechanics that do not have any correspondence in classical world is the **entanglement**. Consider two systems S_1 and S_2 with associated Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Let $\{|i\rangle\}_i$ and $\{|j\rangle\}_j$ be the two basis of the Hilbert spaces. We can consider also the entire system S as $S = S_1 \otimes S_2$ with associated $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Therefore a generic state $|\psi\rangle \in \mathcal{H}$ can be expressed as linear combination of the two basis.

$$|\psi\rangle = \sum_{ij} C_{ij} |i\rangle \otimes |j\rangle$$

$|\psi\rangle$ is called entangled if is not possible to describe it as tensor product of two other states

$$|\psi\rangle \neq |\phi\rangle \otimes |\chi\rangle$$

where

$$\begin{cases} |\phi\rangle \in \mathcal{H}_1 \\ \\ |\chi\rangle \in \mathcal{H}_2 \end{cases}$$

Otherwise if we can do it

$$|\psi\rangle = |\phi\rangle \otimes |\chi\rangle$$

the state $|\psi\rangle$ is called separable or product state.

Example Let $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$, where the two Hilbert spaces are isomorphic to $\mathbb{C}^2$, be

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big[|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\big]$$

Consider two generic states living each one in one of the two Hilbert spaces

$$\begin{cases} |\phi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \quad \in \mathcal{H}_1 \\ \\ |\chi\rangle = a\,|0\rangle + b\,|1\rangle \quad \in \mathcal{H}_2 \end{cases}$$

Since the Hilbert spaces are two dimensional, we used the set $\{\,|0\rangle\,,|1\rangle\,\}$ as basis for each of the spaces. This is the basis that is typically used for a two dimensional space. Therefore we can consider the tensor product of this two states

$$|\phi\rangle \otimes |\chi\rangle = \alpha a\,|0\rangle \otimes |0\rangle + \alpha b\,|0\rangle \otimes |1\rangle + \beta a\,|1\rangle \otimes |0\rangle + \beta b\,|1\rangle \otimes |1\rangle$$

So this product is equal to $|\psi\rangle$ only if

$$\begin{cases} \alpha a = \beta b = \dfrac{1}{\sqrt{2}} \\ \\ \alpha b = \beta a = 0 \end{cases}$$

But we are not able to satisfy both the two conditions together. Therefore, since we define $|\phi\rangle$ and $|\chi\rangle$ as totally generic, the state $|\psi\rangle$ can not be expressed as tensor product of two other states and for definition is an entangled state.

Example Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be the same as the previous example. Let $|\psi\rangle$ be define as

$$\begin{aligned} |\psi\rangle &= \frac{1}{\sqrt{2}}\big[|1\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\big] \\ &= |1\rangle \otimes \frac{1}{\sqrt{2}}\big[|0\rangle + |1\rangle\big] \\ &= |\phi\rangle \otimes |\chi\rangle \end{aligned}$$

Therefore the state $|\psi\rangle$ is a separated state.

1.2 The Density Matrix

The previous axioms assume that the state of the system is perfectly known. This is not true in reality. Like in classical mechanics (where one resorts to statistical mechanics), in general we have only a partial knowledge of the state of the system. What we know about the system is an ensemble of possible states associated to a probability:

$$\{ \psi_k, p_k \} \qquad \text{with} \quad \sum_k p_k = 1$$

where ψ_k are the possible states of the system and p_k are the (classical) probabilities about the state occupied by the system.

In principle, we can continue to use the previous formalism, paying attention to average over the distribution $\{ p_k \}$.

The three processes which determine the evolution of a state are:

$$\begin{cases} \text{EVOLUTION:} & i\hbar \dfrac{d}{dt}\psi_k(t) = H\psi_k(t) \\ \text{PROBABILITIES:} & P[a_n] = \sum_k p_k |\langle a_n|\psi_k\rangle|^2 \\ \text{COLLAPSE:} & |\psi_k\rangle \xrightarrow[\text{MEASUREMENT}]{} |a_n\rangle \end{cases}$$

Before we measure, the system is described by the state $|\psi_k(t)\rangle$, after the measurement by the state $|a_n\rangle$ with a probability $P[a_n]$. The measurement process is an instantaneous process. After the measure the system evolves again as described by the Schrödinger equation, which is a slow process.

But there is another way, which is more convenient from the practical point of view, it is the **density matrix** formalism:

$$\rho = \sum_k p_k |\psi_k\rangle \langle\psi_k|$$

ρ is the statistical operator. $\{ p_k \}$ give us information about the probabilities and $\{ |\psi_k\rangle \langle\psi_k| \}$ the information about the states. Let $\{ |a_n\rangle \}$ be a basis of $\mathcal{H}$ of dimension N. Then there are N basis states.

On this basis we can define a representation of the statistical operator ρ

$$\rho_{nm} = \begin{pmatrix} \langle a_1|\rho|a_1\rangle & \langle a_1|\rho|a_2\rangle & \dots & \langle a_1|\rho|a_N\rangle \\ \langle a_2|\rho|a_1\rangle & \langle a_2|\rho|a_2\rangle & \dots & \langle a_2|\rho|a_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle a_N|\rho|a_1\rangle & \langle a_N|\rho|a_2\rangle & \dots & \langle a_N|\rho|a_N\rangle \end{pmatrix}$$

ρ_{nm} is called the **density matrix** relative to the basis $\{ |a_n\rangle \}$. There is a conceptual difference between the statistical operator and the density matrix.

The explicit form of ρ_{nm} depends on the chosen basis in which we describe the system, but is ever a representation of the statistical operator ρ.

Example Let us consider a system with two degrees of freedom, the simplest non trivial system. $\mathrm{Dim}\{\mathcal{H}\} = 2$, where $\mathcal{H}$ is the Hilbert space associated to the system.

This system could be a particle in a potential well that allows only two states, or the first two states of a harmonic oscillator, or a state of spin.

Let us fix a basis $\{ |0\rangle, |1\rangle \}$ in $\mathcal{H}$. Let us consider just one state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big[|0\rangle + |1\rangle\big] \equiv |+\rangle$$

This state can be associated with:

- **statistical operator**

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}\big[|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|\big]$$

- **density matrix** in the $\{ |0\rangle, |1\rangle \}$ basis

$$\rho_{nm} = \begin{pmatrix} \langle 0|\rho|0\rangle & \langle 0|\rho|1\rangle \\ \langle 1|\rho|0\rangle & \langle 1|\rho|1\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

  where $\langle i|\rho|i\rangle$ are the probabilities of getting the outcome "i" in a measurement and $\langle i|\rho|j\rangle$, $i \neq j$, are the interference terms. In fact

$$\langle a_n|\rho|a_n\rangle = \langle a_n|\psi\rangle\langle\psi|a_n\rangle = |\langle a_n|\psi\rangle|^2 = P[a_n] = \text{PROBABILITY}$$

  here is shown for simple case with $\rho = |\psi\rangle\langle\psi|$, but it works in general.

$$\langle a_n|\rho|a_m\rangle = \langle a_n|\psi\rangle\langle\psi|a_m\rangle \neq 0$$

  $|\psi\rangle$ has non-vanishing component along both $|a_n\rangle$ e $|a_m\rangle$. There is a superposition and when there is superposition one can do interference.

Example From the previous example let's consider two state with the same probability

$$\begin{cases} |+\rangle \equiv \dfrac{1}{\sqrt{2}}\big[|0\rangle + |1\rangle\big] \\ \\ |-\rangle \equiv \dfrac{1}{\sqrt{2}}\big[|0\rangle - |1\rangle\big] \end{cases}$$

This two states[1] are superpositions of other two states: $|0\rangle$ e $|1\rangle$. In this case the statistical operator is

[1] The states $|+\rangle$ and $|-\rangle$ are the eigenvectors of Pauli's matrix σ_x.

$$\rho = \frac{1}{2} |+\rangle \langle +| + \frac{1}{2} |-\rangle \langle -|$$

In fact we associated the same probability to both states, i.e. 1/2. Turns out, however, that ρ can be expressed in terms of $|0\rangle$ and $|1\rangle$, obtaining

$$\rho = \frac{1}{2} \left[|0\rangle \langle 0| + |1\rangle \langle 1| \right]$$

Representing ρ on basis $\{ |0\rangle, |1\rangle \}$ we obtain a matrix density of the form

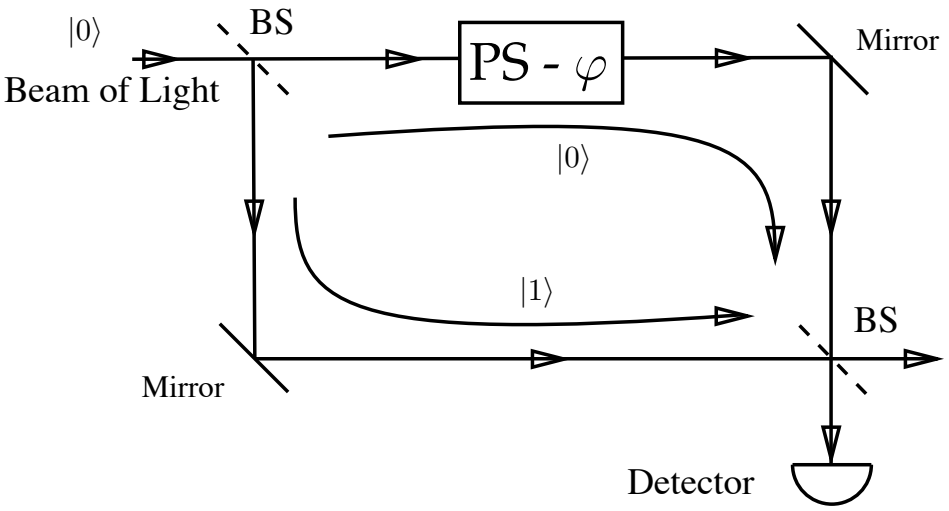
$$\rho_{nm} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

It follows that the system is always in a superposition of states $|0\rangle$ and $|1\rangle$, but it is never possible to see the phenomenon of interference because

$$\langle 0|\rho|1\rangle = \frac{1}{2} \langle 0|+\rangle \langle +|0\rangle + \frac{1}{2} \langle 0|-\rangle \langle -|0\rangle = 0$$

Example Mach-Zender Interferometer

Let's consider the experiment known as the Mach-Zender interferomenter, the scheme is reported in figure.



where $|0\rangle$ is the electric beam propagating in the upper arm and $|1\rangle$ in the lower. BS are Beam-Splitters, physically half silvered mirrors. PS - φ is a phase shift, mathematically is just a multiplication by a phase.

We can represent mathematically BS with an operator, that with the basis set $\{ |0\rangle, |1\rangle \}$ have the form:

$$U_{\text{BS}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

If we represent due two states on the same basis, we can study the action of the operator U_{BS}.

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

Therefore the action of U_{BS} is

$$U_{\mathrm{BS}}\,|0\rangle = \frac{1}{\sqrt{2}}\big[|0\rangle + |1\rangle\big] = |+\rangle$$

$$U_{\mathrm{BS}}\,|1\rangle = \frac{1}{\sqrt{2}}\big[|0\rangle - |1\rangle\big] = |-\rangle$$

Notice that the operator U_{BS} is unitary, as it should be, in fact otherwise it will not act as a quantum transformation.

$$U_{\mathrm{BS}}^{\dagger} U_{\mathrm{BS}} = U_{\mathrm{BS}}^{-1} U_{\mathrm{BS}} = \mathrm{I}_2$$

where I_2 is the identity matrix 2×2

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Let's consider how the state of incoming beam, $|0\rangle$, change inside the interferometer:

$$|0\rangle \quad \xrightarrow[U_{\mathrm{BS}}]{} \quad \frac{1}{\sqrt{2}}\big[|0\rangle + |1\rangle\big] = |+\rangle$$

The second operator acts on the beam is a phase shifter, U_{PS}, that acts only on the state $|0\rangle$, as we see in figure.

$$|+\rangle \quad \xrightarrow[U_{\mathrm{PS}}]{} \quad \frac{1}{\sqrt{2}}\big[e^{i\varphi}\,|0\rangle + |1\rangle\big] = |\psi\rangle$$

If we suppose that mirrors are perfect and don't imply variation of the state of the system, the next operator we have to apply is again U_{BS}

$$|\psi\rangle \quad \xrightarrow[U_{\mathrm{BS}}]{} \quad \frac{1 + e^{i\varphi}}{2}\,|0\rangle - \frac{1 - e^{i\varphi}}{2}\,|1\rangle$$

It has so that the state who detector analyze is a superposition. The probabilities to have on the detector just one of the two states $|0\rangle$ and $|1\rangle$ area $\mathrm{P}^{+}[0]$ e $\mathrm{P}^{+}[1]$ respectively:

$$\begin{cases} \mathrm{P}^{+}[0] = \left|\dfrac{1 + e^{i\varphi}}{2}\right|^2 = \dfrac{1 + \cos\varphi}{2} \\[2ex] \mathrm{P}^{+}[1] = \left|\dfrac{1 - e^{i\varphi}}{2}\right|^2 = \dfrac{1 - \cos\varphi}{2} \end{cases}$$

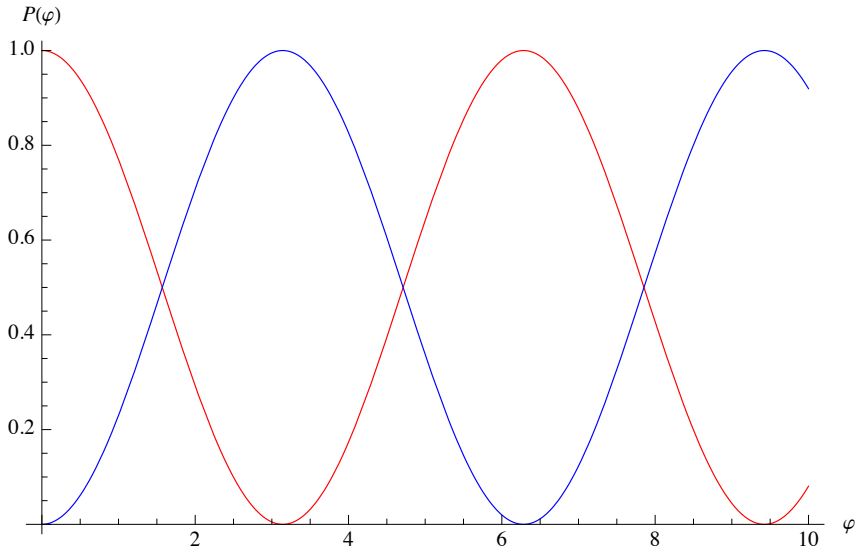
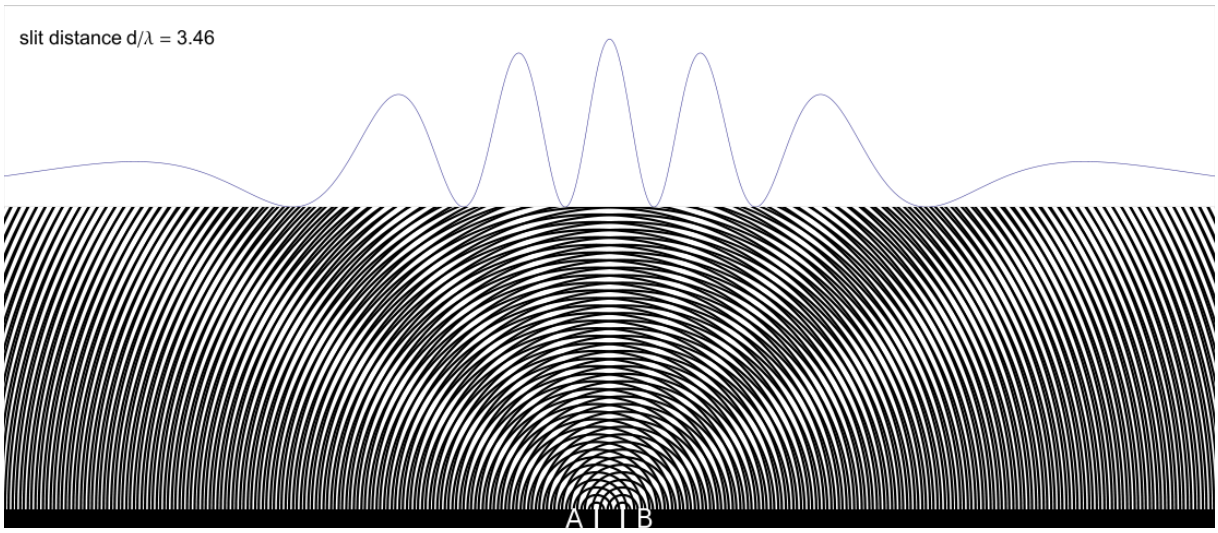


Figure 1.1: $P^+[0]$ in rosso e $P^+[1]$ in blu.

The oscillation present in $P^+[0]$ and $P^+[1]$ respect φ is due to the interference between the two terms of the superposition.

Example Let's consider the double-slit or Young's experiment, the scheme is reported in figure.



Suppose that the state that passes through slit A is $|0\rangle$ and through slit B is $|1\rangle$. The superposition of the two states is shown in interference pattern on the screen. If we close one of the two slit we will not able to see the interference fringes.

This is why the off-diagonal elements are also called **interference terms**.

Note that the information that density matrix give us is always relative to the basis on which we have decided to represent the statistical operator. Let us change basis. We consider $\{ |+\rangle, |-\rangle \}$ basis, in this case the statistical operator $\rho = |+\rangle \langle +|$ is reppresented with

$$\rho_{nm} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

In fact the probability to find the state of our system in $|+\rangle$ is equal to 1. Our state is certainly in $|+\rangle$ state and is not in the $|-\rangle$ state. There are no interference terms. There is no superposition, with respect to $|+\rangle$ and $|-\rangle$, so it cannot be used to create interference.

Example Let us suppose now that the system can be in one of the two states:

$$\begin{cases} |0\rangle & \text{with probability } 50\% \\ \\ |1\rangle & \text{with probability } 50\% \end{cases}$$

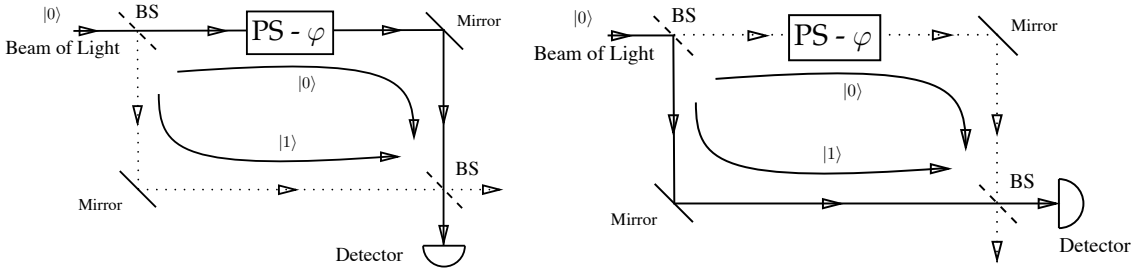
Then we have statistical operator

$$\rho = \frac{1}{2}\,|0\rangle\,\langle 0| + \frac{1}{2}\,|1\rangle\,\langle 1|$$

and the density matrix in the $\{\,|0\rangle\,, |1\rangle\,\}$ basis

$$\rho_{nm} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The probabilities are the same as in the previous case, but now there are no off-diagonal elements, because there is no superposition between $|0\rangle$ and $|1\rangle$, so the interference cannot be created. In the Mach-Zender interferometer we can see this each time the beam either goes up or down.



In the (a) case the state of the system is

$$\begin{cases} |0\rangle \quad \xrightarrow[U_{\mathrm{PS}}]{} \quad e^{i\varphi}\,|0\rangle \quad \xrightarrow[U_{\mathrm{BS}}]{} \quad \dfrac{1}{\sqrt{2}} e^{i\varphi}\big[|0\rangle + |1\rangle\big] \\ \\ \mathrm{P}^{(a)}[0] = \left|\dfrac{1}{\sqrt{2}} e^{i\varphi}\right|^2 = \dfrac{1}{2} \end{cases}$$

In the (b) case instead

$$\begin{cases} |1\rangle \quad \xrightarrow[U_{\mathrm{PS}}]{} \quad |1\rangle \quad \xrightarrow[U_{\mathrm{BS}}]{} \quad \dfrac{1}{\sqrt{2}}\big[|0\rangle - |1\rangle\big] \\ \\ \mathrm{P}^{(b)}[0] = \left|\dfrac{1}{\sqrt{2}}\right|^2 = \dfrac{1}{2} \end{cases}$$

If we close randomly one or the other arm of the interferometer the probability that the state of the system is represented by $|0\rangle$ is

$$\mathrm{P}_{\mathrm{TOT}} = \frac{1}{2}\mathrm{P}^{(a)}[0] + \frac{1}{2}\mathrm{P}^{(b)}[0] = \frac{1}{2}$$

$\mathrm{P}_{\mathrm{TOT}}$ is independent of φ. One cannot do interference.

Example Suppose the system now can be in one of the following two states

$$\begin{cases} |+\rangle & \text{with probability } 50\% \\ |-\rangle & \text{with probability } 50\% \end{cases}$$

Then the statistical operator is

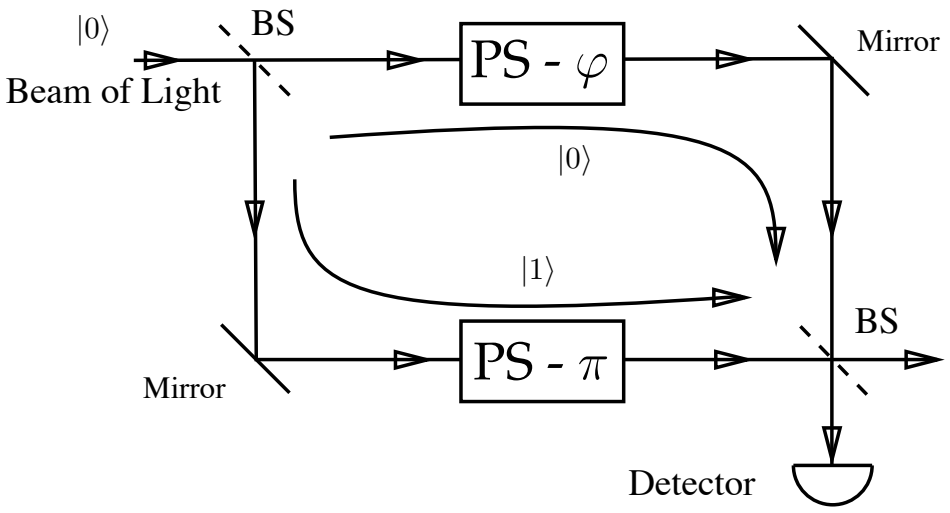
$$\begin{aligned} \rho =& \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| \\ =& \frac{1}{4}\left[|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|\right] + \frac{1}{4}\left[|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|\right] \\ =& \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \end{aligned}$$

same as before. The density matrix in the $\{\,|0\rangle, |1\rangle\,\}$ basis

$$\rho_{nm} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

but now we have superpositions, so why are the off-diagonal elements zero?

Example Let's consider the Mach-Zender interferometer with a second phase shifter of a fixed angle, π, as is shown in figure.



In this case the final state is

$$-\frac{1-e^{i\varphi}}{2}\left|0\right\rangle+\frac{1+e^{i\varphi}}{2}\left|1\right\rangle$$

$$\begin{cases} \mathrm{P}^{-}[0]=\left|\dfrac{1-e^{i\varphi}}{2}\right|^{2}=\dfrac{1-\cos\varphi}{2} \\ \mathrm{P}^{-}[1]=\left|\dfrac{1+e^{i\varphi}}{2}\right|^{2}=\dfrac{1+\cos\varphi}{2} \end{cases}$$

Notice that the coefficients in this case respect the previous are inverted.

Let's suppose we can activate the second phase π-shifter casually. The probability associated to the state $|0\rangle$ become

$$\mathrm{P}[0]=\mathrm{P}^{+}[0]+\mathrm{P}^{-}[0]=\frac{1}{2}$$

The probability P[0] is constant, so we are not able to do an interference measurement.

So, in this case there are superpositions. However, since the phases "1" and "-1" are randomly distributed, and we are not in control of this randomicity, they add destructively and cancel the possibility of seeing interference effects.

Therefore, the fact that the off-diagonal elements of the density matrix are zero does not mean necessary the absence of superpositions. In general it means that, if there are superpositions, they cannot be used to make interference. This because the interference terms ado incoherently and wash away the possibility of making interference.

In previous examples we show we can obtain the same matrix density represented in the same basis, $\{\,|0\rangle\,,|1\rangle\,\}$, for two different prepared systems:

$$\begin{cases} |+\rangle & \text{with probability } 50\% \\ \\ |-\rangle & \text{with probability } 50\% \end{cases} \qquad \longrightarrow \qquad \rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\begin{cases} |0\rangle & \text{with probability } 50\% \\ \\ |1\rangle & \text{with probability } 50\% \end{cases} \qquad \longrightarrow \qquad \rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The systems are different, in the sense that, in order to prepare them, one has to use different procedures. Different ensemble give rise to the same statistical operator. The correspondence between ensembles and the statistical operators in not one to one but many to one. Passing from a statistical mixture to a density matrix we lose information on the system, therefore from a density matrix we can't reconstruct a statistical mixture, i.e. how the state has been prepared.

1.3 Propriesties of the Statistical Operator

The more general definition of a statistical operator is

$$\rho = \sum_k p_k \left|\psi_k\right\rangle \left\langle\psi_k\right|$$

where p_k is the probability that the system is described by the state $|\psi_k\rangle$. ρ has the following proprieties:

- It is a **linear operator**: $\rho : \mathcal{H} \to \mathcal{H}$ This is the reason for the name statistical "operator"

$$|\psi\rangle \in \mathcal{H} \Rightarrow \rho\left|\psi\right\rangle = \sum_k p_k \left|\psi_k\right\rangle \left\langle\psi_k|\psi\right\rangle = \sum_k p_k \left\langle\psi_k|\psi\right\rangle \left|\psi_k\right\rangle = \sum_k C_k \left|\psi_k\right\rangle$$

  Linearity is obvious.

- It is a **positive operator**. An operator O is positive if

$$\forall\, |\psi\rangle \in \mathcal{H} \qquad \langle\psi|O|\psi\rangle \geq 0$$

$$\langle\psi|\rho|\psi\rangle = \sum_k p_k \left\langle\psi|\psi_k\right\rangle \left\langle\psi_k|\psi\right\rangle = \sum_k p_k| \left\langle\psi|\psi_k\right\rangle|^2$$

  which is always non-negative. If the Hilbert space $\mathcal{H}$ is finite dimensional, since ρ is representable by a square matrix, then is possible to define its trace as

$$\mathrm{Tr}\left[\rho\right] \equiv \sum_n \langle\phi_n|\rho|\phi_n\rangle \qquad \text{with } \left\{\, |\phi_n\rangle \,\right\}_n \text{ basis of } \mathcal{H}$$

$$\begin{aligned}\mathrm{Tr}\left[\rho\right] &= \sum_n \langle\phi_n| \left[\sum_k p_k \left|\psi_k\right\rangle \langle\psi_k|\right] |\phi_n\rangle \\ &= \sum_{n,k} p_k \left|\langle\phi_n\psi_k\rangle\right|^2\end{aligned}$$

It is a sum of non-negative elements, so it converges somewhere, to a finite number or to infinity

If we consider an other basis of $\mathcal{H}$, $\{\,|\chi_m\rangle\,\}$, which is related to the first according to the following relation

$$|\chi_m\rangle = \sum_n C_{mn} \left|\phi_n\right\rangle \qquad \text{where } C_{mn} = \langle\phi_n|\chi_m\rangle$$

$$\begin{aligned}\mathrm{Tr}\left[\rho\right] &= \sum_m \langle\chi_m|\rho|\chi_m\rangle \\ &= \sum_{m,n,n'} C^*_{mn'} C_{mn} \langle\phi_{n'}|\rho|\phi_n\rangle \\ &= \sum_{n,n'} \left(\sum_m C^*_{mn'} C_{mn}\right) \langle\phi_{n'}|\rho|\phi_n\rangle\end{aligned}$$

where

$$\sum_m C^*_{mn'} C_{mn} = \sum_m \langle\phi_n|\chi_m\rangle \langle\chi_m|\phi_{n'}\rangle = \langle\phi_n|\phi_{n'}\rangle = \delta_{nn'}$$

Then

$$\mathrm{Tr}\left[\rho\right] = \sum_n \langle\phi_n|\rho|\phi_n\rangle$$

The trace does not depend on the choice of the basis.

- The **trace is equal to one**

$$\begin{aligned}\mathrm{Tr}\left[\rho\right] &= \sum_n \langle\phi_n| \left[\sum_k p_k \left|\psi_k\right\rangle \langle\psi_k|\right] |\phi_n\rangle \\ &= \sum_k p_k \left[\sum_n \left|\langle\phi_n|\psi_k\rangle\right|^2\right] \\ &= \sum_k p_k ||\psi_k||^2 = \sum_k p_k = 1\end{aligned}$$

Notice that in the last expression the sum $\sum_k p_k$ is the sum of the probabilities that the system is described by the state $|\psi_k\rangle$. This is a fundamental point of this formalism.

Actually, **these three conditions are sufficient to characterize a statistical operator**. Suppose ρ is a linear and positive operator on finite dimensional $\mathcal{H}$

$$\begin{aligned} \langle\phi|\rho\phi\rangle \geq 0 \quad \Rightarrow \quad \langle\phi|\rho\phi\rangle &= \langle\phi\rho|\phi\rangle \quad \text{for the positivity} \\ &= \langle\phi|\rho^\dagger\phi\rangle \quad \text{because the adjoint exists} \\ \Rightarrow \quad \rho = \rho^\dagger & \qquad \text{self-adjointness} \end{aligned}$$

Being self-adjoint it admits the spetral decomposition

$$\rho = \sum_k \lambda_k \left|\psi_k\right\rangle \left\langle\psi_k\right|$$

where $\{\ \lambda_k\ \}$ are non negative eigenvalues and $\{\ |\psi_k\rangle\ \}$ are eigenstates, they are orthonormal.

From the trace condition we have $\sum_k \lambda_k = 1$, which means that we can interpret the $\{\ \lambda_k\ \}$ as probabilities, for this reason we call it statistical operator. Remember that the decomposition in general is not unique, just if we do the decomposition on the eigenstate basis.

Therefore

$$\boldsymbol{\rho \Longleftrightarrow \text{Linear, Positive, Trace-1 Operators}}$$

In the case of infinite dimensional Hilbert spaces, one has to be a little more careful, but nothing substantial changes.

Typically the states of a system are normalized vectors in a Hilbert space $\mathcal{H}$ and are defined at least by a phase. There are systems that this description is insufficient, for example the final state of a particle that can decay in various branches with a certain associated probabilities. Therefore there are two types of states described by a statistical operator:

$$\begin{cases} \rho = \left|\psi\right\rangle \left\langle\psi\right| & \textbf{Pure states} \\ \\ \rho = \sum_k p_k \left|\psi_k\right\rangle \left\langle\psi_k\right| & \textbf{Statistical mixture} \end{cases}$$

In the first case we know exactly the state of the system. In the second case no, we can just associate a certain probability to each state. How can they be differentiated? Let's consider the square of the statistical operator: For a pure state

$$\rho^2 = \rho$$

for a statistical mixture we consider the spectral decomposition Considering the spectral decom-

position the $\{ |\psi_k\rangle \}$ are orthonormal.

$$\rho^2 = \left[\sum_k p_k |\psi_k\rangle \langle\psi_k|\right] \left[\sum_n p_n |\psi_n\rangle \langle\psi_n|\right]$$

$$= \sum_{nk} p_n p_k |\psi_k\rangle \langle\psi_k|\psi_n\rangle \langle\psi_n| = \sum_{nk} p_n p_k \delta_{k,n} |\psi_k\rangle \langle\psi_n|$$

$$= \sum_k p_k^2 |\psi_k\rangle \langle\psi_k| \neq \rho$$

Theorem Let ρ be a statistical operator. Then

$$\mathrm{Tr}\left[\rho^2\right] \leq 1$$

$$\mathrm{Tr}\left[\rho^2\right] = 1 \quad \Longleftrightarrow \quad \rho \text{ is a pure state}$$

Proof. Si considera la decomposizione spettrale

$$\rho = \sum_k p_k |\psi_k\rangle \langle\psi_k|$$

and as we show before

$$\rho^2 = \sum_k p_k^2 |\psi_k\rangle \langle\psi_k|$$

$$\mathrm{Tr}\left[\rho^2\right] = \sum_k p_k^2 \leq \left(\sum_k p_k\right)^2 = 1$$

in fact

$$\left(\sum_k p_k\right)^2 = \sum_k p_k^2 + \sum_{k \neq j} p_k p_j$$

where $p_k p_j \geq 0$. In the case of a pure state the inequality becomes an equality.

$$\sum_k p_k^2 = 1 \quad \Longleftrightarrow \quad \sum_{k \neq j} p_k p_j = 0$$

In effect there is just a p_k different from 0, and equal to 1.

Is in common use identify both the statistical operator and density matrix with the same notation ρ and rarely the name statistical operator is used in literature. Density matrix indicates both statistical operator and density matrix.

1.4 The Bloch Sphere

Let us consider a two dimensional Hilbert space $\mathcal{H}$. The system has two degrees of freedom. Let $\{ |0\rangle, |1\rangle \}$ denote a basis of $\mathcal{H}$. A generic density matrix on $\mathcal{H}$ has the form:

$$\rho = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad a, b, c, d \in \mathbb{C}$$

Therefore in principle there are eight degrees of freedom, but we can apply the proprieties of statistical operator

- ρ is self-adjoint

  $$\rho^\dagger = \rho \quad \Rightarrow \quad \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

  these represents four constrains:

  $$\begin{cases} a^* = a = p_1 \\ \\ d^* = d = p_2 \\ \\ b = c^* \equiv \dfrac{r_x - i r_y}{2} \end{cases}$$

  therefore

  $$\rho = \begin{pmatrix} p_1 & \dfrac{r_x - i r_y}{2} \\ \\ \dfrac{r_x + i r_y}{2} & p_2 \end{pmatrix}$$

  So now we have four degrees of freedom.

- Trace of ρ is equal to 1

  $$\mathrm{Tr}\,[\rho] = 1 \quad \Rightarrow \quad p_1 + p_2 = 1$$

  This is one further constrain, so we can re-define them

  $$\begin{cases} p_1 = \dfrac{1 + r_z}{2} \\ \\ p_2 = \dfrac{1 - r_z}{2} \end{cases}$$

So we have

$$\rho = \frac{1}{2}\begin{pmatrix} 1+r_z & r_x - ir_y \\ r_x + ir_y & 1-r_z \end{pmatrix}$$

$$= \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + r_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + r_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + r_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]$$

$$= \frac{I + \mathbf{r}\cdot\boldsymbol{\sigma}}{2}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\mathbf{r} = (x, y, z)$. This is the generic form of a two dimensional density matrix. Let's consider the square or ρ

$$\rho^2 = \left(\frac{I + \mathbf{r}\cdot\boldsymbol{\sigma}}{2}\right)^2 = \frac{1}{4}\left(I + 2\mathbf{r}\cdot\boldsymbol{\sigma} + \sum_{ij} r_i r_j \sigma_i \sigma_j\right)$$
$$= \frac{1}{4}\left(I + 2\mathbf{r}\cdot\boldsymbol{\sigma} + ||\mathbf{r}||^2 + i\sum_{ij} r_i r_j \epsilon_{ijk}\sigma_k\right)$$

in fact

$$\sigma_i \sigma_j = \delta_{i,j} I + i\epsilon_{ijk}\sigma_k$$

So we have

$$\mathrm{Tr}\left[\rho^2\right] = \frac{1}{2}\left(1 + ||\mathbf{r}||^2\right)$$

because

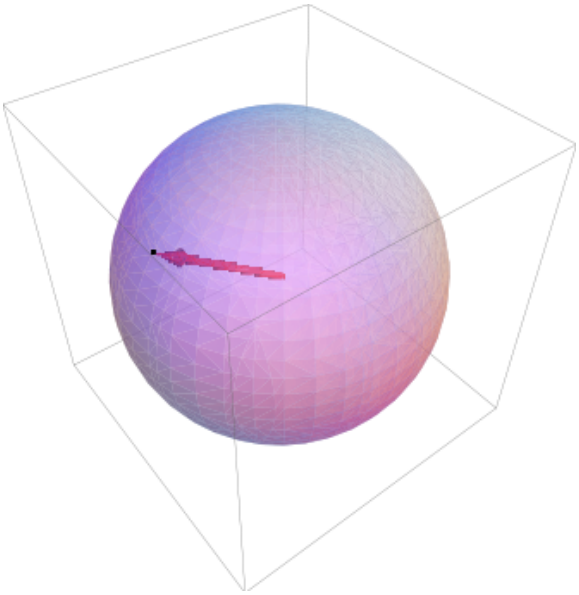
$$\begin{cases} \mathrm{Tr}\left[I\right] = 2 \\ \\ \mathrm{Tr}\left[\sigma_i\right] = 0 \end{cases}$$

But we have seen that the trace of ρ^2 is bounded

$$\mathrm{Tr}\left[\rho^2\right] \leq 1 \quad \Longrightarrow \quad ||\mathbf{r}||^2 \leq 1$$

and it is equal to 1 for a pure state.

Since $\mathbf{r}$ is bounded in modulus, give us a natural representation of the states in a sphere with radius equal to 1. Every point inside the sphere or on its surface it is a state. This sphere is called Bloch sphere. The state of the system is completely determinate from $\mathbf{r}$ called Bloch vector. If $\mathbf{r}$ indicates a point on the surface then the state is pure, if $\mathbf{r}$ points inside the sphere then the system is in a statistical mixture.



We can represent the identity matrix I with

$$\rho = \frac{I}{2} \quad \Longrightarrow \quad \mathbf{r} = 0 \quad \text{is the center of the sphere}$$

or a generic pure state

$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle \qquad \text{with} \quad \begin{cases} a, b \in \mathbb{C} \\ \\ |a|^2 + |b|^2 = 1 \end{cases}$$

expressing a and b as

$$\begin{cases} a = \alpha e^{i\varphi} \\ \\ b = \beta e^{i\chi} \end{cases} \quad \Longrightarrow \quad \alpha^2 + \beta^2 = 1$$

so we can express

$$\begin{cases} \alpha = \cos\frac{\theta}{2} \\ \\ \beta = \sin\frac{\theta}{2} \end{cases}$$

and we obtain the form for a generic pure state

$$|\psi\rangle = e^{i\varphi}\cos\frac{\theta}{2}\,|0\rangle + e^{i\chi}\sin\frac{\theta}{2}\,|1\rangle = e^{i\varphi}\left[\cos\frac{\theta}{2}\,|0\rangle + e^{i(\chi-\varphi)}\sin\frac{\theta}{2}\,|1\rangle\right]$$

where $e^{i\varphi}$ is an unimportant phase, therefore redefining φ we obtain the most general representation for a pure state for a two dimensional system

$$|\psi\rangle \equiv \cos\frac{\theta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|1\rangle$$

The density matrix associated to it has the form

$$\rho = |\psi\rangle\langle\psi| = \cos^2\frac{\theta}{2}\ |0\rangle\langle 0| + e^{-i\varphi}\cos\frac{\theta}{2}\ \sin\frac{\theta}{2}\ |0\rangle\langle 1| + e^{i\varphi}\cos\frac{\theta}{2}\ \sin\frac{\theta}{2}\ |1\rangle\langle 0| + \sin^2\frac{\theta}{2}\ |1\rangle\langle 1|$$

So in represented form

$$\rho = \begin{pmatrix} \cos^2\frac{\theta}{2} & e^{-i\varphi}\cos\frac{\theta}{2}\ \sin\frac{\theta}{2} \\ e^{-i\varphi}\cos\frac{\theta}{2}\ \sin\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix} \equiv \frac{I + \mathbf{r}\cdot\boldsymbol{\sigma}}{2}$$

Therefore

$$\begin{cases} \dfrac{1+r_z}{2} = \cos^2\frac{\theta}{2} & \Longrightarrow \quad r_z = 2\cos^2\frac{\theta}{2} - 1 = \cos\theta \\ \dfrac{r_x}{2} = \cos\varphi\ \cos\frac{\theta}{2}\ \sin\frac{\theta}{2} & \Longrightarrow \quad r_x = \cos\varphi\left(2\cos\frac{\theta}{2}\ \sin\frac{\theta}{2}\right) = \sin\theta\ \cos\varphi \\ \dfrac{r_y}{2} = \sin\varphi\ \cos\frac{\theta}{2}\ \sin\frac{\theta}{2} & \Longrightarrow \quad r_x = \sin\theta\ \sin\varphi \end{cases}$$

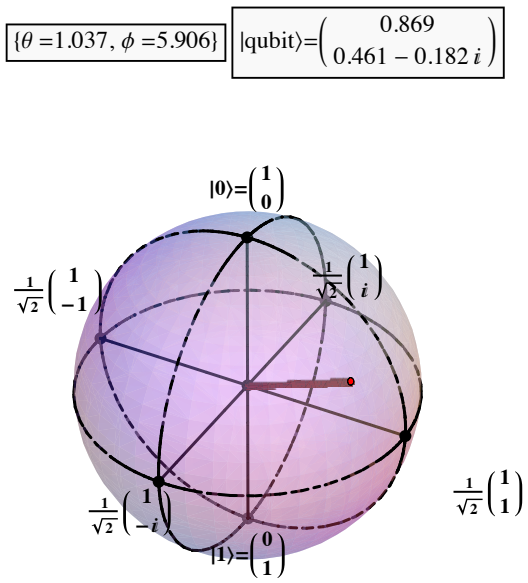
So

$$\mathbf{r} = (\sin\theta\ \cos\varphi\ , \sin\theta\ \sin\varphi\ , \cos\theta)$$

This is the representation of $\mathbf{r}$ in spherical coordinates, with $||\mathbf{r}|| = 1$. The basis $\{\,|0\rangle\,, |1\rangle\,\}$ is represented in Bloch sphere with

$$\begin{cases} |0\rangle \mapsto (0,0,1) \\ |1\rangle \mapsto (0,0,-1) \end{cases}$$

Next is shown an example of a pure state on the Bloch sphere.



1.5 Quantum Mechanics In The Language Of Density Matrices

We can now rephrase the axioms of quantum mechanics in the language of density matrices.

1. **States** To every physical system is associated an Hilbert space $\mathcal{H}$. The possible states of the system are represented by density matrices ρ.

$$\rho = \sum_k p_k \left|\psi_k\right\rangle \left\langle\psi_k\right|$$

2. **Evolution** The density matrix evolves according to the Schrödinger equation:

$$i\hbar \frac{d}{dt}\rho_t = \sum_k p_k \left\{ \left[i\hbar \frac{d}{dt} \left|\psi_k\right\rangle \right] \left\langle\psi_k\right| + i\hbar \left|\psi_k\right\rangle \left[\frac{d}{dt} \left\langle\psi_k\right| \right] \right\}$$

where

$$\begin{cases} i\hbar \dfrac{d}{dt} \left|\psi_k\right\rangle = H \left|\psi_k\right\rangle \\ \\ -i\hbar \dfrac{d}{dt} \left\langle\psi_k\right| = \left\langle\psi_k\right| H \end{cases}$$

Therefore

$$i\hbar \frac{d}{dt}\rho_t = [H, \rho_t] \qquad \text{with initial condition } \rho_0 = \rho$$

This is the **von-Neumann-Liouville equation**. Nothing to be surprised about. It is nothing more than the Schrödinger equation just expressed in another formalism.

Let be U_t the unitary evolution operator associated with the Schrödinger equation.

$$U_t = \exp\left[-\frac{iHt}{\hbar}\right]$$

So we have

$$|\psi_t\rangle = U_t\,|\psi_0\rangle$$

then

$$\rho_t = U_t \rho_0 U_t^\dagger$$

In fact if we suppose to have

$$\rho_0 = \sum_k p_k \left|\psi_0^{(k)}\right\rangle \left\langle\psi_0^{(k)}\right|$$

then

$$\begin{aligned}\rho_t &= \sum_k p_k \left|\psi_t^{(k)}\right\rangle \left\langle\psi_t^{(k)}\right| \\ &= \sum_k p_k U_t \left|\psi_0^{(k)}\right\rangle \left\langle\psi_0^{(k)}\right| U_t^\dagger \\ &= U_t \rho_0 U_t^\dagger\end{aligned}$$

This relation is obtained just applying the linearity of U_t. Let note that for the ciclicity of the trace one have

$$\mathrm{Tr}\left[\rho_t\right] = \mathrm{Tr}\left[U_t \rho_0 U_t^\dagger\right] = \mathrm{Tr}\left[\rho_0\right] = 1$$

because U_t is unitary then

$$U_t^\dagger U_t = I$$

The trace is preserved, as it should be. Physically, it means that the probabilities are conserved. The Schrödinger equation shares this property.

Also the trace of the square density matrix is conserved:

$$\mathrm{Tr}\left[\rho_t^2\right] = \mathrm{Tr}\left[U_t \rho_0 U_t^\dagger U_t \rho_0 U_t^\dagger\right] = \mathrm{Tr}\left[U_t \rho_0 \rho_0 U_t^\dagger\right] = \mathrm{Tr}\left[\rho_0^2\right]$$

this means that

– Pure states are mapped in pure states according to Schrödinger dynamics. This is not a surprise, since a vector remains a vector under the Schrödinger evolution. It does not become a mixture.
– Statistical mixtures are mapped into statistical mixture under the Schrödinger dynamics. They cannot become pure. This is also not a surprise, for the same reason as before.

The main difference between Standard quantum mechanics and quantum mechanics for the open quantum systems is that the dynamics is no longer expressed by the von Neumann-Liouville equation but by a different one. Its results that a pure state can become a statistical mixture and reverse a statistical mixture can become a pure state.

3. **Observable Quantities** The observable quantities are represented by self-adjoint operators on $\mathcal{H}$:

$$A \longrightarrow \hat{A} : \hat{A} \left| a_n \right\rangle = a_n \left| a_n \right\rangle$$

This operators can be expressed in spectral decomposition form:

$$\hat{A} = \sum_n a_n \left| a_n \right\rangle \left\langle a_n \right|$$

4. **Outcomes of measurements** The possible outcome of a measurement of an observable A are the given values of the corresponding self-adjoint operator $\hat{A}$. The outcomes are randomly distributed, and the probability of obtaining the outcome a_n, when the system is represented by state vector ρ, is $P[a_n]$.

With

$$\rho = \sum_k p_k \left| \psi_k \right\rangle \left\langle \psi_k \right|$$

one have

$$P[a_n] = \sum_k p_k | \left\langle a_n | \psi_k \right\rangle |^2 = \sum_k p_k \left\langle a_n | \psi_k \right\rangle \left\langle \psi_k | a_n \right\rangle = \left\langle a_n | \rho | a_n \right\rangle$$

We can define $\mathcal{P}_n$ as the projection operator associated to the eigenvalue a_n.

$$\mathcal{P}_n = \left| a_n \right\rangle \left\langle a_n \right|$$

then we have

$$P[a_n] = \sum_k p_k \mathrm{Tr} \left[\mathcal{P}_n \left| \psi_k \right\rangle \left\langle \psi_k \right| \right]$$

because if we consider a basis $\{ \left| \alpha_m \right\rangle \}$ of $\mathcal{H}$ that contains also $\left| a_n \right\rangle$ we have

$$\langle \alpha_m | a_n \rangle = \delta_{|\alpha_m\rangle,|a_n\rangle}$$

therefore

$$\begin{aligned}
\mathrm{Tr}\left[|a_n\rangle \langle a_n|\psi_k\rangle \langle \psi_k|\right] &= \sum_m \langle \alpha_m|a_n\rangle \langle a_n|\psi_k\rangle \langle \psi_k|\alpha_m\rangle \\
&= \sum_m \delta_{|\alpha_m\rangle,|a_n\rangle} \langle a_n|\psi_k\rangle \langle \psi_k|\alpha_m\rangle \\
&= \langle a_n|\psi_k\rangle \langle \psi_k|a_n\rangle
\end{aligned}$$

So

$$P[a_n] = \sum_k p_k \mathrm{Tr}\left[\mathcal{P}_n |\psi_k\rangle \langle \psi_k|\right] = \mathrm{Tr}\left[\mathcal{P}_n \rho\right]$$

where we use the linearity of the trace.

The average value of an observable A for a pure state $|\psi\rangle$ is

$$\langle \hat{A} \rangle_{|\psi\rangle} = \sum_n a_n |\langle a_n|\psi\rangle|^2$$

this is the same result we obtain for standard quantum mechanics. For the reason before we can express that average like

$$\langle \hat{A} \rangle_{|\psi\rangle} = \sum_n a_n \mathrm{Tr}\left[\mathcal{P}_n \rho\right] = \mathrm{Tr}\left[\sum_n a_n \mathcal{P}_n \rho\right]$$

therefore

$$\langle \hat{A} \rangle_{|\psi\rangle} = \mathrm{Tr}\left[\hat{A}\rho\right]$$

This results is also valid for a statistical mixture.

5. **Collapse of the wave function** At the end of a measurement process, where the outcome a_n has been obtained, the system collapses to

$$\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k| \quad \Rightarrow \quad |a_n\rangle \langle a_n|$$

The collapse of each vector $|psi_k\rangle$ in $|a_n\rangle$ is equivalent to the collapse of ρ in $\mathcal{P}_n = |a_n\rangle \langle a_n|$. It can be written also as

$$\rho \quad \Rightarrow \quad \frac{\mathcal{P}_n \rho \mathcal{P}_n}{\mathrm{Tr}\left[\mathcal{P}_n \rho\right]}$$

This is called **selective measurement**. The division by the trace is necessary for keeping the trace of ρ equal to one. One now can easily describe also a **non selective measurement**, when more that one outcome is retained. We suppose that in a measurement of a observable A, all the outcomes are retained:

$$|\psi\rangle \xrightarrow[\text{MEASUREMENT}]{} |a_n\rangle \qquad \text{with probability } P[a_n] = |\langle a_n|\psi\rangle|^2$$

Then

$$\rho \quad \Rightarrow \quad \sum_n \text{Tr}\left[\mathcal{P}_n\rho\right] \frac{\mathcal{P}_n\rho\mathcal{P}_n}{\text{Tr}\left[\mathcal{P}_n\rho\right]}$$

we generate a statistical mixture, where there is a probability of $\text{Tr}\left[\mathcal{P}_n\rho\right]$ to collapse in the state $\frac{\mathcal{P}_n\rho\mathcal{P}_n}{\text{Tr}[\mathcal{P}_n\rho]}$, therefore the non selective measurement is expressed as

$$\rho \quad \Rightarrow \quad \sum_n \mathcal{P}_n\rho\mathcal{P}_n$$

In this case, a pure state can be turned into a statistical mixture

$$\text{Tr}\left[\left(\sum_n \mathcal{P}_n\rho\mathcal{P}_n\right)^2\right] = \text{Tr}\left[\sum_{nm} \mathcal{P}_n\rho\mathcal{P}_n\mathcal{P}_m\rho\mathcal{P}_m\right]$$

but $\mathcal{P}_n\mathcal{P}_m = \mathcal{P}_n\delta_{n,m}$

$$\begin{aligned}\text{Tr}\left[\left(\sum_n \mathcal{P}_n\rho\mathcal{P}_n\right)^2\right] &= \text{Tr}\left[\sum_n \mathcal{P}_n\rho\mathcal{P}_n\rho\right] \\ &= \sum_n \text{Tr}\left[|a_n\rangle\langle a_n|\rho|a_n\rangle\langle a_n|\,\rho\right]\end{aligned}$$

where $\langle a_n|\rho|a_n\rangle \in \mathbb{C}$

$$\begin{aligned}\text{Tr}\left[\left(\sum_n \mathcal{P}_n\rho\mathcal{P}_n\right)^2\right] &= \sum_n \langle a_n|\rho|a_n\rangle \,\text{Tr}\left[\sum_n \mathcal{P}_n\rho\right] \\ &= \sum_n |\langle a_n|\rho|a_n\rangle|^2\end{aligned}$$

but $|\langle a_n|\rho|a_n\rangle| \leq 1$, therefore

$$\begin{aligned}\text{Tr}\left[\left(\sum_n \mathcal{P}_n\rho\mathcal{P}_n\right)^2\right] &\leq \sum_n \langle a_n|\rho|a_n\rangle \\ &= \sum_n \text{Tr}\left[\mathcal{P}_n\rho\right] = \text{Tr}\left[\rho\right] = 1\end{aligned}$$

So we have

$$\mathrm{Tr}\left[\left(\sum_n \mathcal{P}_n \rho \mathcal{P}_n\right)^2\right] \leq 1$$

i.e. we can have a statistical mixture after a non selective measurement starting from a pure state.

1.5.1 Entanglement

Such as we consider the entangled states in the standard quantum mechanics, we can consider the entanglement in density matrix formalism. For a bipartite system, i.e. the total Hilbert space $\mathcal{H}$ is define as $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, if the statistical operator of the entire system can not be expressed as linear combination of statistical operators of the two systems alone

$$\rho \neq \sum_{ij} \lambda_{ij} \rho_i^{(1)} \otimes \rho_j^{(2)}$$

therefore it is a entangled state. If ρ can be instead expressed in that way, with conditions

$$\begin{cases} \lambda_{ij} \geq 0 \quad \in \mathbb{R} \\ \sum_{ij} \lambda_{ij} = 1 \\ \rho_i^{(1)} \text{ and } \rho_j^{(2)} \quad \forall i,j \quad \text{are good statistical operators} \end{cases}$$

therefore ρ is a separated state.

Example Consider the state $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ as

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big[|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\big]$$

The associated statistical operator is

$$\begin{aligned} \rho = |\psi\rangle\langle\psi| &= \frac{1}{2}\big[|0\rangle|0\rangle\langle 0|\langle 0| + |1\rangle|1\rangle\langle 1|\langle 1| + |0\rangle|0\rangle\langle 1|\langle 1| + |1\rangle|1\rangle\langle 0|\langle 0|\big] \\ &= \frac{1}{2}\big[|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0|\big] \end{aligned}$$

If there was be just

$$\frac{1}{2}\big[|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|\big] = \sum_{ij} \lambda_{ij} \rho_i^{(1)} \otimes \rho_j^{(2)}$$

the state will be separable. But there are also terms as $|1\rangle\langle 0|$ that are not statistical operators. Therefore the state ρ is entangled.

In general to understand if a state is entangled or separable is not so easy as we see. There are some criteria for study it, for example Schmidt decomposition or the partial transposition, but is not the aim of this course.

Example Consider the hamiltonian H of a two dimensional system.

$$H = \sigma_z = \begin{pmatrix} 1 & 0 \\ & \\ 0 & -1 \end{pmatrix}$$

Let be, just for the example, $\hbar = 1$. The state ρ of the system can be represented by the Bloch vector $\mathbf{r}$:

$$\rho = \frac{I + \mathbf{r} \cdot \boldsymbol{\sigma}}{2} \quad \Rightarrow \quad \dot{\rho} = \frac{\dot{\mathbf{r}} \cdot \boldsymbol{\sigma}}{2}$$

Therefore, equating with the von Neumann-Liouville equation

$$\dot{\rho} = -i \left[H, \rho \right] = \frac{\dot{\mathbf{r}} \cdot \boldsymbol{\sigma}}{2}$$

we obtain

$$\frac{\dot{\mathbf{r}} \cdot \boldsymbol{\sigma}}{2} = -\frac{i}{2} \left[\sigma_z, I \right] - \frac{i}{2} \sum_k r_k \left[\sigma_z, \sigma_k \right]$$

but $[\sigma_z, I] = 0$ and $[\sigma_z, \sigma_k] = 2i \sum_j \epsilon_{z,k,j} \sigma_j$. So one obtain

$$\frac{\dot{\mathbf{r}} \cdot \boldsymbol{\sigma}}{2} = r_x \sigma_y + r_y (-\sigma_x)$$

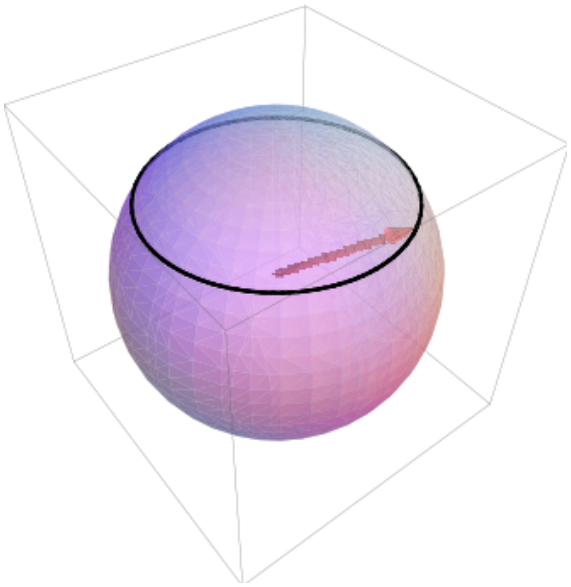
Since the set $\{ I, \sigma_x, \sigma_y, \sigma_z \}$ is a basis of space of 2×2 matrices, therefore we can express the three coefficients along the three components of $\boldsymbol{\sigma}$ by themselves.

$$\begin{cases} \dot{r}_x = -2 r_y \\ \dot{r}_y = 2 r_x \\ \dot{r}_z = 0 \end{cases}$$

So r_x and r_y have a oscillatory behavior:

$$\begin{cases} r_x = \cos 2t \\ r_y = \sin 2t \\ rz \equiv \text{CONSTANT} \end{cases}$$

The dynamic is an oscillation around the z axis of the Bloch sphere, both for pure states and for statistical mixtures.



1.6 The Reduce Density Matrix

Perhaps the most important application of the density matrix formalism is to describe a **subsystem** of a composite system.

We have two systems A and B. Their Hilbert spaces are $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively, suppose their dimensions are respectively N and M. Let $\left\{ \left|\phi_n^A\right\rangle \right\}_{n=1}^{N}$ be a basis of $\mathcal{H}_A$ and $\left\{ \left|\phi_m^B\right\rangle \right\}_{m=1}^{M}$ a basis of $\mathcal{H}_B$. This basis are between the othonormal, i.e.

$$\langle \phi_m^B | \phi_n^A \rangle = 0$$

A generic statistical operator describing the composite system is

$$\rho_{AB} = \sum_{kj} p_{kj} \left|\psi_k^A\right\rangle \left|\psi_j^B\right\rangle \left\langle \psi_k^A\right| \left\langle \psi_j^B\right|$$

This statistical operator can be represented by a square $(N \cdot M) \times (N \cdot M)$ density matrix.

Suppose we are interested only in the properties of subsystem A, for example because we cannot control or we have not direct access to system B. Therefore, the observable quantities we are interested in have the form

$$\hat{A} \otimes \hat{I}_B$$

The average value of this kind of observables is

$$\begin{aligned}
\langle \hat{A} \otimes \hat{I}_B \rangle &= \mathrm{Tr}\left[(\hat{A} \otimes \hat{I}_B) \rho_{AB} \right] = \sum_{nm} \left\langle \phi_n^A \right| \left\langle \phi_m^B \right| \left[(\hat{A} \otimes \hat{I}_B) \rho_{AB} \right] \left|\phi_m^B\right\rangle \left|\phi_n^A\right\rangle \\
&= \sum_{nm} \sum_{kj} p_{kj} \left\langle \phi_n^A \right| \left\langle \phi_m^B \right| \left[(\hat{A} \otimes \hat{I}_B) \left|\psi_k^A\right\rangle \left|\psi_j^B\right\rangle \left\langle \psi_k^A\right| \left\langle \psi_j^B\right| \right] \left|\phi_m^B\right\rangle \left|\phi_n^A\right\rangle
\end{aligned}$$

Here $\hat{A}$ applies to $\left|\psi_k^A\right\rangle$ and $\hat{I}_B$ to $\left|\psi_j^B\right\rangle$. So we obtain

$$\langle \hat{A} \otimes \hat{I}_B \rangle = \sum_n \langle \phi_n^A | \hat{A} \left[\sum_m \langle \phi_m^B | \rho_{AB} | \phi_m^B \rangle \right] | \phi_n^A \rangle$$

Therefore

$$\langle \hat{A} \rangle = \mathrm{Tr}^{(A)} \left[\hat{A} \, \rho^{(A)} \right]$$

where we define $\rho^{(A)}$ as **reduce density matrix**

$$\rho^{(A)} \equiv \mathrm{Tr}^{(B)} \left[\rho_{AB} \right]$$

This is a statistical operator acting on $\mathcal{H}_A$ and can be represented by a square $(N \cdot 1) \times (N \cdot 1)$ density matrix. Unlike the typical trace operation, the partial trace gives an operator and not a scalar value.

- **Comment 1.** The reduce density matrix is the matrix obtained by performing a **partial trace** over the degrees of freedom of the second system, i.e. system B. Unlike the typical trace operation, the partial trace gives an operator and not a scalar value.

  For compute the partial trace we have to consider the if the is factorized or entangled:

  a. For a factorized state we can express

  $$\rho_{AB} = \rho_A \otimes \rho_B$$

  for example this state can be $|0_A\rangle \langle 0_A| \otimes |0_B\rangle \langle 0_B|$. Then the partial trace is

  $$\rho^{(A)} = \mathrm{Tr}^{(B)} \left[\rho_{AB} \right] = \mathrm{Tr}^{(B)} \left[\rho_A \otimes \rho_B \right] = \rho_A \, \mathrm{Tr}^{(B)} \left[\rho_B \right] = \rho_A$$

  as we would expect $\rho^{(A)} = \rho_A$.

  b. For a entangled state we cannot express the total density matrix as shown before. There is without sense consider the density matrix of the system A or B alone. In this case if we want describe only the A system we have to consider the reduce density matrix. For example consider the totally entangled pure state $|\psi_+\rangle$

  $$|\psi_+\rangle \equiv \frac{|0_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle}{\sqrt{2}}$$

  the associated density matrix is

  $$\begin{aligned} \rho_{AB} = |\psi_+\rangle \langle \psi_+| &= \frac{|0_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle}{\sqrt{2}} \frac{\langle 0_A| \langle 0_B| + \langle 1_A| \langle 1_B|}{\sqrt{2}} \\ &= \frac{1}{2} \left[|0_A\rangle |0_B\rangle \langle 0_A| \langle 0_B| + |0_A\rangle |0_B\rangle \langle 1_A| \langle 1_B| + |1_A\rangle |1_B\rangle \langle 0_A| \langle 0_B| + |1_A\rangle |1_B\rangle \langle 1_A| \langle 1_B| \right] \end{aligned}$$

Then performing the partial trace we obtain

$$\begin{aligned}\rho^{(A)} &= \mathrm{Tr}^{(B)}\left[\rho_{AB}\right] = \langle 0_B|\rho_{AB}|0_B\rangle + \langle 1_B|\rho_{AB}|1_B\rangle \\ &= \frac{1}{2}\left[|0_A\rangle\langle 0_A| + |1_A\rangle\langle 1_A|\right] = \frac{1}{2}I_A\end{aligned}$$

Note that ρ_{AB} is a pure state, while $\rho^{(A)}$ is a mixed state. The partial trace can transform pure states into mixed states.

Of course, in order to be a good definition, $\rho^{(A)} = \mathrm{Tr}^{(B)}\left[\rho_{AB}\right]$ must still represent a density matrix.

- Of course it is a **linear** operator, since the partial trace preserves linearity.
- It is **positive**

$$\begin{aligned}\langle\psi_A|\rho^{(A)}|\psi_A\rangle &= \langle\psi_A|\mathrm{Tr}^{(B)}\left[\rho_{AB}\right]|\psi_A\rangle \\ &= \sum_m \langle\psi_A|\langle\phi_m^B|\rho_{AB}|\phi_m^B\rangle|\psi_A\rangle \geq 0\end{aligned}$$

because ρ_{AB} is a positive operator, so

$$\forall\,|\psi_A\rangle\left|\phi_m^B\right\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \qquad \langle\psi_A|\langle\phi_m^B|\rho_{AB}|\phi_m^B\rangle|\psi_A\rangle \geq 0$$

- the **trace is one**

$$\begin{aligned}\mathrm{Tr}^{(A)}\left[\rho^{(A)}\right] &= \sum_n \langle\phi_n^A|\rho^{(A)}|\phi_n^A\rangle = \sum_n \langle\phi_n^A|\mathrm{Tr}^{(B)}\left[\rho_{AB}\right]|\phi_n^A\rangle \\ &= \sum_{nm}\langle\phi_n^A|\langle\phi_m^B|\rho_{AB}|\phi_m^B\rangle|\phi_n^A\rangle = \mathrm{Tr}\left[\rho_{AB}\right] = 1\end{aligned}$$

So it is a good definition

- **Comment 2.** The above formula states a very important property. If we want to compute physical predictions regarding subsystem A alone, we do not have to consider the entire density matrix ρ_{AB}. It is sufficient to work with the reduce density matrix $\rho^{(A)}$.

  $\rho^{(A)}$ contains all physical information about the subsystem A, when we are not interested in knowing the properties of subsystem B, i.e. the observables have the form $\hat{A} \otimes \hat{I}_B$.

- **Comment 3.** The partial trace is the unique way of obtaining the desired information about subsystem A starting from the density matrix ρ_{AB}. In fact, physical consistency requires that, given the association

$$\rho_{AB} \quad \Rightarrow \quad \tilde{\rho}^{(A)} = F(\rho_{AB})$$

then it must be

$$\mathrm{Tr}^{(A)}\left[A\tilde{\rho}^{(A)}\right] = \mathrm{Tr}\left[(A \otimes I_B)\rho_{AB}\right] \qquad \forall A \text{ observables acting on } \mathcal{H}_A$$

The physical quantities computed in the two ways, with $\rho^{(A)}$ and $\tilde{\rho}^{(A)}$, must be the same. The space of the bounded hermitian operators is a Hilbert-Schmidt space $\mathcal{B}(\mathcal{H})$ associated to the Hilbert space $\mathcal{H}$, where $\mathcal{B}$ stands for bounded operators space. $\mathcal{B}(\mathcal{H})$ is defined as

$$\mathcal{B}(\mathcal{H}) = \mathcal{H} \otimes \mathcal{H}^*$$

where $\mathcal{H}^*$ is the dual Hilbert space associated to $\mathcal{H}$. In $\mathcal{B}(\mathcal{H})$ the inner product is defined as

$$\langle X, Y \rangle = \mathrm{Tr}\left[XY\right]$$

Let $\{ M_n \}$ be a basis of $\mathcal{B}(\mathcal{H}_A)$, so we can decompose $\tilde{\rho}^{(A)}$ on this basis

$$\tilde{\rho}^{(A)} = \sum_n M_n \mathrm{Tr}\left[M_n \tilde{\rho}^{(A)}\right]$$

this decomposition is the equivalent of the decomposition in standard quantum mechanics of state $|\psi\rangle$ on a basis $\{ |j\rangle \}$ of $\mathcal{H}$

$$|\psi\rangle = \sum_j |j\rangle \langle j|\psi\rangle$$

Notice that the composition on a fixed basis is unique. Since we have the above property for all operators acting on $\mathcal{H}_A$ theirs mean value is

$$\mathrm{Tr}^{(A)}\left[A\tilde{\rho}^{(A)}\right] = \mathrm{Tr}\left[(A \otimes I_B)\rho_{AB}\right]$$

therefore this is valid also for each M_n

$$\mathrm{Tr}^{(A)}\left[M_n\tilde{\rho}^{(A)}\right] = \mathrm{Tr}\left[(M_n \otimes I_B)\rho_{AB}\right]$$

so we have

$$\tilde{\rho}^{(A)} = \sum_n M_n \mathrm{Tr}\left[(M_n \otimes I_B)\rho_{AB}\right]$$

Consider the reduce density matrix $\rho^{(A)}$ and consider its decomposition on the same basis $\{ M_n \}$

$$\rho^{(A)} = \sum_n M_n \mathrm{Tr}^{(A)} \left[M_n \rho^{(A)} \right]$$

applying the definition of reduce density matrix we obtain

$$\begin{aligned} \rho^{(A)} &= \sum_n M_n \mathrm{Tr}^{(A)} \left[M_n \mathrm{Tr}^{(B)} \left[\rho_{AB} \right] \right] \\ &= \sum_n M_n \mathrm{Tr} \left[(M_n \otimes I_B) \rho_{AB} \right] \end{aligned}$$

this is the same result we obtain above, so

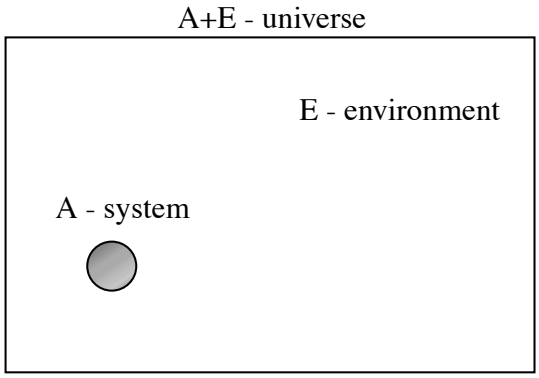
$$\rho^{(A)} = \tilde{\rho}^{(A)} = F(\rho_{AB})$$

Therefore the partial trace is the unique map from total density matrix ρ_{AB} to the reduce one $\rho^{(A)}$ that satisfy the relation for the mean value of the operator A acting on $\mathcal{H}$.

Chapter 2

Axiomatic Approach To Open Quantum System

In this chapter we want apply the reduce density formalism to study a very common situation in nature: a physical system A interacting with the surrounding environment E as in the next figure. This is an **open quantum system**.



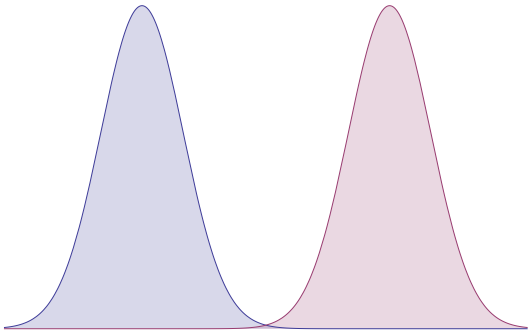
2.1 Decoherence

In many experimental situations, it is impossible, or difficult or not strictly necessary, to isolate the system under interest from the noise coming from the environment. We want to take these effects into account. Consider the above figure with system A represented by a particle interacting with an environment E made of gas. We want to study the dynamic of the reduce density matrix $\rho^{(A)}$ of the open system A.

Considering the system A isolated its states is suppose to be

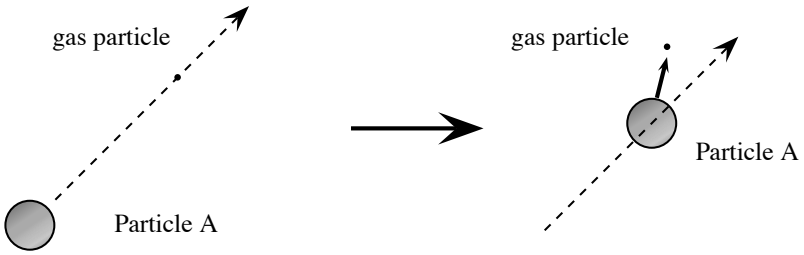
$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[|u\rangle + |d\rangle\right]$$

where we are supposing that $|u\rangle$ and $|d\rangle$ represents some wave functions well localized in space and are not necessarily orthonormal. For example can have little tails going to infinity as gaussians in next figure.



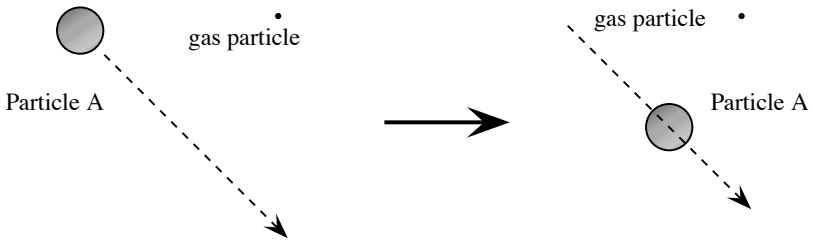
$|u\rangle$ represents the state of the particle A going upwards and $|d\rangle$ those going downwards. Suppose from a certain time the system A hits a molecule of the surrounding gas. If the state of A is just one of the two above states and the interaction with the environment do not imply big changes in the state of A, we obtain without consider the time evolution

$$|\psi_0\rangle = |u\rangle \otimes |\phi_E\rangle \quad \Rightarrow \quad |\psi\rangle = |u\rangle \otimes |\phi_E^u\rangle$$



The gas particle is scattered away from the particle A. Otherwise we have

$$|\psi_0\rangle = |d\rangle \otimes |\phi_E\rangle \quad \Rightarrow \quad |\psi\rangle = |d\rangle \otimes \left|\phi_E^d\right\rangle$$



The gas particle is not scattered away.

If we suppose that the particle travels in the superposition of this two states for linearity we obtain

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}\left[|u\rangle + |d\rangle\right] \otimes |\phi_E\rangle \quad \Rightarrow \quad |\Psi\rangle = \frac{1}{\sqrt{2}}\left[|u\rangle \otimes |\phi_E^u\rangle + |d\rangle \otimes \left|\phi_E^d\right\rangle\right]$$

this state is entangle, in fact if we do a measurement of the state of the particle and we get $|u\rangle$ therefore is certain the state of the environment is $|\phi_E^u\rangle$. Analogue it happen if we obtain state $|d\rangle$ from the measurement, the state of the environment collapse in $\left|\phi_E^d\right\rangle$.

Suppose we do not have direct access to the state of the environment and we want to study just the A system. We have to consider the **reduce density matrix**, i.e. the partial trace over the degree of freedom of the environment. Suppose the Hilbert space $\mathcal{H}_E$ of the environment is two dimension and $\left\{ |\phi_E^u\rangle, \left|\phi_E^d\right\rangle \right\}$ is basis of this space and ρ_{AE} is the density matrix of entire system (particle A and environment E), we can compute the partial trace as

$$\rho_{AE} = |\Psi\rangle\langle\Psi| = \frac{1}{\sqrt{2}}\left[|u\rangle \otimes |\phi_E^u\rangle + |d\rangle \otimes \left|\phi_E^d\right\rangle\right] \cdot \frac{1}{\sqrt{2}}\left[\langle u| \otimes \langle\phi_E^u| + \langle d| \otimes \left\langle\phi_E^d\right|\right]$$

$$\begin{aligned}\rho^{(A)} &= \mathrm{Tr}^{(E)}\left[\rho_{AE}\right] = \langle\phi_E^u|\rho_{AE}|\phi_E^u\rangle + \langle\phi_E^d|\rho_{AE}|\phi_E^d\rangle \\ &= \mathrm{Tr}^{(E)}\left[\frac{1}{2}\left[|u\rangle\langle u| + \langle\phi_E^d|\phi_E^u\rangle\,|u\rangle\langle d| + \langle\phi_E^u|\phi_E^d\rangle\,|d\rangle\langle u| + |d\rangle\langle d|\right]\right]\end{aligned}$$

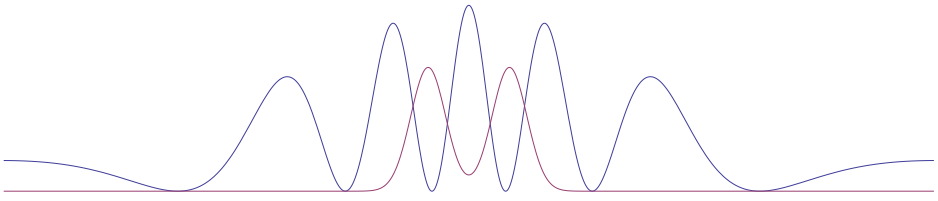
Considering the basis $\left\{ |u\rangle, |d\rangle \right\}$ of $\mathcal{H}_A$ therefore we can represent the reduce density matrix at initial state, $\rho_0^{(A)} = |\Psi_0\rangle\langle\Psi_0|$, and after the interaction with environment, $\rho^{(A)} = |\Psi\rangle\langle\Psi|$:

$$\begin{array}{ll} \text{Before} & \text{After} \\ \rho_0^{(A)} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} & \Rightarrow \quad \rho^{(A)} = \frac{1}{2}\begin{pmatrix} 1 & \langle\phi_E^d|\phi_E^u\rangle \\ \langle\phi_E^u|\phi_E^d\rangle & 1 \end{pmatrix} \end{array}$$

The effect of the interaction with the environment is to modify the off-diagonal elements of the density matrix, with represent the interference terms. The diagonal terms remain the same, in general can vary but trace must be conserved. Since in our example $|\phi_E^u\rangle$ and $\left|\phi_E^d\right\rangle$ represent two different states with a little overlap, as shown in figure above, therefore we have

$$|\langle\phi_E^u|\phi_E^d\rangle| = \left|\int dx\ \phi_E^{u*}(x)\phi_E^d(x)\right| \sim 0$$

Then **the effect of decoherence is to suppress the off-diagonal elements**. Since the off-diagonal elements represent the possibility to measuring interference among the different terms of the superposition, the effect of decoherence is to destroy such interference terms. In fact in typical double slit experiment we have



where the blue graph represents the experiment without an interacting environment and red graph represent the absence of interference terms do the presence of a strong environment.

- **Comment 1.** Our assumption of $|\langle\phi_E^u|\phi_E^d\rangle| \sim 0$ is often exaggerated. Not always the effect on one particle of the environment is so dramatic, we can consider

$$|\langle\phi_E^u|\phi_E^d\rangle| \lesssim 1$$

But then one has to take into account that there are many particles in the environment, therefore

$$\langle\phi_E^u|\phi_E^d\rangle \quad \Rightarrow \quad \langle\phi_{E1}^u|\phi_{E1}^d\rangle\langle\phi_{E2}^u|\phi_{E2}^d\rangle\ldots\langle\phi_{En}^u|\phi_{En}^d\rangle$$

where $\langle\phi_{Ei}^u|\phi_{Ei}^d\rangle$ is the term relative to i-particle of the environment. So we have

$$\begin{cases} |\langle\phi_{Ei}^u|\phi_{Ei}^d\rangle| \lesssim 1 \\ \\ \left|\prod_{i=1}^{N}\langle\phi_{Ei}^u|\phi_{Ei}^d\rangle\right| \xrightarrow{N\to+\infty} 0 \end{cases}$$

we see therefore a dynamical effect. As time passes, more and more particles of the environment interact with the particle A and cause decoherence, i.e. $t \propto N$. So we expect a behavior of the type

$$\rho_0^{(A)} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \xrightarrow{t\to+\infty} \rho^{(A)} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

there is a complete loss of coherence.

- **Comment 2.** the density matrix diagonalizes in the **position basis**. In fact the two states $|u\rangle$ and $|d\rangle$ refer to two different configuration in space of the particle.

  The reason is that most interactions in nature mainly depend of the **position** of the two systems interacting to each other. For this reason, position is selected as the natural basis where diagonalize the density matrix.

One of the effects of decoherence is to transform pure states into statistical mixtures. This means, as we have seen before, that **the dynamics of the reduce density matrix cannot be given by the Schrödinger equation**. The evolution of the reduce density matrix can not be obtained from the action of a unitary operator as in the Schrödinger i.e. von Neumann-Liouville equation

$$i\hbar\frac{d}{dt}\rho_t = \big[H, \rho_t\big]$$

In presence of an interaction it is not like that. This is not a surprise, because the particle is not isolated, but interacts with the environment, and we trace the environment away. We have

to asking ourself **what is the proper dynamics for the reduce density matrix?**

There are two approaches:

- Derive the general form, from general considerations. This is the axiomatic approach. We are looking for equations that we can always apply. This approach will be next describe.
- Derive the effective dynamics from the underlying microscopic dynamics, i.e. from the Schrödinger equation for the total system. This approach we be describe in the next chapter.

2.2 Linear Evolution

We start our analysis on the general form of the evolution equations for density matrices.

Let S be the physical (open) quantum system under study and $\mathcal{H}$ the associated Hilbert space.

Let $\mathrm{T}(\mathcal{H})$ be the Banach space of self-adjoint trace-class operators equipped with the trace norm. Density matrices belong to this space, since a positive operator is automatically self-adjoint and a trace-class must have a finite trace as a density matrix.

Let ρ be a density matrix and $T_t(\rho)$ represent its time evolution, as an operator applied to ρ. $T_t(\rho)$ is a temporal map such that

$$\begin{aligned} T_t \ &: \mathrm{T}(\mathcal{H}) \to \mathrm{T}(\mathcal{H}) \\ \rho \ &\mapsto T_t(\rho) \qquad \forall t \in \mathbb{R}^+ \end{aligned}$$

We want to argue that $T_t(\rho)$ must be a **linear operator**.

Lemma Let $\mathcal{H}$ be a finite Hilbert space and $\{ |\phi_i\rangle \}_{i=1\ldots n}$ and $\{ |\psi_j\rangle \}_{j=1\ldots m}$ two sets of vectors of $\mathcal{H}$.

Let be $p_i \in]0,1]$, $i = 1 \ldots n$ and $q_j \in]0,1]$, $j = 1 \ldots m$.

Let also

$$\sum_{i=1}^{n} p_i \, |\phi_i\rangle \langle\phi_i| = \sum_{j=1}^{m} q_j \, |\psi_j\rangle \langle\psi_j|$$

This equality describes equivalent ensembles. Then there exists a Hilbert space $\mathcal{H}'$, a vector $|\chi\rangle \in \mathcal{H} \otimes \mathcal{H}'$ and two orthonormal basis $\{ |\alpha_i\rangle \}$ and $\{ |\beta_j\rangle \}$ of $\mathcal{H}$ such that

$$|\chi\rangle = \sum_i \sqrt{p_i} \, |\phi_i\rangle \otimes |\alpha_i\rangle = \sum_j \sqrt{q_j} \, |\psi_j\rangle \otimes |\beta_j\rangle$$

Proof. Assume $n > m$.

Let be $\mathcal{H}' = \mathbb{C}^n$ and $\{ |\alpha_i\rangle \}$ a basis of $\mathcal{H}'$.

Let E be the space spanned by the set $\{ |\phi_i\rangle \}$. Obviously one obtain

$$E = \left\{ |v\rangle \in \mathcal{H} \middle| \langle v| \left[\sum_i p_i |\phi_i\rangle \langle \phi_i| \right] v\rangle = 0 \right\}^{\perp}$$

Therefore E is also the space spanned by the set $\{ |\psi_j\rangle \}$. Consequently exist a transformation from the set $\{ |\phi_i\rangle \}$ and $\{ |\psi_j\rangle \}$ and reverse.

$$|\phi_i\rangle = \sum_j b_{ij} |\psi_j\rangle \qquad \forall i = 1 \dots n$$

where $b_{ij} = \langle \psi_j | \phi_i \rangle$ and hence

$$\begin{aligned} |\chi\rangle \equiv \sum_i \sqrt{p_i} |\phi_i\rangle \otimes |\alpha_i\rangle &= \sum_{ij} \sqrt{p_i} b_{ij} |\psi_j\rangle \otimes |\alpha_i\rangle \\ &= \sum_j |\psi_j\rangle \otimes \left[\sum_i \sqrt{p_i} b_{ij} |\alpha_i\rangle \right] \end{aligned}$$

so we can define

$$\left| \tilde{\beta}_j \right\rangle \equiv \sum_i \sqrt{p_i} b_{ij} |\alpha_i\rangle$$

this set of vectors must be normalized

$$\begin{aligned} \langle \tilde{\beta}_j | \tilde{\beta}_l \rangle &= \sum_{ik} \sqrt{p_i} \sqrt{p_k} b^*_{ij} b_{kl} \langle \alpha_i | \alpha_k \rangle \\ &= \sum_{ik} \sqrt{p_i} \sqrt{p_k} b^*_{ij} b_{kl} \delta_{i,k} \\ &= \sum_i p_i b^*_{ij} b_{il} \end{aligned}$$

Without loss any generality, we can assume the set $\{ |\psi_j\rangle \}$ to be orthonormal. In fact we can orthonormalize this set defining

$$\sum_{j=1}^{m} q_j |\psi_j\rangle \langle \psi_j| = \sum_k \lambda_k \left| \tilde{\psi}_k \right\rangle \left\langle \tilde{\psi}_k \right|$$

where λ_k are the eigenvalues of projectors $\left| \tilde{\psi}_k \right\rangle \left\langle \tilde{\psi}_k \right|$, this is a spectralization of the set. If the following equations are valid for $\left\{ \left| \tilde{\psi}_k \right\rangle \right\}$ therefore are valid for $\{ |\psi_j\rangle \}$. So we do not lose generality and we obtain

$$\langle \psi_m | \psi_l \rangle = \delta_{m,l}$$

Applying the above definition of b_{ij} of the transformation we obtain

$$\begin{aligned}\langle\tilde{\beta}_j|\tilde{\beta}_l\rangle &= \sum_i p_i \langle\phi_i|\psi_j\rangle \langle\psi_l|\phi_i\rangle \\ &= \langle\psi_l| \left[\sum_i p_i |\phi_i\rangle \langle\phi_i|\right] |\psi_j\rangle \\ &= \langle\psi_l| \left[\sum_j q_j |\psi_j\rangle \langle\psi_j|\right] |\psi_j\rangle = q_j \delta_{j,l}\end{aligned}$$

therefore we have the normalized set $\{ |\beta_j\rangle \}$

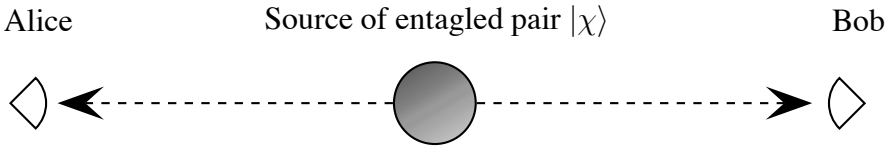
$$|\beta_j\rangle \equiv \frac{1}{\sqrt{q_j}} \left|\tilde{\beta}_j\right\rangle$$

So

$$|\chi\rangle = \sum_i \sqrt{p_i} |\phi_i\rangle \otimes |\alpha_i\rangle = \sum_j \sqrt{q_j} |\psi_j\rangle \otimes |\beta_j\rangle$$

Theorem Linearity of the evolution map T_t

Consider the following situation



There is a source of an entangled state $|\chi\rangle$ as defined in above lemma that send a part of the pair of particles to Alice and the second part to Bob, who is long far away from Alice.

Alice can do measurement of two operators, $\hat{A}$ and $\hat{B}$, and Bob just observe his part of the state of the system.

$$\begin{cases} \hat{A} = \sum_i \alpha_i |\alpha_i\rangle \langle\alpha_i| \\ \\ \hat{B} = \sum_j \beta_j |\beta_j\rangle \langle\beta_j| \end{cases}$$

Suppose if Alice do a measurement of $\hat{A}$, therefore Bob observe

$$\hat{A} \quad \Rightarrow \quad \rho = \sum_i p_i |\phi_i\rangle \langle\phi_i|$$

Bob do not know the result of the measurement, so he have a statistical mixture. If Alice do a measurement of $\hat{B}$

$$\hat{B} \quad \Rightarrow \quad \rho = \sum_j q_i \left|\psi_j\right\rangle \left\langle\psi_j\right|$$

All the statistical mixture Bob can obtain are prepared in this way from Alice starting always from a entangled state $|\chi\rangle \in \mathcal{H}_{Alice} \otimes \mathcal{H}_{Bob}$. Obviously that statistical mixture are between them equivalent because, for the impossibility to send informations faster then light, Bob can not know what Alice measure.

Suppose Bob do not do any measure but his particle go into a gas. Therefore will be an interaction with it and the particle evolves with T_t. Since we don not know in which state is the particle we have to maintain the structure of statistical mixture and apply the evolution to the basis $\{ |\phi_i\rangle \}$ and $\{ |\psi_j\rangle \}$. So we obtain

$$\begin{cases} \sum_i p_i \left|\phi_i\right\rangle \left\langle\phi_i\right| & \xrightarrow{T_t} \quad \sum_i p_i T_t \left[\left|\phi_i\right\rangle \left\langle\phi_i\right|\right] = \rho_1 \\ & \qquad\qquad\qquad\qquad\qquad\qquad \Rightarrow \quad \rho_1 = \rho_2 \\ \sum_j q_j \left|\psi_j\right\rangle \left\langle\psi_j\right| & \xrightarrow{T_t} \quad \sum_j q_j T_t \left[\left|\psi_j\right\rangle \left\langle\psi_j\right|\right] = \rho_2 \end{cases}$$

We have the equivalence of the two density matrices after the evolution do the interaction with the gas, in fact otherwise Bob can know what Alice measure. Therefore T_t must map equivalent ensembles into equivalent ensembles.

$$T_t \ : \ \rho \mapsto T_t(\rho) = \sum_i p_i T_t(\left|\phi_i\right\rangle \left\langle\phi_i\right|)$$

where this is valid for any decomposition of ρ. This is a good definition of T_t such as do not depends from the chosen basis.

There we can consider two possible decompositions of ρ

$$\begin{cases} \rho = \sum_i p_i \left|\phi_i\right\rangle \left\langle\phi_i\right| \\ \\ \rho = \lambda_1 \rho_1 + \lambda_2 \rho_2 \end{cases}$$

where

$$\rho_j = \sum_k p_k^{(j)} \left|\phi_k^{(j)}\right\rangle \left\langle\phi_k^{(j)}\right|$$

So the evolution of ρ can be done in two equivalent ways, the first one is the direct evolution of ρ, i.e.

$$T_t(\rho) = \sum_i p_i T_t \left(\left|\phi_i\right\rangle \left\langle\phi_i\right|\right)$$

The second one the evolution of the two density matrices ρ_1 and ρ_2:

$$\begin{aligned} T_t(\rho) &= \lambda_1 T_t(\rho_1) + \lambda_2 T_t(\rho_2) \\ \\ &= \lambda_1 \sum_k p_k^{(1)} T_t \left(\left|\phi_k^{(1)}\right\rangle \left\langle\phi_k^{(1)}\right|\right) + \lambda_2 \sum_k p_k^{(2)} T_t \left(\left|\phi_k^{(2)}\right\rangle \left\langle\phi_k^{(2)}\right|\right) \end{aligned}$$

As we show this two evolutions are equivalent therefore

$$T_t(\rho) = T_t\left(\lambda_1\rho_1 + \lambda_2\rho_2\right) = \lambda_1 T_t(\rho_1) + \lambda_2 T_t(\rho_2)$$

So T_t is a linear evolution map. For physical reasons the linearity of T_t is stronger of the linearity of Schrödinger equation, in fact is not possible to do a similar proof using $|\psi\rangle \in \mathcal{H}$ instead of ρ.

2.3 Quantum Dynamical Semigroups

Let $\mathcal{B}$ be a Banach space. A family $\{\, T_t, t \in [0, +\infty[\,\}$ of **bounded**[1] **linear operators** on $\mathcal{B}$ is called a strongly continuous semigroup of operators if:

1)
$$T_{t+s} = T_t T_s \qquad \forall t, s \geq 0$$

2)
$$T_0 = I \quad \text{identity operator}$$

3)
$$\lim_{h \to 0^+} ||T_{t+h}(x) - T_t(x)|| = 0 \qquad \forall t, h \geq 0,\ \forall x \in \mathcal{B}$$

There we call that group strongly continuous because there exist a weakly continuity but we do not use it. The $\{\, T_t \,\}$ as above defined is a group, i.e. a semigroup such the time parameter t is non-negative defined, $t \geq 0$. In general a group G is defined such that

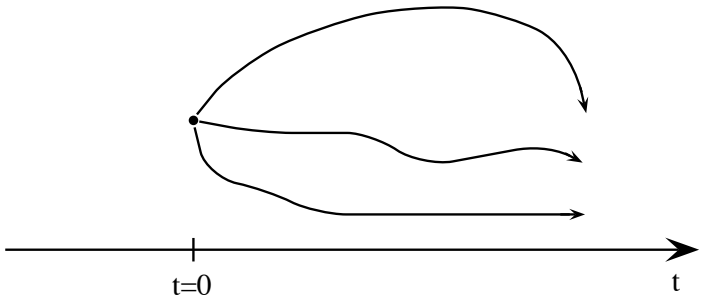
$$\forall g \in G\ \exists \overline{g} \in G \quad \text{such that} \quad \overline{g}g = 0$$

- **Comment 1.** T_t is to be physically interpreted as the time evolution operator which brings the state x from time $t = 0$ to time t. This is the reason for assumption 2), for $t = 0$ we have to obtain the same state ρ

$$T_{t=0}(\rho) \equiv \rho \Rightarrow T_0 = I$$

- **Comment 2.** Assumption 3) implies **continuity**, from the right, of the evolution, which is also a reasonable assumption. Usually we work with continuous dynamics, there are non-continuous ones but we are not going to work with them.
- **Comment 3.** Assumption 1) implies the **Markovian nature of the evolution**. Consider a system at $t = 0$, how evolves in time?

[1] A bounded operator T is such that $||Tx|| \leq C||x|| \quad \forall x \in \mathcal{D}(T)$, where $\mathcal{D}(T)$ stands for domain of T.



There are two possible dynamics:

- **Markovian dynamics**: The knowledge of the state of the system at $t = 0$ is sufficient to predict the future evolution. The future is separated from the past. In this kind of dynamic we find the newtonian mechanics, the electromagnetism, statistical physics and Schrödinger evolution. The property of this kind of dynamics derive from the properties of differential equations: known the initial conditions one can derive the solution for every time $t \geq 0$.
- **Non-Markovian dynamics**: The knowledge of the state of the system at $t = 0$ is not sufficient to predict the future. This kind of dynamics typically is related to integral-differential equations as

$$\frac{d}{dt}x_t = \int_{-\infty}^{t} ds\ F(x(s))$$

The nature follows a markovian dynamic, but nothing tell us different. In case of interactions with the environment in general there are non-markovian dynamics. Consider a particle who go into an environment. Suppose the environment interfere on the particle as function of how the particle changes the environment when it entering in the environment. If the change that particle imply are less of the typical fluctuations of the environment therefore the dynamic is still markovian. If the change is grater then the dynamic can become non-markovian.

We define the **generator** of the semigroup as

$$L(x) \equiv \lim_{h\to 0^+} \frac{T_h(x) - x}{h}$$

where

$$x \in \mathcal{D}(L) \equiv \left\{ y \in \mathcal{B},\ \exists \lim_{h\to 0^+} \frac{T_h(y) - y}{h} \right\}$$

Then one can prove that

a) $\mathcal{D}(L)$ is a linear submanifold of $\mathcal{B}$ and L is a **linear operator**.

b) Let $x \in \mathcal{D}(L)$, then $x_t = T_t(x) \in \mathcal{D}(L)$ for all $t \geq 0$. Then

$$\frac{d}{dt}x_t = L(x_t) \qquad \forall t \geq 0$$

In this sense L is the generator of the semigroup. Physically this equation is very important. Therefore

$$x_t = T_t(x) ='' \, e^{Lt} \, '' \, x$$

It is at the generalization of the exponent formula. It is not the usually exponential but behaves as that.

This is a differential equation, with means that the future evolution is determinate by the present state only, not by its past. This is a strong assumption, not always true in nature (non-markovian dynamics). But it is convenient for modeling many important physical situations. In our case, this assumption is true when environment correlation time is much shorter that the relaxation time of the reduce system. Also, we consider only first order differential equations for density matrix, not higher order ones. It happens that the typical equations of the dynamic are expressed in terms of $\frac{d^2}{dt^2}$ and not just $\frac{d}{dt}$. There one can always bring back from a problem of second order to a system of equations of first order.

In case of Schrödinger equation we have as generator

$$L = -\frac{i}{\hbar}\left[H, \cdot\right]$$

in fact

$$\frac{d}{dt}\rho_t \equiv L(\rho_t) = \frac{i}{\hbar}\left[H, \rho_t\right]$$

is the von Neumann-Liouville equation. So L is the generator of the Schrödinger dynamic.

c) $\mathcal{D}(L)$ is dense on $\mathcal{B}$, and L on $\mathcal{D}(L)$ is a closed operator.

An important question is to give necessary and sufficient conditions for an operator L to be the infinitesimal generator of a semigroup. In functional analysis the theorem of Hille-Yosida impose this conditions on L to be a good generator of the semigroup, i.e. impose conditions to the hamiltonian to be a good hamiltonian.

Let A be a bounded operator. A is called **trace-class** operator if exist and is bounded its **trace norm** $||A||$

$$||A|| = \mathrm{Tr}\left[\sqrt{A^\dagger A}\right]$$

Since A is bounded, $A^\dagger$ exist. Then $A^\dagger A$ is a positive operator and one can define the square root operator, so $\sqrt{A^\dagger A}$ exist. The set of all trace class operators $\mathrm{T}(\mathcal{H})$ is a Banach space with associated trace norm $||A||$.

Statistical operators are a special type of trace class operators. They are also positive, thus self-adjoint.

A family $\{ T_t,\ t \in [0, +\infty[\}$ of bounded linear operators on $\mathrm{T}(\mathcal{H})$ is called a **quantum dynamical semigroup** if:

1. It is a strongly continuous semigroup
2. If $\rho \geq 0$ then

$$T_t(\rho) \geq 0 \qquad \forall \rho \in \mathrm{T}(\mathcal{H}) \text{ and } \forall t \in [0, +\infty[$$

3. The trace is conserved

$$\mathrm{Tr}\left[T_t(\rho)\right] = \mathrm{Tr}\left[\rho\right] \qquad \forall \rho \in \mathrm{T}(\mathcal{H}) \text{ and } \forall t \in [0, +\infty[$$

The last two conditions imply that density matrices are mapped into density matrices.

The next step is to characterize the generator of a quantum dynamical semigroup. This is the content of the Lindblad theorem.

2.4 The Lindblad Equation

Consider a system associated to a N dimensional Hilbert space $\mathcal{H}$. Let $\rho \in \mathrm{T}(\mathcal{H})$ be the density matrix of the system. The density matrix at fixed time t is

$$\rho' = T_t(\rho)$$

where T_t belongs to a quantum dynamical semigroup. Since T_t is a linear operator, temporal map of a markovian evolution, with respect to some convenient orthonormal basis $\{ |\phi_i\rangle \}$ of $\mathcal{H}$ we can express the matrix elements of ρ' in terms of the matrix elements of ρ.

$$\rho'_{ij} = \sum_{rs}^{N} A_{ir,js} \rho_{rs}$$

This is not the standard way of writing it. It is a good way, because we are treating ρ as a vector of the Banach space $\mathrm{T}(\mathcal{H})$.

Note that $\{ A_{ir,js} \}$ consists of N^4 complex constants, so there are $2N^4$ degrees of freedom. For determine the form of this coefficients we have to impose the conditions on ρ' to be a density matrix.

- **hermiticity** $(\rho')^\dagger = \rho'$

$$(\rho'_{ij})^\dagger = \sum_{rs}^{N} A^*_{js,ir} \rho_{sr}$$

because for a generic operator $\hat{A}$ we have

$$(\hat{A})_{ij} = a_{ij} \quad \Rightarrow \quad (\hat{A}^\dagger)_{ij} = a^*_{ji}$$

And

$$\rho'_{ij} = \sum_{rs}^{N} A_{ir,js}\rho_{rs} = \sum_{rs}^{N} A_{ir,js}\rho_{sr}$$

because ρ is hermitian. So we obtain

$$A^*_{js,ir} = A_{ir,js}$$

since ρ_{rs} are arbitrary. Therefore, considering js and ir as a unique index, A can be viewed as a $N^2 \times N^2$ hermitian matrix. It has N^2 real eigenvalues λ^α and N^2 complex eigenvectors E^α_{ir} which satisfy the orthonormality condition

$$\sum_{ir} E^\alpha_{ir} E^{\beta *}_{ir} = \delta^{\alpha\beta}$$

If we view E^α_{ir} as the component $|i, r\rangle$ of a square $N \times N$ matrix $\vec{E}^\alpha$, we can write the above condition as

$$\mathrm{Tr}\left[\vec{E}^\alpha \vec{E}^{\beta\dagger}\right] = \delta^{\alpha\beta}$$

as product of two matrices. Therefore

$$\mathrm{Tr}\left[\vec{E}^\alpha \vec{E}^{\beta\dagger}\right] = \sum_{i}^{N}\sum_{r}^{N} E^\alpha_{ir}(\vec{E}^{\beta\dagger})_{ir} = \sum_{i}^{N}\sum_{r}^{N} E^\alpha_{ir} E^{\beta *}_{ir}$$

So we can write ρ'_{ij} in the spectral decomposition

$$\rho'_{ij} = \sum_{\alpha=1}^{N^2} \lambda^\alpha \sum_{rs=1}^{N} E^\alpha_{ir} E^{\alpha *}_{js} \rho_{rs} \quad \Rightarrow \quad \rho' = \sum_{\alpha=1}^{N^2} \lambda^\alpha \vec{E}^\alpha \rho \vec{E}^{\alpha\dagger}$$

- **trace constraint** $\mathrm{Tr}\,[\rho'] = \mathrm{Tr}\,[\rho] = 1$

  For the linearity and the ciclicity of the trace one obtain

$$\mathrm{Tr}\left[\left(\sum_{\alpha=1}^{N^2} \lambda^\alpha \vec{E}^{\alpha\dagger}\vec{E}^\alpha - I\right)\rho\right] = 0$$

  This must be true $\forall \rho \in \mathrm{T}(\mathcal{H})$, therefore

$$\sum_{\alpha=1}^{N^2} \lambda^\alpha \vec{E}^{\alpha\dagger} \vec{E}^\alpha = I$$

- **positivity** $\rho' \geq 0$

  So if we define for all $|v\rangle \in \mathcal{H}$

$$|v^\alpha\rangle = \vec{E}^{\alpha\dagger} |v\rangle \quad \Rightarrow \quad \langle v|\rho'|v\rangle = \sum_{\alpha=1}^{N^2} \lambda^\alpha \langle v^\alpha|\rho|v^\alpha\rangle$$

  but $\langle v|\rho|v\rangle \geq 0$ for all $|v\rangle \in \mathcal{H}$, $|v^\alpha\rangle$ too. The condition $\lambda^\alpha \geq 0$ for all $\alpha = 1 \dots N^2$ is therefore sufficient for ρ' to be positive, but **not necessary**.

  Example Let $\mathcal{H}$ be a two dimensional Hilbert space and

$$\left\{ \vec{E}^\alpha \right\}_\alpha \longrightarrow \begin{cases} \vec{E}^1 = \dfrac{1}{\sqrt{2}}\sigma_1 \\ \vec{E}^2 = \dfrac{1}{\sqrt{2}}\sigma_2 \\ \vec{E}^3 = \dfrac{1}{\sqrt{2}}\sigma_3 \\ \vec{E}^4 = \dfrac{1}{\sqrt{2}}I \end{cases}$$

  with relative eigenvalues $\lambda^1 = \lambda^2 = -\lambda^3 = \lambda^4 = 1$. Therefore

$$\rho' = \frac{1}{2}\left[\sigma_1\rho\sigma_1 + \sigma_2\rho\sigma_2 - \sigma_3\rho\sigma_3 + \rho\right]$$

  If we consider ρ as

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \\ \rho_{21} & \rho_{22} \end{pmatrix}$$

  we obtain for ρ'

$$\rho' = \begin{pmatrix} \rho_{22} & \rho_{12} \\ \\ \rho_{21} & \rho_{11} \end{pmatrix}$$

  i.e. ρ' is just ρ with its diagonal elements exchanged. Thus, since ρ is positive, also ρ' is positive, though λ^3 is negative.

  So the condition that for all $\alpha = 1 \dots N$ we have $\lambda^\alpha \geq 0$ is sufficient for the positivity of ρ', but is not a necessary condition.

Above we impose just the conditions on ρ' to be a density matrix. We have to impose also the conditions that ρ' is a state obtained by a good time evolution map starting from ρ.

- **identity at** $t = 0$

  A, i.e. $A_{ir,js}$, must be the identity matrix. Therefore we can take for $t = 0$

$$\begin{cases} \lambda^{\alpha=N^2}(0) = N & \vec{E}^{\alpha=N^2}(0) = \dfrac{1}{\sqrt{N}} I \\ \\ \lambda^{\alpha\neq N^2}(0) = 0 & \vec{E}^{\alpha\neq N^2}(0) = \vec{K}^{\alpha} \text{ chosen arbitrary} \end{cases}$$

  For $\alpha \neq N^2$ the vectors $\vec{E}^{\alpha}$ are associated to the eigenvalue zero, therefore must be orthonormal to $\vec{E}^{N^2}$ and have to spam all the rest of the associated Banach space.

- **continuity of evolution** We have to impose the continuity of the evolution, therefore for infinitesimal time dt we must have for $\rho' = T_{dt}(\rho)$

$$\begin{cases} \lambda^{N^2}(dt) = N\left[1 - C^{N^2}dt\right] & \vec{E}^{N^2}(dt) = \dfrac{1}{\sqrt{N}}\left[I + \vec{B}dt\right] \\ \\ \lambda^{\alpha\neq N^2}(dt) = C^{\alpha}dt & \vec{E}^{\alpha\neq N^2}(dt) = \vec{K}^{\alpha} + \vec{R}^{\alpha}dt \end{cases}$$

  Like in a Taylor expansion, we consider just the terms to first order in dt. Therefore we obtain

$$\begin{aligned} \rho' = T_{dt}(\rho) = \rho(dt) &= \sum_{\alpha=1}^{N^2} \lambda^{\alpha}\left(\vec{E}^{\alpha}\rho\vec{E}^{\alpha\dagger}\right) \\ &= N\left[1 - C^{N^2}dt\right]\frac{1}{\sqrt{N}}\left[I + \vec{B}dt\right]\rho\frac{1}{\sqrt{N}}\left[I + \vec{B}^{\dagger}dt\right] + \\ &+ \sum_{\alpha=1}^{N^2-1} C^{\alpha}dt\left[\vec{K}^{\alpha} + \vec{R}^{\alpha}dt\right]\rho\left[\vec{K}^{\alpha\dagger} + \vec{R}^{\alpha\dagger}dt\right] \end{aligned}$$

  At first order in dt we have

$$\rho(dt) = \rho - C^{N^2}\rho dt + \vec{B}\rho dt + \rho\vec{B}^{\dagger}dt + \sum_{\alpha=1}^{N^2-1} C^{\alpha}dt\left[\vec{K}^{\alpha}\rho\vec{K}^{\alpha\dagger}\right]$$

  So applying the limit

$$\lim_{dt\to 0}\frac{\rho(dt) - \rho}{dt} = \frac{d\rho}{dt}$$

  we obtain

$$\frac{d\rho}{dt} = -C^{N^2}\rho + \vec{B}\rho + \rho\vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\left[\vec{K}^{\alpha}\rho\vec{K}^{\alpha\dagger}\right]$$

Because of the structure of a dynamical semigroup, this differential equation holds true not only for $t = 0$, but for any time t. We want to simplify this equation so we can apply another proprieties that a good evolution must have

- **trace constraint** The trace must be conserved, that implies

$$\begin{aligned}\mathrm{Tr}\left[\rho(dt) - \rho\right] &\equiv 0 \\ &= \mathrm{Tr}\left[-C^{N^2}\rho dt + \vec{B}\rho dt + \rho\vec{B}^{\dagger}dt + \sum_{\alpha=1}^{N^2-1} C^{\alpha} dt\left[\vec{K}^{\alpha}\rho\vec{K}^{\alpha\dagger}\right] - \rho\right]\end{aligned}$$

Applying the linearity and the ciclicity of the trace one obtain

$$C^{N^2} I = \vec{B} + \vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\vec{K}^{\alpha\dagger}\vec{K}^{\alpha}$$

Since the commutator between $C^{N^2} I$ and ρ is zero we can consider

$$\begin{aligned}C^{N^2}\rho &= \frac{1}{2}C^{N^2} I\rho + \frac{1}{2}\rho C^{N^2} I \\ &= \frac{1}{2}\left[\vec{B} + \vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\vec{K}^{\alpha\dagger}\vec{K}^{\alpha}\right]\rho + \frac{1}{2}\rho\left[\vec{B} + \vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\vec{K}^{\alpha\dagger}\vec{K}^{\alpha}\right]\end{aligned}$$

So we can replace this expression in the differential equation above

$$\begin{aligned}\frac{d\rho}{dt} &= -\frac{1}{2}\left[\vec{B} + \vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\vec{K}^{\alpha\dagger}\vec{K}^{\alpha}\right]\rho - \frac{1}{2}\rho\left[\vec{B} + \vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\vec{K}^{\alpha\dagger}\vec{K}^{\alpha}\right] \\ &\quad + \vec{B}\rho + \rho\vec{B}^{\dagger} + \sum_{\alpha=1}^{N^2-1} C^{\alpha}\left[\vec{K}^{\alpha}\rho\vec{K}^{\alpha\dagger}\right] \\ &= \left[\frac{1}{2}\left(\vec{B} - \vec{B}^{\dagger}\right), \rho\right] - \frac{1}{2}\sum_{\alpha=1}^{N^2-1} C^{\alpha}\left[\vec{K}^{\alpha}\vec{K}^{\alpha\dagger}\rho + \rho\vec{K}^{\alpha}\vec{K}^{\alpha\dagger} - 2\vec{K}^{\alpha}\rho\vec{K}^{\alpha\dagger}\right]\end{aligned}$$

Defininig an self-adjoint operator H as

$$-\frac{i}{\hbar}H = \frac{1}{2}\left(\vec{B} - \vec{B}^{\dagger}\right)$$

we obtain the **Lindblad form of the equation**.

Example Consider the two dimensional case with

$$\begin{cases} \vec{E}^1 = \dfrac{1}{\sqrt{2}}\sigma_1 \\ \vec{E}^2 = \dfrac{1}{\sqrt{2}}\sigma_2 \end{cases} \qquad \begin{cases} \vec{E}^3 = \dfrac{1}{\sqrt{2}}\sigma_3 \\ \vec{E}^4 = \dfrac{1}{\sqrt{2}}I \end{cases}$$

We can consider a representation of $\left\{ \vec{E}^\alpha \right\}$ as vectors:

$$\vec{E}^1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \quad \vec{E}^2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ i \\ 0 \end{pmatrix} \quad \vec{E}^3 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \vec{E}^4 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

As we show above we have

$$\rho'_{ij} = \sum_{rs}^{N} A_{ir,js}\rho_{rs}$$

For $t = 0$ we must have $\rho' = \rho$ therefore

$$A_{ir,js} = \delta_{ir}\delta js$$

So if we consider just two indices $m = (i, r)$ and $n = (j, s)$ we can represent A as

$$A_{m,n} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}_{m,n}$$

The matrix A is not the identity matrix, but lets ρ unchanged. Its eigenvalues are

$$\mathrm{Det}\left[A_\lambda I\right] \equiv 0 \quad \Rightarrow \quad \lambda^2(1-\lambda)^2 - \lambda^2 = 0$$

therefore we obtain

$$\begin{cases} \lambda = 0 & \text{with degeneration 3} \\ \lambda = 2 & \text{without degeneration} \end{cases}$$

The eigenvalue $\lambda = 2$ is the one associated to $\vec{E}^4 = \vec{E}^{N^2}$.

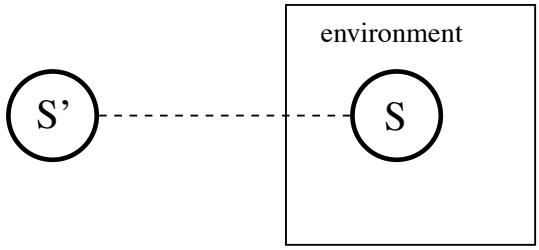
Return to the equation, we notice that this form is too generic, we have to impose the last condition

- **positivity** ρ' must be positive, i.e. the map should preserve positivity. Since the conservation of the positivity is an algebraic problem that became heavier and heavier going forward with the integration, actually we need a stronger requirement than that, which is the **complete positivity**.

  Let $\rho \in \mathrm{T}(\mathcal{H})$ be a density matrix and T_t a quantum dynamical semigroup. The positivity requirement implies

  $$T_t(\rho) \geq 0 \qquad \forall t \geq 0$$

  However, consider the following situation. Suppose we have a system S immersed in an environment. The interaction between the system and the environment leads to a time evolution that is different from that Schrödinger equation describe. Suppose we have a copy of the system S' in the vacuum as in the following figure.

  Suppose that S' do not evolve in time. Let $\mathcal{H}$ and $\mathcal{H}'$ be respectively the Hilbert space associated S and S'. The total density matrix of the two systems is $\overline{\rho} \in \mathrm{T}(\mathcal{H}') \otimes \mathrm{T}(\mathcal{H})$. The evolution of entire system will be a compose map $\overline{T}_t$

  $$\overline{T}_t = I \otimes T_t$$

  If the map T_t is positive,i.e. the predictions on final state of system S have positive probabilities, therefore $T_t(\rho) \geq 0$ for all times $t \geq 0$. Although T_t and I are positive, that does not imply that also $I \otimes T_t$ is positive. Indeed S and S' are no interacting between them they can be correlated, i.e. can form a entangled state. So in this case the evolution of the system S imply an evolution also of the system S'. Therefore we can not factorize the action of $\overline{T}_t$ on the single states, but we have to consider the evolution of the entire system. So the request of positivity of the map T_t is not sufficient in a general case. We have to consider the condition of positivity of the map $\overline{T}_t = I \otimes T_t$. That condition if is true for all dimension of $\mathcal{H}'$ imply the complete positivity of T_t.

  The compete positivity of the temporal map is not a physical request, but also mathematical, so in this way one can characterize the positive maps, in our case the temporal ones. Considering the mapped state $\overline{\rho}'$ as

  $$\overline{\rho}' = (I \otimes T_t)(\overline{\rho}) = \sum_{\alpha=1}^{N^2} \lambda^\alpha \left(I \otimes \vec{E}^\alpha\right) \overline{\rho} \left(I \otimes \vec{E}^\alpha\right)^\dagger$$

  we have to impose that $\overline{\rho}'$ have to be positive, so for all $|\omega\rangle \in \mathcal{H}' \otimes \mathcal{H}$

$$\langle\omega|\overline{\rho}'|\omega\rangle = \sum_{\alpha=1}^{N^2} \lambda^\alpha \langle\omega| \left(I \otimes \vec{E}^\alpha\right) \overline{\rho} \left(I \otimes \vec{E}^\alpha\right)^\dagger |\omega\rangle \geq 0$$

Considering $\{ \chi_n \}_n$ and $\{ \phi_m \}_m$ as basis respectively of $\mathcal{H}'$ and $\mathcal{H}$, we can decompose $|\omega\rangle$ on this basis as

$$|\omega\rangle = \sum_{mn} \lambda_{nm} |\chi_n\rangle \otimes |\phi_m\rangle$$

So

$$\langle\omega|\overline{\rho}'|\omega\rangle = \sum_{\alpha=1}^{N^2} \lambda^\alpha \sum_{mn,m'n'} \lambda^*_{m'n'}\lambda_{mn} \langle\chi_{n'}| \langle\phi_{m'}| \left(I \otimes \vec{E}^\alpha\right) \overline{\rho} \left(I \otimes \vec{E}^\alpha\right)^\dagger |\chi_n\rangle |\phi_m\rangle$$

Expressing $\overline{\rho}$ a general linear combination of the two basis

$$\overline{\rho} = \sum_{kl,k'l'} C_{kl}C^*_{k'l'} |\chi_l\rangle |\phi_k\rangle \langle\chi_{l'}| \langle\phi_{k'}|$$

therefore

$$\langle\omega|\overline{\rho}'|\omega\rangle = \sum_{\alpha=1}^{N^2} \lambda^\alpha \sum_{mn,m'n'} \lambda^*_{m'n'}\lambda_{mn} \sum_{kl,k'l'} C_{kl}C^*_{k'l'}\vec{E}^\alpha_{m'k}\vec{E}^{\alpha*}_{mk'}\delta_{n'l}\delta_{nl'}$$

Let $\vec{C}$ and $\vec{D}$ be the matrices that

$$\begin{cases} (\vec{C})_{kl} = C_{kl} \\ \\ (\vec{D})_{mn} = \lambda_{mn} \end{cases}$$

So we can use the matrix notation

$$\langle\omega|\overline{\rho}'|\omega\rangle = \sum_{\alpha=1}^{N^2} \lambda^\alpha \mathrm{Tr}\left[\vec{C}\vec{D}^\dagger\vec{E}^\alpha\right] \mathrm{Tr}\left[\vec{E}^{\alpha\dagger}\vec{D}\vec{C}^\dagger\right]$$

Choose

$$\vec{E}^\beta = \frac{\vec{D}\vec{C}^\dagger}{\sqrt{N}} \qquad \text{with index } \beta \text{ arbitrary but fixed}$$

We can define $\vec{E}^\beta$ in this way, in fact $\vec{D}$ is the matrix of coefficients of $|\omega\rangle$, an arbitrary vector of $\mathcal{H}' \otimes \mathcal{H}$. And $\vec{C}$ is the matrix of coefficients of $\overline{\rho}$, but $\overline{\rho}$ is also a generic state. The only restriction is the trace constrain

$$\mathrm{Tr}\left[\overline{\rho}\right] = 1 = \mathrm{Tr}\left[\vec{C}^\dagger\vec{C}\right]$$

therefore we have just two choices

1)

$$\vec{C}^{\dagger} = \frac{\vec{E}^{\beta}}{\sqrt{N}} \quad \text{and} \quad \vec{D} = I$$

2)

$$\vec{C}^{\dagger} = \frac{I}{\sqrt{N}} \quad \text{and} \quad \vec{D} = \vec{E}^{\beta}$$

In both cases we have satisfy the trace constrain and also we obtain

$$\langle \omega | \overline{\rho}' | \omega \rangle = \sum_{\alpha=1}^{N^2} \lambda^{\alpha} \left(\delta^{\alpha\beta} \right)^2 = \lambda^{\beta}$$

but β is a arbitrary index, so for all $\beta = 1 \dots N^2$ we have

$$\lambda^{\beta} \geq 0$$

The eigenvalues λ^{β} of A are non-negative. For $t = 0$ this eigenvalues are defined as

$$\begin{cases} \lambda^{\alpha=N^2}(0) = N \\ \\ \lambda^{\alpha\neq N^2}(0) = 0 \end{cases}$$

So for λ^{N^2} there is no any problem for infinitesimal dt, but for $\alpha \neq N^2$ we have to be sure that λ^{α} are still non-negative. For infinitesimal dt we defined

$$\lambda^{\alpha\neq N^2}(dt) = C^{\alpha} dt$$

therefore the coefficients $\{ C^{\alpha} \}_{\alpha}$ of the **Kossakowski matrix** have to be positive to maintain the complete positivity of T_t, i.e. the positivity of $\overline{T}_t$.

The complete positivity is a condition more restrictive that the simply positivity. Moreover, like for positivity, the complete positivity is a propriety not just for temporal maps but for maps in general. For give a general mathematical definition of positivity consider a positive map Λ from $\mathrm{T}(\mathcal{H})$ to $\mathrm{T}(\mathcal{H})$

$$\begin{aligned} \Lambda \ : \mathrm{T}(\mathcal{H}) &\to \mathrm{T}(\mathcal{H}) \\ \rho \qquad &\mapsto \rho' = \Lambda(\rho) \end{aligned}$$

The map Λ is called n-positive if

$$(\mathrm{id}_n \otimes \Lambda) \geq 0$$

where id_n is n dimensional identity map. If

$$(\mathrm{id}_n \otimes \Lambda) \geq 0 \qquad \forall n$$

therefore the map Λ is a complete positive map. The condition that $(\mathrm{id}_n \otimes \Lambda)$ must be positive for all n is required because we do not know if in the past of the our system was be some interaction with another system and it was created an entangled state. We neither know the dimension of the possible entangled system, therefore we require to the map the most general condition, i.e. $\forall n$.

Notice that one can use the difference between the condition of the simply positivity and the complete positivity for understands if a state is entangled or not. There in fact some criteria that use this. The idea is to use a positive but not completely positive map Λ and act with its extended map $(\mathrm{id}_n \otimes \Lambda)$ on a density matrix ρ. Therefore if

$$(\mathrm{id}_n \otimes \Lambda)(\rho) < 0$$

the density matrix ρ describe a bipartite entangled state. The map Λ is called entanglement witness. Otherwise if

$$(\mathrm{id}_n \otimes \Lambda)(\rho) \geq 0$$

we can not know if the state ρ is entangled.

We return on the derivation of Lindblad equation. Since the Kossakowski matrix is positive, we can define

$$L^\alpha = \sqrt{C^\alpha}\vec{K}^\alpha$$

Therefore we obtain the **Lindblad master equation**

$$\frac{d}{dt}\rho_t = -\frac{i}{\hbar}[H, \rho_t] - \frac{1}{2}\sum_{\alpha=1}^{N^2-1}\left[L^\alpha L^{\alpha\dagger}\rho_t + \rho_t L^\alpha L^{\alpha\dagger} - 2L^\alpha \rho_t L^{\alpha\dagger}\right]$$

This is the equation for a completely positive dynamic of a quantum dynamical semigroup, is the equivalent of the Schrödinger evolution but for an open system. The first term is the von Neumann-Liouville equation, i.e. the generator of a rotation made by the unitary operator $\exp[-it[H, \rho_t]/\hbar]$. The second term is the action of the environment on the system. The H is not the hamiltonian of the system alone, but is the effective one, its consider the environment in interaction too. It is possible to write the Lindblad equation also in a different way

$$\frac{d}{dt}\rho_t = -\frac{i}{\hbar}[H, \rho_t] + \sum_\alpha \left[L^\alpha \rho_t L^{\alpha\dagger} - \frac{1}{2}\left\{L^{\alpha\dagger}L^\alpha, \rho_t\right\}\right]$$

- **Comment 1.** It is a consequence of this derivation that the Lindblad operators L^α are not arbitrary operators, because they are restricted by the orthonormality conditions

$$\mathrm{Tr}\left[\vec{E}^\alpha \vec{E}^{\beta\dagger}\right] = \delta^{\alpha\beta} \quad \Rightarrow \quad \begin{cases} \mathrm{Tr}\left[\vec{B} + \vec{B}^\dagger\right] = 0 & \text{when } \alpha = \beta = N^2 \\ \mathrm{Tr}\left[\vec{K}^\alpha\right] = 0 & \text{when } \alpha \neq N^2, \beta = N^2 \\ \mathrm{Tr}\left[\vec{K}^\alpha \vec{K}^{\beta\dagger}\right] = \delta^{\alpha\beta} & \text{when } \alpha \neq N^2, \beta \neq N^2 \end{cases}$$

The first condition says that the hermitian part of $\vec{B}$ vanishes. There is no restriction on H, which is the anti-hermitian part of $\vec{B}$.

The second condition says that $\mathrm{Tr}\left[\vec{K}^\alpha I\right] = 0$, which implies that $I/\sqrt{N}$ completes the orthonormal set operators, vectors in the Banach space.

The third condition says that the vectors $\vec{K}^\alpha$ are orthonormal.

One can prove that a Lindblad equation with arbitrary Lindblad operators, i.e. with no constrains on the number of the operators and no orthonormality constrains, can be reduced to a constrained Lindblad equation. This is because we can always redefine L'^α as a unitary transformation of L^α

$$L'^\alpha \equiv \sum_\beta U^{\alpha\beta} L^\beta$$

Therefore

$$\begin{aligned} \sum_\alpha L'^\alpha L'^{\alpha\dagger} &= \sum_{\alpha\beta\gamma} L^\beta U^{\alpha\beta} U^{\alpha\gamma\dagger} L^{\gamma\dagger} \\ &= \sum_{\beta\gamma} L^\beta \left(\sum_\alpha U^{\alpha\beta} U^{\alpha\gamma\dagger} \right) L^{\gamma\dagger} \\ &= \sum_{\beta\gamma} L^\beta \delta^{\beta\gamma} L^{\gamma\dagger} \\ &= \sum_\beta L'^\beta L'^{\beta\dagger} \end{aligned}$$

because $U^{\alpha\beta}$ are unitary operators which are acting on a different Hilbert space that acts L^α, we can consider them as coefficient of the expansion of L'^α on the basis $\left\{ L^\beta \right\}_\beta$. In similar way

$$\begin{cases} \rho L'^{\alpha} L'^{\alpha\dagger} & \Rightarrow \quad \rho L^{\alpha} L^{\alpha\dagger} \\ L'^{\alpha} L'^{\alpha\dagger} \rho & \Rightarrow \quad L^{\alpha} L^{\alpha\dagger} \rho \\ L'^{\alpha} \rho L'^{\alpha\dagger} & \Rightarrow \quad L^{\alpha} \rho L^{\alpha\dagger} \end{cases}$$

- **Comment 2.** The proof of the theorem was given by Gorini, Kossakowski and Sudarshan in 1976 for the case of a finite-dimensional Hilbert space, and by Lindblad in 1976, the same year, for a bounded generator of a quantum dynamical semigroup in a separable Hilbert space and with index α allowed to run over a countable set. Special proofs for unbounded operators also exist.

2.5 Example Of Lindblad Dynamics

Example 1) Pure dephasing
Consider the following dynamics for a two dimensional system

$$\frac{d}{dt}\rho_t = -\frac{i\omega}{2}\left[\sigma_z, \rho_t\right] - \frac{\lambda}{2}\left[\rho_t - \sigma_z \rho_t \sigma_z\right]$$

i.e. a system with an effective hamiltonian $H = \omega\sigma_z/2$ and just one Lindblad operator defined as $L = \sqrt{\lambda/2}\ \sigma_z$. Inserting the Bloch vector

$$\rho_t = \frac{I + \mathbf{r}_t \cdot \boldsymbol{\sigma}}{2}$$

in the above equation one obtain

$$\dot{\mathbf{r}} \cdot \boldsymbol{\sigma} = -i\omega \left[\sigma_z, \frac{I + \mathbf{r} \cdot \boldsymbol{\sigma}}{2}\right] - \lambda \left[\frac{I + \mathbf{r} \cdot \boldsymbol{\sigma}}{2} - \sigma_z \frac{I + \mathbf{r} \cdot \boldsymbol{\sigma}}{2} \sigma_z\right]$$

The first term gives us

$$\left[\sigma_z, \frac{I + \mathbf{r}_t \cdot \boldsymbol{\sigma}}{2}\right] = i r_x \sigma_y - i r_y \sigma_x$$

and the last one

$$\sigma_z \frac{I + \mathbf{r}_t \cdot \boldsymbol{\sigma}}{2} \sigma_z = \frac{1}{2}\left[I + r_x(-\sigma_x) + r_y(-\sigma_y) + r_z \sigma_z\right]$$

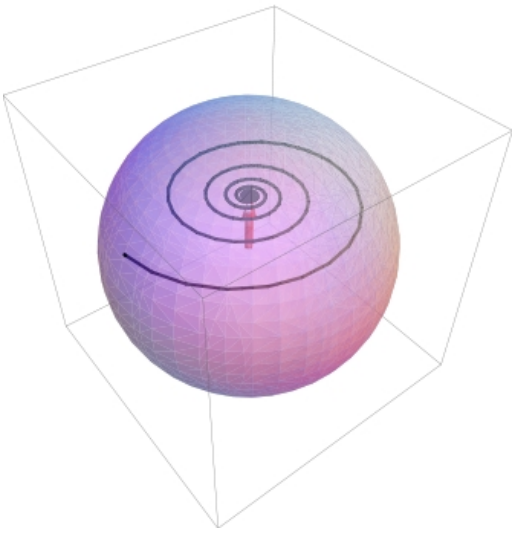
Therefore

$$\dot{\mathbf{r}} \cdot \boldsymbol{\sigma} = \sigma_x\left(-\omega r_y - \lambda r_x\right) + \sigma_y\left(\omega r_x - \lambda r_y\right)$$

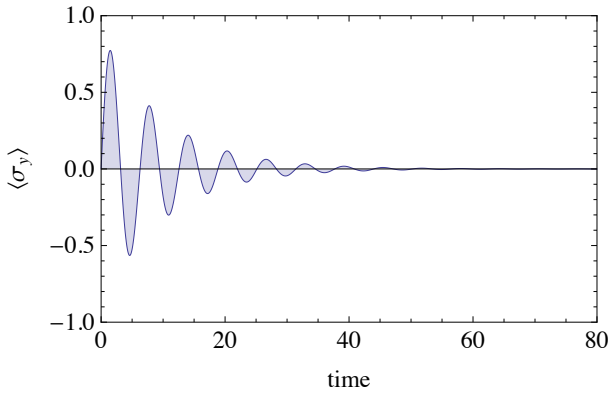
equating the coefficient of the three Pauli's matrices one obtain

$$\begin{cases} \dot{r}_x = -\omega r_y - \lambda r_x \\ \\ \dot{r}_y = \omega r_x - \lambda r_y \\ \\ \dot{r}_z = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} r_x = \left[r_x^0 \cos(\omega t) - r_y^0 \sin(\omega t)\right] e^{-\lambda t} \\ \\ r_y = \left[r_x^0 \sin(\omega t) + r_y^0 \cos(\omega t)\right] e^{-\lambda t} \\ \\ r_z = r_z^0 \end{cases}$$

In following figures are shown the dynamic on the Bloch sphere and the evolution in time of mean value of σ_y.



(a)



(b)

So the oscillatory behavior in x and y components is damped. The system tends towards a mixed state. There is loss of quantum coherence. Only the off-diagonal elements are affected and exponential damped. The diagonal elements,i.e. r_z, do not change. It is a pure dephasing.

Example 2) Damped harmonic oscillator
Consider the following dynamic for a two dimensional system

$$\frac{d}{dt}\rho_t = -i\frac{\omega}{2}\left[\sigma_x, \rho_t\right] - \frac{\lambda}{2}\left(\rho_t - \sigma_z \rho_t \sigma_z\right)$$

Notice that the master equation is of Lindblad type. Therefore inserting the Bloch vector in the master equation

$$\begin{aligned} \frac{d}{dt}\rho_t &= \frac{\dot{\mathbf{r}}_t \cdot \boldsymbol{\sigma}}{2} \\ &= -i\frac{\omega}{2}\left[\sigma_x, \frac{I + \mathbf{r}_t \cdot \boldsymbol{\sigma}}{2}\right] - \frac{\lambda}{2}\left\{\frac{I + \mathbf{r}_t \cdot \boldsymbol{\sigma}}{2} - \sigma_z \frac{I + \mathbf{r}_t \cdot \boldsymbol{\sigma}}{2}\sigma_z\right\} \end{aligned}$$

The second term is equal to the second term of the previous example and also the first term is quite similar.

so we obtain

$$\frac{\lambda}{2}\left\{\frac{I+\mathbf{r}_t\cdot\boldsymbol{\sigma}}{2}-\sigma_z\frac{I+\mathbf{r}_t\cdot\boldsymbol{\sigma}}{2}\sigma_z\right\}=\frac{\lambda}{2}\left\{r_x\sigma_x+r_y\sigma_y\right\}$$

Therefore equating with $d\rho_t/dt$ one obtain

$$\frac{d}{dt}\rho_t=\sigma_x\left(-\frac{\lambda}{2}r_x\right)+\sigma_y\left(-\frac{\omega}{2}r_z-\frac{\lambda}{2}r_y\right)+\sigma_z\left(\frac{\omega}{2}r_y\right)$$

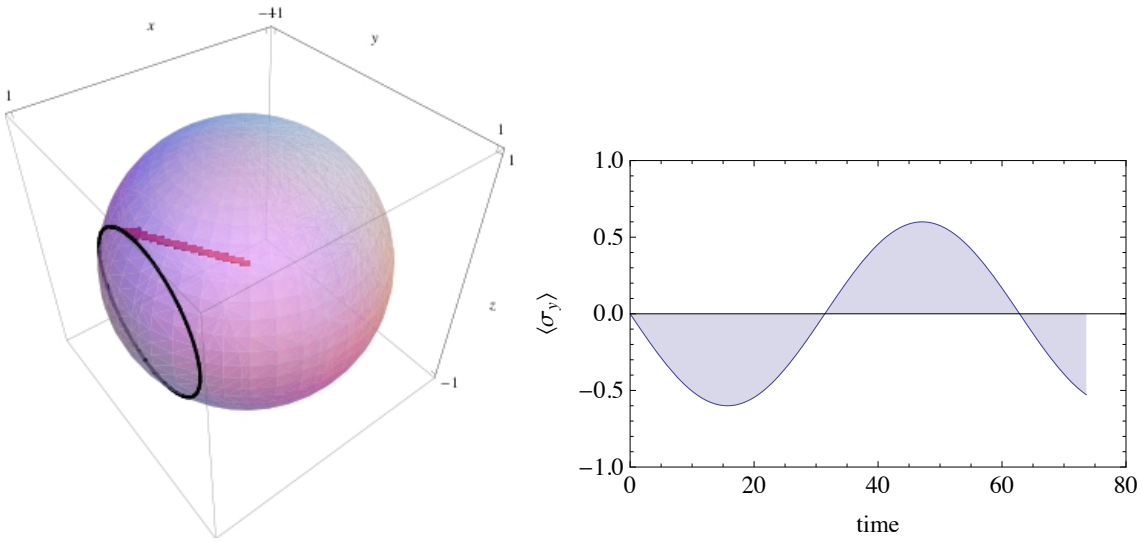
So we obtain how the Bloch vector components evolve in time

$$\begin{cases}\dot{r}_x=-\lambda r_x\\ \dot{r}_y=-\lambda r_y-\omega r_z\\ \dot{r}_z=\omega r_z\end{cases}$$

If we consider $\lambda=0$ we get

$$\begin{cases}\dot{r}_x=0 & r_x=\text{CONSTANT}\\ \dot{r}_y=-\omega r_z & r_y=\cos(\omega t)\\ \dot{r}_z=\omega r_z & r_z=\sin(\omega t)\end{cases}$$

is an oscillation along the x axis of the Bloch sphere.

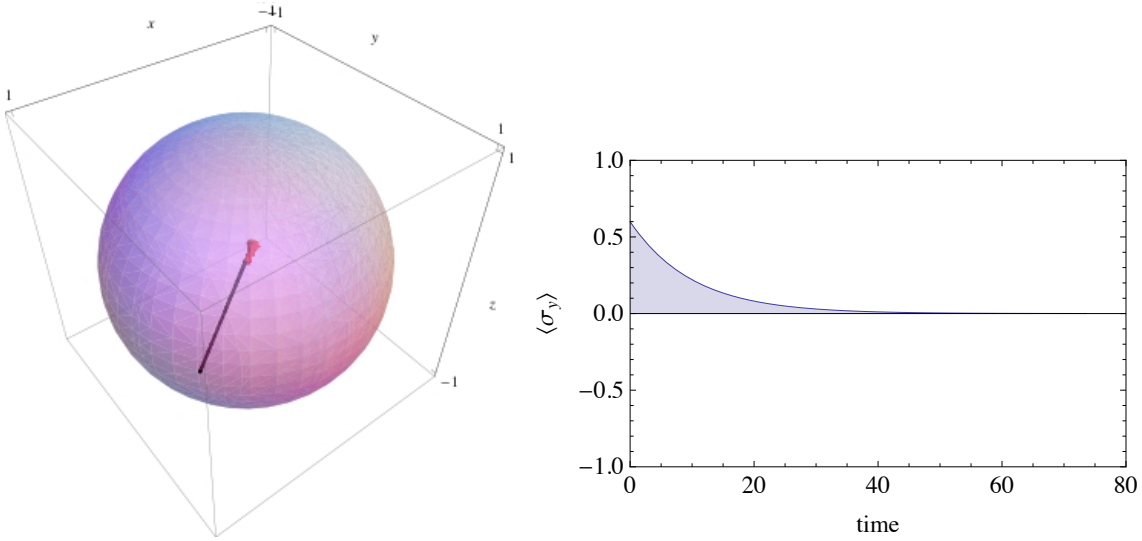


(a) (b)

If we put instead $\omega=0$ we obtain

$$\begin{cases} \dot{r}_x = -\lambda r_x & r_x = r_x^0 e^{-\lambda t} \\ \dot{r}_y = -\lambda r_y & r_y = r_y^0 e^{-\lambda t} \\ \dot{r}_z = 0 & r_z = \text{CONSTANT} \end{cases}$$

we obtain an damped dynamic, i.e. an exponential decay of x and y components of Bloch vector. A pure state can become a mixed state. We loose information about superposition in the x and y directions.



(a) (b)

The general solution can be obtained considering the second time derivative of one of this two components, for example r_y

$$\ddot{r}_y = -\omega \dot{r}_z - \lambda \dot{r}_y = -\omega r_z^2 - \lambda \dot{r}_y$$

This is the equation for a damped harmonic oscillator

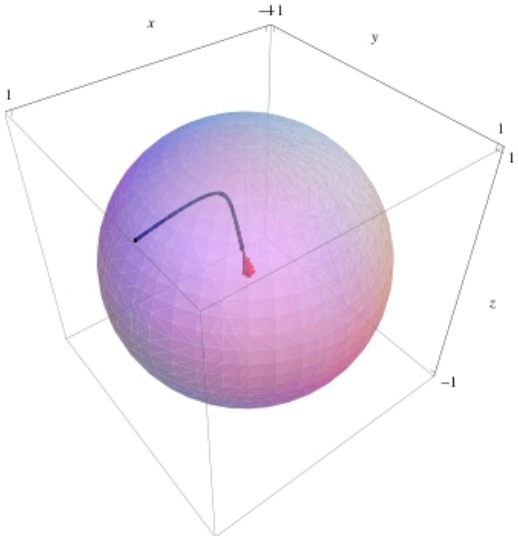
$$\ddot{r}_y + \omega^2 r_y + \lambda \dot{r}_y = 0$$

The roots of the equation are

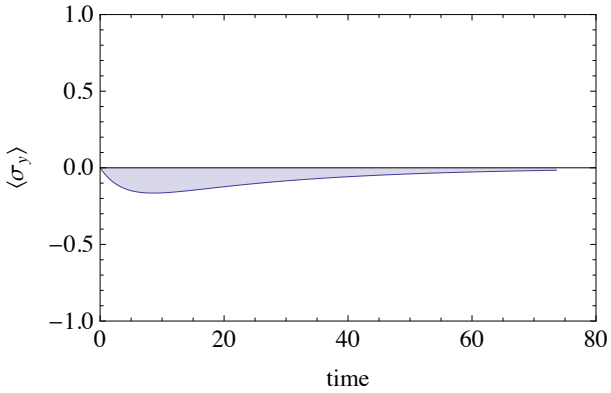
$$\alpha^2 + \lambda\alpha + \omega^2 = 0 \qquad \Rightarrow \qquad \alpha_{1,2} = \frac{-\lambda \pm \sqrt{\lambda^2 - 4\omega}}{2}$$

Therefore there are three cases

$$1) \qquad \lambda > 2\omega \quad \Rightarrow \quad \text{Overdamped case}$$

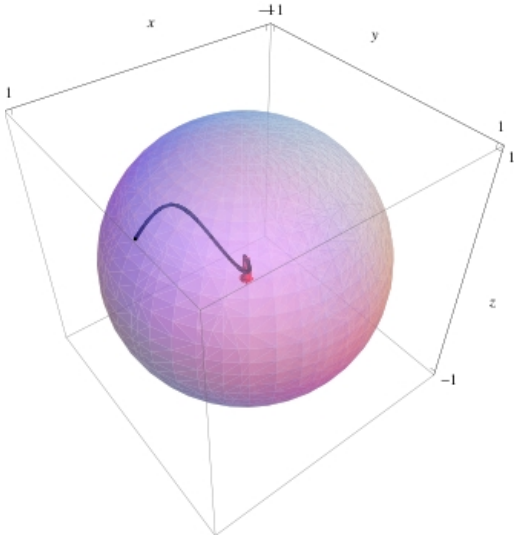


(a)

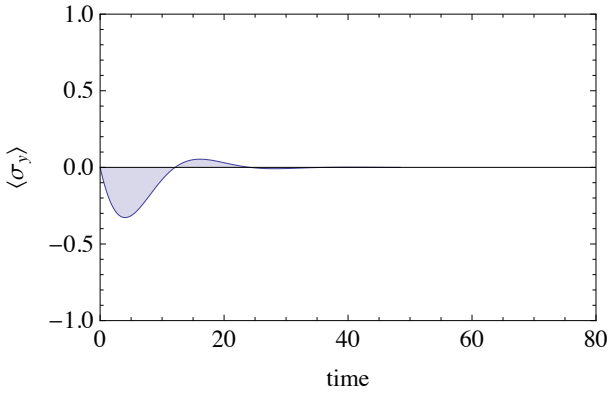


(b)

2) $\lambda = 2\omega \quad \Rightarrow \quad$ Critical damping case

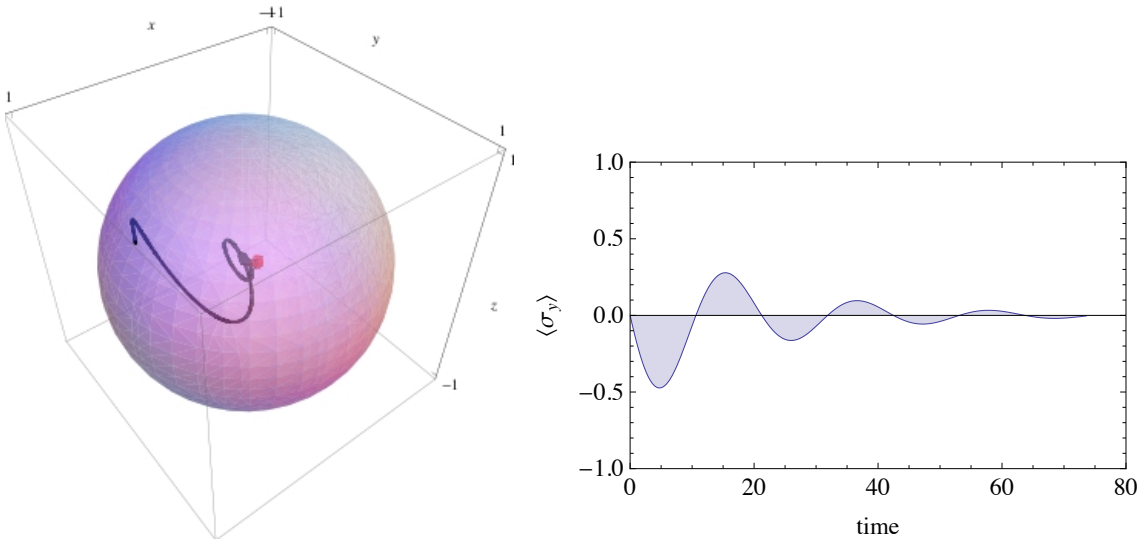


(a)



(b)

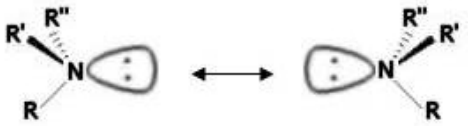
3) $\lambda < 2\omega \quad \Rightarrow \quad$ Underdamped case



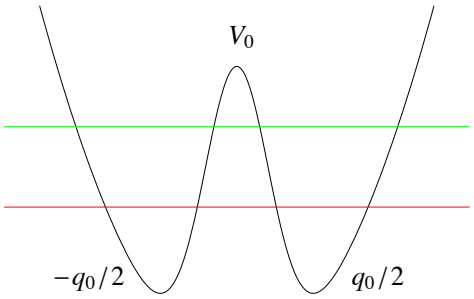
(a) (b)

Example 3) Chiral molecule

The chiral molecules are important in chemistry and biology. Consider a ammonia molecule in an ammonia gas. The ammonia, NH_3, is a molecule that oscillating between two states called chiral with a frequency ω_0. An idea is given by the following figure



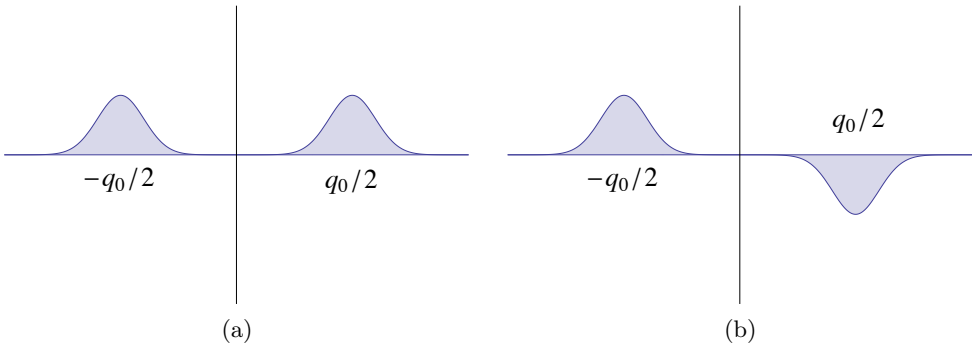
A good way to represent the problem is a potential double-well with two minima in $q = \pm q_0/2$ separated by a barrier V_0 as shown in figure.



In the limit of low temperature, i.e.

$$V_0 \gg \hbar\omega_0 \gg K_B T$$

where T is the temperature of the gas and K_B is the Boltzmann constant, the system is well approximated from a two dimensional hamiltonian H. As custom we denote as $|+\rangle$ the ground state and $|-\rangle$ the first excited. Since the parity operator P commutes with the hamiltonian H this two states are also eigenstates of P. Therefore they cannot be localized states. Their typical shape is shown in the next figure: in (a) is represented $\langle x|+\rangle$ and in (b) $\langle x|-\rangle$.



(a) (b)

But usually molecules are found in **chiral states**, which are localized states:

$$\begin{cases} |L\rangle \dfrac{1}{\sqrt{2}}\big[|+\rangle + |-\rangle\big] \\ \\ |R\rangle \dfrac{1}{\sqrt{2}}\big[|+\rangle - |-\rangle\big] \end{cases}$$

i.e. the state $|L\rangle$ is localized in $q = -q_0/2$ and $|R\rangle$ in $q = q_0/2$. In this two dimensional approximation the hamiltonian becomes

$$H = -\frac{1}{2}\omega_0\sigma_x$$

therefore the two eigenstates of H are the eigenstates of σ_x:

$$\sigma_x\,|\pm\rangle = \pm\,|\pm\rangle$$

Notice that the position operator $\hat{q}$ in this approximation can be expressed as

$$\hat{q} = \frac{q_0}{2}\sigma_z$$

therefore the two localized states $|L\rangle$ and $|R\rangle$ are eigenstates of σ_z.

As we tell above, molecules are usually found in chiral states and not in the energy eigenstates. The reason of this paradox, called Hund's paradox, is the decoherence that the external environment implies on our chiral molecule with scattering processes. Since the scattering process occurs in space therefore the decoherence occurs in space. So if we consider a real chiral system in interaction with the environment, we found its states in position eigenstates. For describing the interaction with environment we can consider the following form for the Lindblad equation.

$$\frac{d}{dt}\rho_t = -i\frac{\omega_0}{2}\left[\sigma_x, \rho_t\right] - \frac{\lambda}{2}\left[\rho_t - \sigma_z\rho_t\sigma_z\right]$$

where the first term indicates the hamiltonian evolution and the second one the decoherence in position. Solving this equation one find

$$r_z(t) = \frac{e^{-\lambda t/2}}{2\omega}\left[2r_z(0)\omega\cos(\omega t) + (r_z(0)\lambda + 2r_y(0)\omega_0)\sin(\omega t)\right]$$

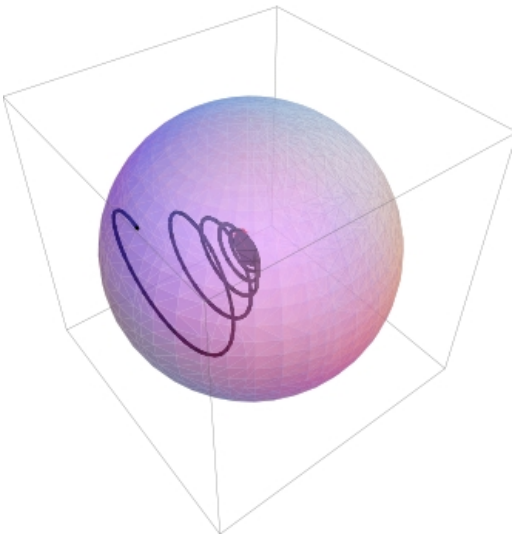
where ω is the characteristic inversion frequency, defined as

$$\omega = \omega_0\sqrt{1 - \left(\frac{p}{p_{cr}}\right)^2}$$

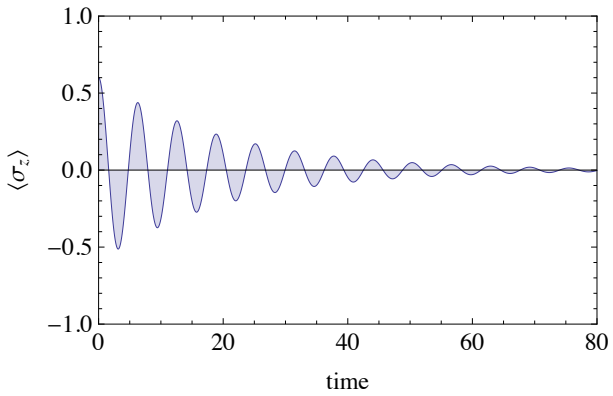
where p is the pressure of the environment, i.e. the gas, and p_{cr} is a critical pressure

$$p_{cr} = \frac{\sqrt{2\omega_0^2 m K_B T}}{\sigma_{TOT}(\bar{q})}$$

defined in terms of the total cross section σ_{TOT} as function of the most probable momentum of the gas $\bar{p} = \sqrt{2mK_BT}$.

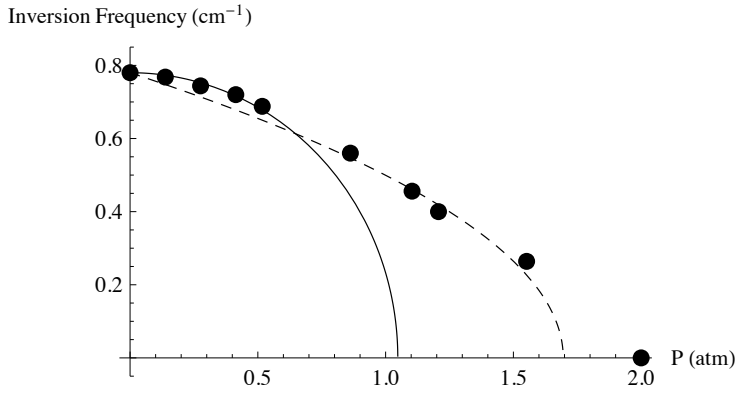


(a)



(b)

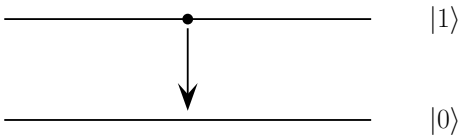
This model have a limit of validity, the model works well for pressure values between 0 and 0.7 atmospheres, as shown in figure.



Example 4) Relaxation to zero temperature
Consider a two dimensional system with hamiltonian eigenstates that are also eigenstates of σ_z, i.e. $|0\rangle$ as ground state and $|1\rangle$ as first exited. The hamiltonian H of the isolated system is

$$H = \frac{\hbar\omega}{2}\sigma_z$$

Consider the system is in the state $|1\rangle$, because of the interaction with the environment, the system tends to fall to the ground state, in fact there is no thermal energy, i.e. temperature $T = 0$, that can excite the system, so



The Lindblad operator associated to this phenomena is

$$L = \sqrt{\gamma}\,|0\rangle\langle 1| = \sqrt{\gamma}\sigma^-$$

This operator describe the transition from $|0\rangle$ to $|1\rangle$ with a certain probability. The operator σ^- is defined as

$$\sigma^- = \sigma_x - i\sigma_y$$

Its adjoint operator σ^+ is defining in the similar way with the plus instead the minus.
The Lindblad equation is therefore

$$\frac{d}{dt}\rho_t = -i\frac{\omega}{2}\big[\sigma_z, \rho_t\big] - \frac{\gamma}{2}\left[\sigma^+\sigma^-\rho_t + \rho_t\sigma^+\sigma^- - 2\sigma^-\rho_t\sigma^+\right]$$

With the same procedure as before one obtain

$$\begin{cases} \dot{r}_x = -\omega r_y - \dfrac{\gamma}{2} r_x \\ \dot{r}_y = \omega r_x - \dfrac{\gamma}{2} r_y \\ \dot{r}_z = -\gamma(1 + r_z) \end{cases}$$

Integrating one obtain

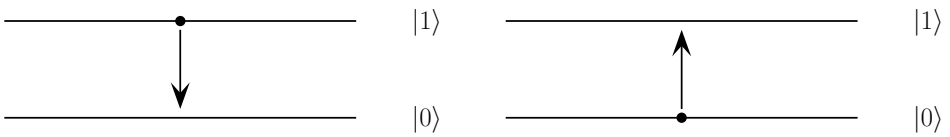
$$\begin{cases} r_x(t) = [r_x(0)\cos(\omega t) - r_y(0)\sin(\omega t)]\, e^{-\gamma t/2} \\ r_y(t) = [r_x(0)\sin(\omega t) + r_y(0)\cos(\omega t)]\, e^{-\gamma t/2} \\ r_z(t) = (r_z(0) - 1)e^{-\gamma t} - 1 \end{cases}$$

The solution have in r_x and r_y damped oscillations with a decay rate of $\gamma/2$, this is a dephasing, i.e. suppression of off-diagonal elements. And for r_z have a relaxation with rate γ.

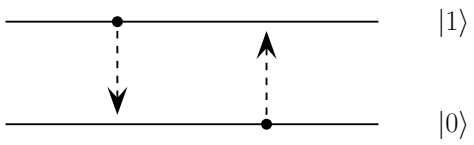
Example 5) Relaxation to finite temperature
A generalization of the previous example is this one. Consider the same two dimensional system with hamiltonian of isolated system H as

$$H = \frac{\hbar\omega}{2}\sigma_z$$

The only difference between this case and the previous is that the temperature T is not zero. Therefore if the system is in the ground state $|0\rangle$ can be excited by the environment to the first excited state $|1\rangle$ and reversal the system can fall from $|1\rangle$ to $|0\rangle$. We have both the phenomena



After enough time the system is described by the **thermal state** ρ_β, i.e. the state in thermal equilibrium with the environment, whatever was be the starting state of the system.



$$\rho_\beta = \frac{e^{-\beta H}}{\mathrm{Tr}\left[e^{-\beta H}\right]}$$

where β is the inverse temperature, i.e. $K_B T = 1/\beta$. Since the hamiltonian is the one described above we have

$$\begin{aligned} e^{-\beta H} &= \exp(-\frac{\beta\hbar\omega}{2}\sigma_z) = \exp(\alpha\sigma_z) = \sum_{n=0}^{+\infty} \frac{(\alpha\sigma_z)^n}{n!} \\ &= I + \alpha\sigma_z + \frac{\alpha^2}{2} I + \frac{\alpha^3}{3!}\sigma_z + \dots \\ &= \left(1 + \frac{\alpha^2}{2} + \frac{\alpha^4}{4!} + \dots\right) I + \left(\alpha + \frac{\alpha^3}{3!} + \dots\right)\sigma_z = \cosh(\alpha) I + \sinh(\alpha)\sigma_z \end{aligned}$$

$$= \begin{pmatrix} \cosh(\alpha) + \sinh(\alpha) & 0 \\ 0 & \cosh(\alpha) + \sinh(\alpha) \end{pmatrix} = \begin{pmatrix} e^{\alpha} & 0 \\ 0 & e^{-\alpha} \end{pmatrix} = \begin{pmatrix} e^{-\beta\hbar\omega/2} & 0 \\ 0 & e^{\beta\hbar\omega/2} \end{pmatrix}$$

Therefore the trace is

$$\mathrm{Tr}\left[e^{-\beta H}\right] = e^{-\beta\hbar\omega/2} + e^{\beta\hbar\omega/2}$$

And we have the final form of ρ_β

$$\rho_\beta = \begin{pmatrix} \dfrac{e^{-\beta\hbar\omega/2}}{e^{-\beta\hbar\omega/2} + e^{\beta\hbar\omega/2}} & 0 \\ 0 & \dfrac{e^{\beta\hbar\omega/2}}{e^{-\beta\hbar\omega/2} + e^{\beta\hbar\omega/2}} \end{pmatrix} = \frac{1}{1 + e^{-\beta\hbar\omega}} \begin{pmatrix} e^{-\beta\hbar\omega} & 0 \\ 0 & 1 \end{pmatrix}$$

From this form we can consider the two asymptotic behavior. The first one is for $T \to 0$, i.e. the above example. Therefore $\beta \to +\infty$ and we obtain

$$\rho_{beta} \quad \xrightarrow[\beta \to +\infty]{} \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

so the system goes into the ground state $|0\rangle$. The second one is the limit for $T \to +\infty$, i.e. $\beta \to 0$. In this case we obtain

$$\rho_{beta} \quad \xrightarrow[\beta \to 0]{} \quad \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

so we lose all the information about the state of the system.

For a finite temperature T we can express ρ_β in the Bloch representation. Therefore one obtain

$$\begin{cases} r_x = 0 \\ \\ r_y = 0 \\ \\ r_z = \dfrac{e^{-\beta\hbar\omega} - 1}{e^{-\beta\hbar\omega} + 1} = -\tanh\left(\dfrac{\beta\hbar\omega}{2}\right) \end{cases}$$

The Lindblad equation that describe this interaction with the environment is

$$\frac{d}{dt}\rho_t = -i\frac{\omega}{2}\left[\sigma_z, \rho_t\right] - \frac{\gamma}{2}\left[\sigma^+\sigma^-\rho_t + \rho_t\sigma^+\sigma^- - 2\sigma^-\rho_t\sigma^+\right] - \frac{\gamma'}{2}\left[\sigma^-\sigma^+\rho_t + \rho_t\sigma^-\sigma^+ - 2\sigma^+\rho_t\sigma^-\right]$$

where the first term is the hamiltonian evolution, the second one is the falling process from $|1\rangle$ to $|0\rangle$ with rate γ and the third term is the rising process from $|0\rangle$ to $|1\rangle$ with rate γ'. As in previous examples one can solve the equation and obtain

$$\begin{cases} \dot{r}_x(t) = -\omega r_y - \dfrac{\gamma + \gamma'}{2} r_x \\ \\ \dot{r}_y(t) = \omega r_x - \dfrac{\gamma + \gamma'}{2} r_y \\ \\ \dot{r}_z(t) = -(\gamma + \gamma')r_z - \gamma + \gamma' \end{cases}$$

Therefore r_x and r_y have damped oscillations, they decay exponentially with rate $(\gamma + \gamma')/2$. This is a dephasing effect, as in previous example. Instead r_z goes asymptotically as $\dot{r}_z = 0$, this is the equilibrium state. From this last observation we can derive

$$\dot{r}_z = 0 = -(\gamma + \gamma')r_z - \gamma + \gamma' \quad \Rightarrow \quad \gamma'\left(1 + \tanh\left(\frac{\beta\hbar\omega}{2}\right)\right) = \gamma\left(1 - \tanh\left(\frac{\beta\hbar\omega}{2}\right)\right)$$

Therefore we obtain a relation between the two rates

$$\gamma' = \gamma e^{-\beta\hbar\omega}$$

Therefore for very large temperature we have $\gamma' \sim \gamma$, i.e. the excitation and de-excitation occur with the same rate, and for long times $t \to +\infty$ we hare $\mathbf{r} \to 0$ exponentially with rate $(\gamma+\gamma')/2$ and we obtain the completely mixed state.

Chapter 3

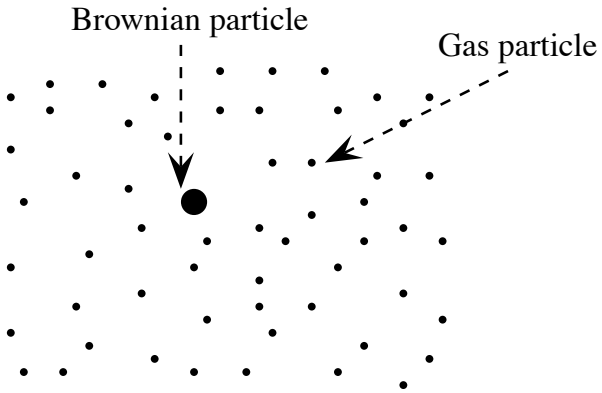
Quantum Brownian Motion

The most important example of open quantum system is a particle, or any other system, interacting with a bath of molecules. This is called **quantum brownian motion**. Because it is the quantum version of the classical brownian motion studied by Brown, Einstien and others.

In this chapter we will devire the master equation from a microscopic situation.

3.1 Collisional Decoherence

Consider a particle in a gas, as in following figure



This is a many particle problem, which cannot be solved exactly. One needs to introduce some approximations.

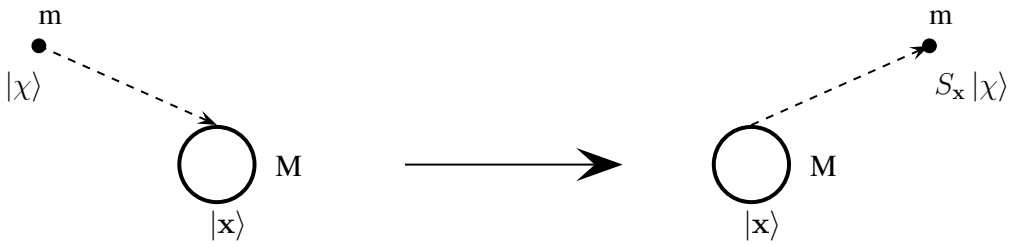
PARTE DA SISTEMARE!!!: LE APPROSSIMAZIONI SONO: GAS DILUITO, M¿¿m

3.2 The Master Equation With Collisional Decoherence

The assumption of heavy particle, i.e. the mass of the brownian particle M is much larger than the mass m of the gas particle ($M >> m$), means that if the brownian particle is on perfectly localized state $|\mathbf{x}\rangle$ and the gas particle in a state $|\chi\rangle$, then the scattering brings in the following change

$$|\mathbf{x}\rangle \otimes |\chi\rangle \quad \xrightarrow{\text{scattering}} \quad |\mathbf{x}\rangle \otimes S_{\mathbf{x}} |\chi\rangle$$

So the heavy particle assumption make that the scattering process change just the gas particle state $|\chi\rangle$ and not the brownian one $|\mathbf{x}\rangle$. $S_{\mathbf{x}}$ is the scattering matrix, is the representation in positions of the unitary operator $\hat{S}$.



If instead the brownian particle is not perfectly localized but is in a state of superposition $|\varphi\rangle$

$$|\varphi\rangle = \int d^3x\ \varphi(\mathbf{x})\,|\mathbf{x}\rangle$$

Then the scattering process is describe from

$$|\varphi\rangle \otimes |\chi\rangle \quad \xrightarrow{\text{scattering}} \quad \int d^3x\ \varphi(\mathbf{x})\,|\mathbf{x}\rangle \otimes S_{\mathbf{x}}\,|\chi\rangle \equiv |F\rangle$$

The density matrix of entire system is

$$\rho = |F\rangle\,\langle F|$$

Therefore the reduce density matrix for the brownian particle changes is

$$\begin{aligned}\rho^{(S)} &= \mathrm{Tr}^{(E)}\left[|F\rangle\,\langle F|\right] \\ &= \mathrm{Tr}^{(E)}\left[\int d^3x d^3x'\ \varphi(\mathbf{x})\varphi^*(\mathbf{x}')\,|\mathbf{x}\rangle\,\langle\mathbf{x}'| \otimes S_{\mathbf{x}}\,|\chi\rangle\,\langle\chi|\,S^\dagger_{\mathbf{x}'}\right]\end{aligned}$$

The partial trace TR^E is the trace applied only on the degrees of freedom of gas, therefore only on $S_{\mathbf{x}}\,|\chi\rangle\,\langle\chi|\,S^\dagger_{\mathbf{x}'}$. If we choose as basis $\{\ S_{\mathbf{x}}\,|\chi\rangle\ \}$ of Hilbert space $\mathcal{H}^E$ associated to the environment (gas) we obtain

$$\rho^{(S)} = \int d^3x d^3x'\ \varphi(\mathbf{x})\varphi^*(\mathbf{x}')\,|\mathbf{x}\rangle\,\langle\mathbf{x}'|\,\langle\chi|S^\dagger_{\mathbf{x}'}S_{\mathbf{x}}|\chi\rangle$$

The representation in the position basis of the density matrix ρ is

$$\rho(\mathbf{x},\mathbf{x}') = \langle\mathbf{x}|\rho|\mathbf{x}'\rangle$$

Therefore before and after the scattering this quantity changes

$$\rho(\mathbf{x},\mathbf{x}') = \varphi(\mathbf{x})\varphi^*(\mathbf{x}') \quad \xrightarrow{\text{scattering}} \quad \rho(\mathbf{x},\mathbf{x}',\tau) = \varphi(\mathbf{x})\varphi^*(\mathbf{x}')\,\langle\chi|S^\dagger_{\mathbf{x}'}S_{\mathbf{x}}|\chi\rangle$$

The last term appears as effect of collision, i.e. we call it **decoherence term** $\eta(\mathbf{x}',\mathbf{x})$. The effect of the scattering is to modify the off-diagonal elements of density matrix. In fact for the diagonal elements we have $\mathbf{x} = \mathbf{x}'$ and we obtain

$$\eta(\mathbf{x}',\mathbf{x}) = \langle\chi|S^\dagger_{\mathbf{x}'}S_{\mathbf{x}}|\chi\rangle = \langle\chi|S^{-1}_{\mathbf{x}}S_{\mathbf{x}}|\chi\rangle = \langle\chi|\chi\rangle = 1$$

because $S_{\mathbf{x}}$ is unitary.

The interaction is **translational invariant**. This means that, if we introduce the translation operator

$$T_{\mathbf{x}} = e^{-i\hat{\mathbf{p}}\cdot\mathbf{x}/\hbar}$$

where $\hat{\mathbf{p}}$ is the momentum operator in three dimension. $T_{\mathbf{x}}$ is defined as

$$T_{\mathbf{x}}\left|\mathbf{x}'\right\rangle = \left|\mathbf{x}+\mathbf{x}'\right\rangle$$

It translates the state in space. Therefore we can express the scattering matrix as

$$S_{\mathbf{x}} = T_{\mathbf{x}}S_0T^\dagger_{\mathbf{x}}$$

where S_0 is the scattering matrix in the origin of the reference system. We want to compute the **decoherence term**

$$\eta(\mathbf{x}',\mathbf{x}) = \langle\chi|S^\dagger_{\mathbf{x}'}S_{\mathbf{x}}|\chi\rangle$$

We has assumed that the gas particle state is in the generic state $|\chi\rangle$. In a typical situation, we have a gas in thermal equilibrium at temperature T. Therefore the gas particle state is a momentum state $|\mathbf{p}\rangle$ with a associated probability related to the Boltzmann distribution $\mu(\mathbf{p})$

$$\mu(\mathbf{p}) = \left(\frac{\beta}{2\pi m}\right)^{3/2}\exp\left[-\frac{\beta p^2}{2m}\right]$$

with $\beta = (KT)^{-1}$ is the inverse temperature. The integration over momentum space give us

$$\int d\mathbf{p}\ \mu(\mathbf{p}) = 1$$

Therefore we obtain

$$\begin{aligned}\eta(\mathbf{x}',\mathbf{x}) &= \int d\mathbf{p}\ \mu(\mathbf{p})\,\langle\mathbf{p}|S^\dagger_{\mathbf{x}'}S_{\mathbf{x}}|\mathbf{p}\rangle \\ &= \int d\mathbf{p}\ \mu(\mathbf{p})\,\langle\mathbf{p}|e^{-i\hat{\mathbf{p}}\cdot\mathbf{x}'/\hbar}\ S_0^\dagger\ e^{i\hat{\mathbf{p}}\cdot\mathbf{x}'/\hbar}\ e^{-i\hat{\mathbf{p}}\cdot\mathbf{x}/\hbar}\ S_0\ e^{i\hat{\mathbf{p}}\cdot\mathbf{x}/\hbar}|\mathbf{p}\rangle \\ &= \int d\mathbf{p}\ \mu(\mathbf{p})e^{-i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\,\langle\mathbf{p}|S_0^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ S_0|\mathbf{p}\rangle\end{aligned}$$

To simply solve this equation we consider the two systems, bath and brownian particle, in a finite box with volume $V = L^3$. Therefore there are not a continuous of momentum states, but only the ones that are supported by the box. This operation is called **box normalization**. We turn the integrals into finite sums

$$\int d\mathbf{p} \quad \longrightarrow \quad \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p}}$$

Moreover because of the position representation of momentum states $|\mathbf{p}\rangle$

$$\langle\mathbf{x}|\mathbf{p}\rangle = \frac{1}{\sqrt{L}}e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$$

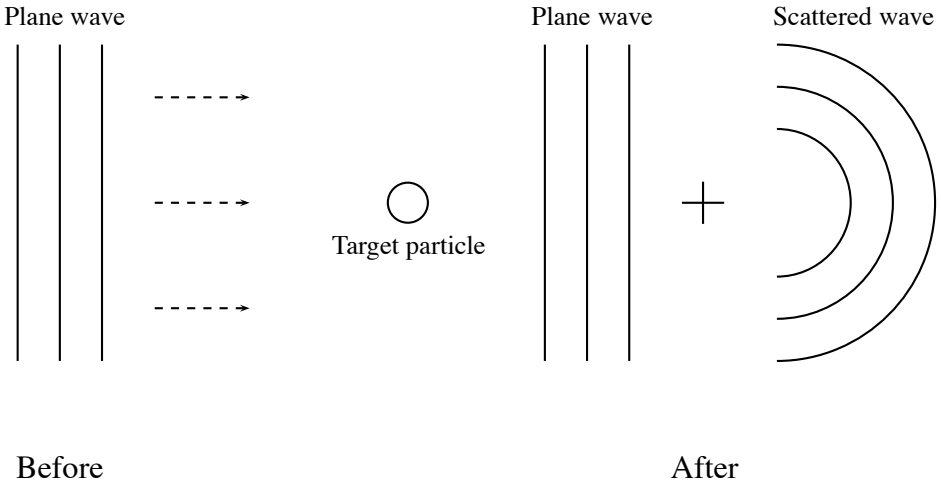
we have for any operator $\hat{A}$

$$\langle\mathbf{p}|\hat{A}|\mathbf{p}\rangle = \int_V d\mathbf{x}\ \frac{1}{\sqrt{L}}e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}A\frac{1}{\sqrt{L}}e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$$

These are the properly normalized wave functions. If we apply the limit $L \to +\infty$ to the sums we obtain again the integral forms. Therefore the decoherence term become

$$\eta(\mathbf{x}',\mathbf{x}) = \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p}} \mu(\mathbf{p})e^{-i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\,\langle\mathbf{p}|S_0^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ S_0|\mathbf{p}\rangle$$

Consider a plane wave that runs over a target particle. The outcome wave is a superposition of a plane wave and a scattered one, i.e. just a part of the original wave change after the interaction with the target.



With this consideration we can consider the operator of scattering S_0 as

$$S_0 = I + i\mathcal{T}$$

$\mathcal{T}$ is the so-called T-matrix. Therefore we can simplify the previous equation

$$\begin{aligned}\langle \mathbf{p}|S_0^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ S_0|\mathbf{p}\rangle &= \langle \mathbf{p}|\left[I - i\mathcal{T}^\dagger\right]\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ \left[I + i\mathcal{T}\right]|\mathbf{p}\rangle \\ &= e^{i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\langle \mathbf{p}|\mathbf{p}\rangle - i\ e^{i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\langle \mathbf{p}|\left(\mathcal{T}^\dagger - \mathcal{T}\right)|\mathbf{p}\rangle + \langle \mathbf{p}|\mathcal{T}^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ \mathcal{T}|\mathbf{p}\rangle\end{aligned}$$

If the two systems will be in the free space the bracket $\langle \mathbf{p}|\mathbf{p}\rangle$ will be a Dirac-δ in 0, i.e. a divergence. Since we are not in free space but in a finite box we have $\langle \mathbf{p}|\mathbf{p}\rangle = 1$. Therefore

$$\langle \mathbf{p}|S_0^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ S_0|\mathbf{p}\rangle = e^{i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\left[1 + i\langle \mathbf{p}|\left(\mathcal{T} - \mathcal{T}^\dagger\right)|\mathbf{p}\rangle\right] + \langle \mathbf{p}|\mathcal{T}^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ \mathcal{T}|\mathbf{p}\rangle$$

As we tell before S_0 is an unitary operator, therefore we can use this property

$$\begin{aligned}I = S_0^\dagger S_0 &= \left[I - i\mathcal{T}^\dagger\right]\left[I + i\mathcal{T}\right] \\ &= I + i\left(\mathcal{T} - \mathcal{T}^\dagger\right) + \mathcal{T}^\dagger\mathcal{T}\end{aligned}$$

So

$$i\left(\mathcal{T} - \mathcal{T}^\dagger\right) = -\mathcal{T}^\dagger\mathcal{T}$$

The previous term become

$$\langle \mathbf{p}|S_0^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ S_0|\mathbf{p}\rangle = e^{i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\left[1 - \langle \mathbf{p}|\mathcal{T}^\dagger\mathcal{T}|\mathbf{p}\rangle\right] + \langle \mathbf{p}|\mathcal{T}^\dagger\ e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\ \mathcal{T}|\mathbf{p}\rangle$$

With tho simplification we can express the decoherence term as

$$\begin{aligned}\eta(\mathbf{x}',\mathbf{x}) &= \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p}} \mu(\mathbf{p}) e^{-i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} \langle \mathbf{p}| S_0^\dagger \; e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} \; S_0|\mathbf{p}\rangle \\ &= \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p}} \mu(\mathbf{p}) - \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p}} \mu(\mathbf{p}) \big[\langle \mathbf{p}|\mathcal{T}^\dagger\mathcal{T}|\mathbf{p}\rangle + e^{-i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} \langle \mathbf{p}|\mathcal{T}^\dagger \; e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} \; \mathcal{T}|\mathbf{p}\rangle \big]\end{aligned}$$

The first term is equal to one, in fact if we consider the limit of $L \to +\infty$

$$\lim_{L\to+\infty} \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p}} \mu(\mathbf{p}) = \int d\mathbf{p} \; \mu(\mathbf{p}) = 1$$

For factorize the $\mathcal{T}$ terms we have to insert an identity in momentum space, i.e. $\sum_{\mathbf{p}'} |\mathbf{p}'\rangle \langle \mathbf{p}'|$, just after $\mathcal{T}^\dagger$.

$$\begin{aligned}\eta(\mathbf{x}',\mathbf{x}) &= 1 - \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p},\mathbf{p}'} \mu(\mathbf{p}) \big[\langle \mathbf{p}|\mathcal{T}^\dagger|\mathbf{p}'\rangle \langle \mathbf{p}'|\mathcal{T}|\mathbf{p}\rangle + e^{-i\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} \langle \mathbf{p}|\mathcal{T}^\dagger|\mathbf{p}'\rangle \langle \mathbf{p}'| \; e^{i\hat{\mathbf{p}}\cdot(\mathbf{x}'-\mathbf{x})/\hbar} \; \mathcal{T}|\mathbf{p}\rangle \big] \\ &= 1 - \left(\frac{2\pi\hbar}{L}\right)^3 \sum_{\mathbf{p},\mathbf{p}'} \mu(\mathbf{p}) \langle \mathbf{p}|\mathcal{T}^\dagger|\mathbf{p}'\rangle \langle \mathbf{p}'|\mathcal{T}|\mathbf{p}\rangle \left[1 - e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{x}'-\mathbf{x})/\hbar}\right]\end{aligned}$$

As we shown before for any operator $\hat{A}$ we have

$$\langle \mathbf{p}|\hat{A}|\mathbf{p}\rangle = \int_V d\mathbf{x} \; \frac{1}{\sqrt{L}} e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} A \frac{1}{\sqrt{L}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$$

So we have to apply this rule for $\mathcal{T}^\dagger$ and $\mathcal{T}$:

$$\begin{cases} \langle \mathbf{p}|\mathcal{T}^\dagger|\mathbf{p}'\rangle = \displaystyle\int_V d\mathbf{y} \; \frac{1}{\sqrt{L}} e^{-i\mathbf{p}\cdot\mathbf{y}/\hbar} \; \mathcal{T}^*(\mathbf{y}) \; \frac{1}{\sqrt{L}} e^{i\mathbf{p}'\cdot\mathbf{y}/\hbar} \\ \\ \langle \mathbf{p}'|\mathcal{T}|\mathbf{p}\rangle = \displaystyle\int_V d\mathbf{z} \; \frac{1}{\sqrt{L}} e^{-i\mathbf{p}'\cdot\mathbf{z}/\hbar} \; \mathcal{T}(\mathbf{z}) \; \frac{1}{\sqrt{L}} e^{i\mathbf{p}\cdot\mathbf{z}/\hbar} \end{cases}$$

Consider the product of these two brackets

$$\begin{aligned}\langle \mathbf{p}|\mathcal{T}^\dagger|\mathbf{p}'\rangle \langle \mathbf{p}'|\mathcal{T}|\mathbf{p}\rangle &= \frac{1}{L^6} \int d\mathbf{y} \int d\mathbf{z} \; e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{y}-\mathbf{z})/\hbar} \mathcal{T}^*(\mathbf{y})\mathcal{T}(\mathbf{z}) \\ &= \left(\frac{2\pi\hbar}{L}\right)^6 \int d\mathbf{y} \int d\mathbf{z} \; e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{y}-\mathbf{z})/\hbar} \frac{\mathcal{T}^*(\mathbf{y})}{(2\pi\hbar)^3} \frac{\mathcal{T}(\mathbf{z})}{(2\pi\hbar)^3} \\ &= \left(\frac{2\pi\hbar}{L}\right)^6 \left| \int d\mathbf{y} \; e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{y})/\hbar} \frac{\mathcal{T}(\mathbf{y})}{(2\pi\hbar)^3} \right|^2 \\ &= \left(\frac{2\pi\hbar}{L}\right)^6 \left|\mathcal{F}(\mathbf{p}-\mathbf{p}')\right|^2\end{aligned}$$

where $\mathcal{F}(\mathbf{p}-\mathbf{p}')$ is the Fourier transformation of $\mathcal{T}(\mathbf{x})$. Therefore the decoherence term become

$$\eta(\mathbf{x}',\mathbf{x}) = 1 - \left(\frac{2\pi\hbar}{L}\right)^9 \sum_{\mathbf{p},\mathbf{p}'} \mu(\mathbf{p}) \left|\mathcal{F}(\mathbf{p}-\mathbf{p}')\right|^2 \left[1 - e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right]$$

Applying the limit for $L \to +\infty$ we obtain

$$\eta(\mathbf{x}',\mathbf{x}) = 1 - \left(\frac{2\pi\hbar}{L}\right)^3 \int d\mathbf{p} \int d\mathbf{p}'\ \mu(\mathbf{p}) \left[1 - e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right] \left|\mathcal{F}(\mathbf{p}-\mathbf{p}')\right|^2$$

We can introduce a time parameter τ which denotes the duration of the scattering interaction. Subsequently we will make $\tau \to 0$. Consider the difference between density matrix, i.e. their representation in position basis, at time τ and at time 0

$$\begin{aligned}
\rho(\mathbf{x},\mathbf{x}',\tau) - \rho(\mathbf{x},\mathbf{x}',0) &= \left[\eta(\mathbf{x}',\mathbf{x}) - 1\right] \rho(\mathbf{x},\mathbf{x}',0) \\
&= -\rho(\mathbf{x},\mathbf{x}',0) \int d\mathbf{p}\ \mu(\mathbf{p}) \left(\frac{2\pi\hbar}{L}\right)^3 \int d\mathbf{p}'\ \left[1 - e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right] \left|\mathcal{F}(\mathbf{p}-\mathbf{p}')\right|^2
\end{aligned}$$

From the scattering theory we know that

$$\langle \mathbf{p}|\mathcal{T}|\mathbf{p}'\rangle = \frac{i}{2\pi\hbar m}\delta(E-E')\mathcal{F}(\mathbf{p},\mathbf{p}')$$

where E is the energy of the brownian particle, i.e. the δ function correspond to the conservation of the energy, and $\mathcal{F}(\mathbf{p},\mathbf{p}')$ is the scattering amplitude function. So we have

$$\left|\langle \mathbf{p}|\mathcal{T}|\mathbf{p}'\rangle\right|^2 = \frac{1}{(2\pi\hbar m)^2}\delta^2(E-E') \left|\mathcal{F}(\mathbf{p},\mathbf{p}')\right|^2$$

We have a problem with the δ^2, which gives rise to an infinity: $\delta^2(E-E') = \delta(E-E')\delta(0)$. If we go back to the calculation about scattering theory, the reason for the Dirac-δ comes from the fact that we have considered the scattering going to $t = -\infty$ to $t = +\infty$, therefore

$$\delta(E-E') = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt\ e^{i(E-E')t/\hbar}$$

To solve the problem, like the previous box quantization, we constraint the interaction in time. We leave a δ for the energy conservation, the other one become

$$\begin{aligned}
\delta^2(E-E') &= \delta(E-E')\delta(0) \\
&= \delta(E-E')\frac{1}{2\pi\hbar}\int_{-\tau/2}^{+\tau/2} e^0 \\
&= \delta(E-E')\frac{\tau}{2\pi\hbar}
\end{aligned}$$

Applying the rules for the change of variables in Dirac-δ, i.e.

$$\delta\left(f(x-x_0)\right) = \left(\left[\frac{df(x-x_0)}{dx}\Big|_{x=x_0}\right)^{-1}\right. \delta(x-x_0)$$

we obtain for $E = p^2/2m$

$$\delta^2(E-E') = \frac{m}{p'}\frac{\tau}{2\pi\hbar}\delta(p-p')$$

With this constrain one have

$$\rho(\mathbf{x},\mathbf{x}',\tau)-\rho(\mathbf{x},\mathbf{x}',0) = -\rho(\mathbf{x},\mathbf{x}',0)\frac{\tau}{L^3}\int d\mathbf{p}\,\mu(\mathbf{p})\int dp'\int d\hat{n}'\,\frac{p'}{m}\left[1-e^{-i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right]\delta(p-p')\left|\mathcal{F}(\mathbf{p},\mathbf{p}')\right|^2$$

where $\int d\mathbf{p}'$ becomes $\int dp' \int d\hat{n}'(p')^2$. Using the Dirac-$\delta$ we have

$$\rho(\mathbf{x},\mathbf{x}',\tau) - \rho(\mathbf{x},\mathbf{x}',0) = -\rho(\mathbf{x},\mathbf{x}',0)\frac{\tau}{L^3}\int d\mathbf{p}\;\mu(\mathbf{p})\frac{p}{m}\int d\hat{n}'\;\left[1-e^{-i(\mathbf{p}-p\hat{n}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right]\left|\mathcal{F}(\mathbf{p},p\hat{n}')\right|^2$$

This equation has two non-well definite terms: τ and L^3. As we consider before the gas is not formed just by one particle. There are N of them. So we have to multiply the righthand side of the above equation by N. We can consider in this form the density of particles of the gas $n = N/L^3$. So instead of using L we use n that is a well defined parameter of the bath. Technically the time of the scattering process is infinite, but for maintain the markovian character of the dynamics we have to consider instantaneous interactions, i.e. the limit of $\tau \to 0$. Therefore the proper way to consider the above equation is

$$\lim_{\tau\to 0}\frac{\rho(\mathbf{x},\mathbf{x}',\tau)-\rho(\mathbf{x},\mathbf{x}',0)}{\tau} = -\rho(\mathbf{x},\mathbf{x}',0)n\int d\mathbf{p}\,\mu(\mathbf{p})\frac{p}{m}\int d\hat{n}'\,\left[1-e^{-i(\mathbf{p}-p\hat{n}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right]\left|\mathcal{F}(\mathbf{p},p\hat{n}')\right|^2$$

That is nothing else that the form of the master equation

$$\frac{d}{dt}\rho(\mathbf{x},\mathbf{x}',t) = -F(\mathbf{x}-\mathbf{x}')\rho(\mathbf{x},\mathbf{x}',t)$$

where

$$F(\mathbf{x}-\mathbf{x}') = n\int d\mathbf{p}\;\mu(\mathbf{p})\frac{p}{m}\int d\hat{n}'\;\left[1-e^{-i(\mathbf{p}-p\hat{n}')\cdot(\mathbf{x}'-\mathbf{x})/h}\right]\left|\mathcal{F}(\mathbf{p},p\hat{n}')\right|^2$$

To this master equation we have to add to the hamiltonian term. Suppose, as usual, that the distribution in momenta is isotropic. So we have

$$\mu(\mathbf{p})d\mathbf{p} = \frac{\nu(p)dpd\hat{n}}{4\pi}$$

where

$$\int_0^{+\infty} dp\ \nu(p) = 1$$

With this assumption we obtain the usual form of the scattering amplitude represented in position basis

$$F(\mathbf{x}-\mathbf{x}') = n\int_0^{+\infty} dp\nu(p)\frac{p}{m}\int\frac{d\hat{n}d\hat{n}'}{4\pi}\left[1-e^{ip(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')/\hbar}\right]\left|\mathcal{F}(p\hat{n},p\hat{n}')\right|^2$$

This is the main result we wanted to arrive at. We have computed the decoherence effect and we turned the whole calculation down to compute a scattering amplitude.

We can consider this master equation in two limits.

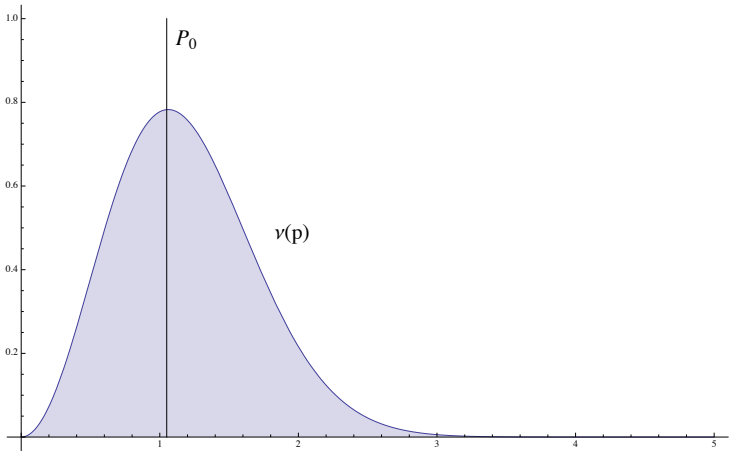
- **Case A: the short wave-length limit or large distance limit**
  Consider the limit

  $$\lambda_0 \ll \Delta x \equiv |\mathbf{x}-\mathbf{x}'|$$

  where λ_0 is the typical wave-length of the bath particle, i.e. for the de Broglie relation

  $$\lambda_0 = \frac{2\pi\hbar}{p_0}$$

  with p_0 the most probable momentum in accord to the density of momenta $\nu(p)$.



  So the typical wave-length is much smaller than the coherent separation. One can see it the way around the coherent separation is very large.

  $$\lambda_0 \ll \Delta x \quad \Rightarrow \quad \frac{p_0\Delta x}{\hbar} \gg 1$$

  In this limit the complex exponential in the integral will oscillate very fast and thus in average not contribute to the integral

$$F\left(|\mathbf{x}-\mathbf{x}'|\to+\infty\right)=n\int_0^{+\infty}dp\;\nu(p)\frac{p}{m}\int\frac{d\hat{n}d\hat{n}'}{4\pi}\left|F(p\hat{n},p\hat{n}')\right|^2$$

but

$$\int d\hat{n}'\;\left|F(p\hat{n},p\hat{n}')\right|^2$$

is the cross section for momentum $\mathbf{p}=p\hat{n}$ and

$$\int\frac{d\hat{n}d\hat{n}'}{4\pi}\left|F(p\hat{n},p\hat{n}')\right|^2\equiv\sigma_{\mathrm{TOT}}(p)$$

is the cross section for momentum p irrespective of direction. Therefore

$$F\left(|\mathbf{x}-\mathbf{x}'|\to+\infty\right)=n\int_0^{+\infty}dp\;\nu(p)\frac{p}{m}\sigma_{\mathrm{TOT}}(p)=n\left\langle v\sigma\right\rangle_{\mathrm{THERMAL}}$$

where $\langle\;\rangle_{\mathrm{THERMAL}}$ denote the average on the distribution of momenta $\nu(p)$. The linearity respect to n is reasonable, in fact the effect of decoherence is much stronger if there are many particle of gas, i.e. the density of particle n is high. There is a finite limit for $\Delta x\to+\infty$ and it sets an **upper bound** to the decoherence rate. This is reasonable for any given separation Δx. There is a wavelength of the environmental particle that allows for complete resolution of the separation and therefore for maximum amount of spatial decoherence. Increasing the separation further cannot lead to stronger decoherence.

- **Case B: the long wave-length limit or short distance limit**

  Consider the opposite limit, $\Delta x\to 0$. In this limit we can express the exponential as series and cut off it at the first non null term that contribute to the integral

$$1-\exp\left(\frac{i}{\hbar}p(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')\right)\simeq-\frac{i}{\hbar}p(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')+\frac{1}{2\hbar^2}p^2\left[(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')\right]^2$$

the first tern is odd with respect the integral variables $\hat{n}$ and $\hat{n}'$ therefore do not contribute to the integral

$$-\frac{i}{\hbar}p(\mathbf{x}-\mathbf{x}')\cdot\int\frac{d\hat{n}d\hat{n}'}{4\pi}(\hat{n}-\hat{n}')\left|F(p\hat{n},p\hat{n}')\right|^2=0$$

So we have as first non null term

$$F\left(\Delta x\to 0\right)=n\int_0^{+\infty}dp\;\nu(p)\frac{p^3}{m}\int\frac{d\hat{n}d\hat{n}'}{8\pi\hbar^2}\left[(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')\right]^2\left|F(p\hat{n},p\hat{n}')\right|^2$$

Let us evaluate the quantity

$$\left[(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')\right]^2=(\mathbf{v}\cdot\Delta\mathbf{x})^2$$

where $\mathbf{v} = \hat{n} - \hat{n}'$ and $\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}'$. We use the isotropy of the problem so that we average over all directions $(\mathbf{x} - \mathbf{x}')$ which is equivalent to averaging over all directions of incident bath particles

$$\begin{aligned}(\mathbf{v}\cdot\Delta\mathbf{x})^2 \quad \Rightarrow \quad & \frac{1}{4\pi}\int d\Omega\ (\mathbf{v}\cdot\Delta\mathbf{x})^2 = \\ & = \frac{v^2(\Delta x)^2}{4\pi}\int_{-1}^{1} d\cos\theta\ \int_0^{2\pi} d\varphi\ \cos^2\theta \\ & = \frac{v^2(\Delta x)^2}{3}\end{aligned}$$

In fact $\mathbf{v}\cdot\Delta\mathbf{x} = v\Delta x\cos\theta$, where θ is the angle between $\mathbf{v}$ and $\mathbf{x}$. Therefore one obtain

$$\begin{aligned}\left[(\hat{n}-\hat{n}')\cdot(\mathbf{x}-\mathbf{x}')\right]^2 \quad \Rightarrow \quad & \frac{1}{3}(\hat{n}-\hat{n}')^2(\mathbf{x}-\mathbf{x}')^2 = \\ & = \frac{2}{3}(\mathbf{x}-\mathbf{x}')^2(1-\hat{n}\cdot\hat{n}') \\ & = \frac{4}{3}(\mathbf{x}-\mathbf{x}')^2\sin^2\frac{\theta}{2}\end{aligned}$$

where θ is the scattering angle between $\hat{n}$ and $\hat{n}'$. So we can express

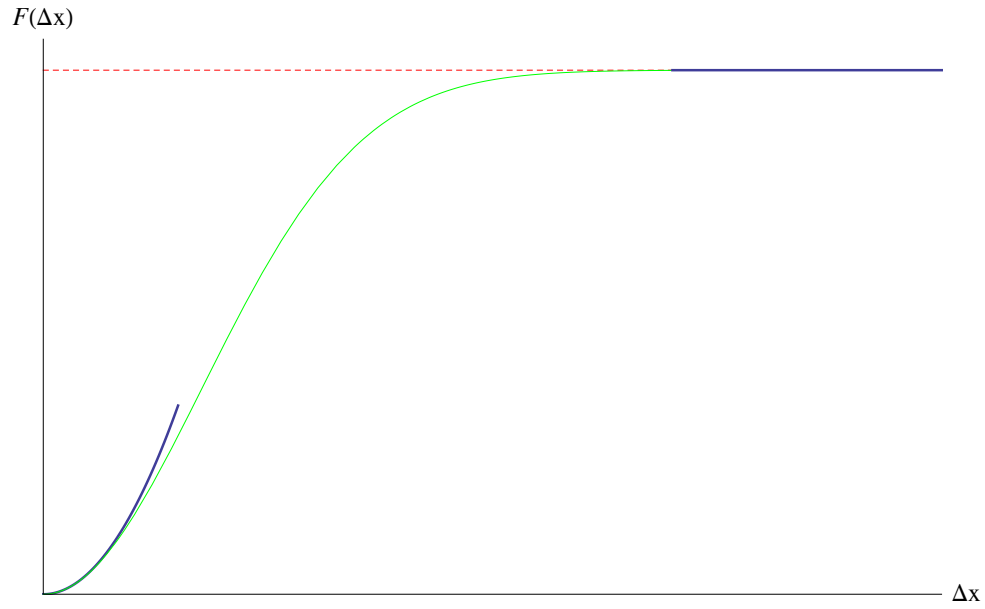
$$F(\Delta x \to 0) = \Lambda(\mathbf{x}-\mathbf{x}')^2$$

where the coherence rate Λ is

$$\Lambda = \frac{2}{3}\frac{n}{\hbar^2}\int_0^{+\infty} dp\ \nu(p)\frac{p^3}{m}\int\frac{d\hat{n}d\hat{n}'}{4\pi}\sin^2\left(\frac{\theta}{2}\right)\ \left|F(p\hat{n},p\hat{n}')\right|^2$$

Without the term $\sin^2(\theta/2)$ it would be the total cross section. We can interpret it as the **effective** or **decoherence** cross section.

To summarize the two cases consider the following graph of the shape of $F(\Delta x)$



Blue graphs represent the two limits of $F(\Delta x)$ for $\Delta x \to 0$ and $\Delta x \to +\infty$, the dashed red line represent the asymptotic shape of F, i.e. $n \langle v\sigma \rangle_{\text{THERMAL}}$. In the intermediate region is difficult to compute the shape of $F(\Delta x)$. A good ansatz is the gaussian one

$$F(\Delta x) = \gamma \left[1 - \exp\left[-\frac{\Delta x^2}{r^2}\right]\right]$$

This function is plotted in above graph in green. It have to interpolate the two limits, therefore for $\Delta x \to +\infty$ we have

$$\lim_{\Delta x \to +\infty} F(\Delta x) = \gamma \equiv n \langle v\sigma \rangle_{\text{THERMAL}}$$

On the other hand for $\Delta x \to 0$ we consider

$$F(\Delta x) \simeq \gamma \left[1 - \left(1 - \frac{\Delta x^2}{r^2}\right)\right] = \frac{\gamma}{r^2}\Delta x^2 \equiv \Lambda \ \Delta x^2$$

so one obtain

$$r = \sqrt{\frac{\gamma}{\Lambda}}$$

Therefore $F(\Delta x)$ in this ansatz depends from two parameters that are related to the two limits.

3.3 Scattering Of Air Molecules

One of the most important sources of decoherence is represented by an environment of air molecules. The typical thermal de Broglie wavelength is very short, for example for oxygen O_2 molecule

$$\lambda_{\rm dD} = \frac{\hbar}{\sqrt{2mK_BT}} \simeq \begin{cases} 2 \times 10^{-11} \text{ m} & \text{at room temperature} \\ \\ 2 \times 10^{-10} \text{ m} & \text{at } T \simeq 3\text{K} \end{cases}$$

Consider "dust" particles, with dimension $r \sim 10^{-8} - 10^{-5}$ m, as the brownian particle. In this case, it is a good approximation to take the scattering amplitude to be a constant. Such that the cross section integrated over all directions is simply equal to the geometric cross section πr^2 of the object

$$\int d\hat{n} \ |F|^2 = 4\pi |F|^2 = \pi r^2 \quad \Rightarrow \quad |F|^2 = \frac{r^2}{4}$$

Assume that the coherent separation Δx is much shorter that the typical wavelength of the bath particle. So we use the long wavelength approximation in this case and we obtain

$$\Lambda = \frac{\pi r^2}{3\hbar^2} \frac{n}{m} \langle p^3 \rangle_{\rm THERMAL}$$

where

$$\langle p^3 \rangle_{\rm THERMAL} = \int_0^{+\infty} dp \ \nu(p) p^3 = \frac{4}{\sqrt{\pi}} (2mK_BT)^{3/2}$$

with

$$\nu(p) = 4\pi p^2 \left(\frac{\beta}{2\pi m} \right)^{3/2} \exp\left[-\frac{\beta p^2}{2m} \right]$$

Notice that $\nu(p)$ is obtained by

$$\int d^3p \ \mu(\mathbf{p}) = \int_0^{+\infty} dp \ 4\pi p^2 \mu(p)$$

So the coherence rate Λ is

$$\Lambda = \frac{8}{3\hbar^2} n \sqrt{2\pi m} r^2 (K_BT)^{3/2}$$

So the dependence of Λ to the parameters is

$$\Lambda \propto n \ r^2 \ T^{3/2}$$

So for air with normal pressure (1 atm) one have

$$\Lambda \sim 10^{39} \text{ cm}^{-2}\text{s}^{-1} \left(\frac{r}{\text{cm}} \right)^2 \left(\frac{T}{\text{K}} \right)^{3/2}$$

Therefore consider some examples

- **dust grain** ($r \sim 10^{-3}$ cm) at room temperature ($T \sim 300$ K) we have

$$\Lambda \sim \begin{cases} 10^{37}\ \mathrm{cm}^{-2}\mathrm{s}^{-1} & \text{normal pressure} \\ \\ 10^{20}\ \mathrm{cm}^{-2}\mathrm{s}^{-1} & \text{laboratory vacuum} \end{cases}$$

- **large molecule** ($r \sim 10^{-6}$ cm) at room temperature ($T \sim 300$ K) we have

$$\Lambda \sim \begin{cases} 10^{31}\ \mathrm{cm}^{-2}\mathrm{s}^{-1} & \text{normal pressure} \\ \\ 10^{14}\ \mathrm{cm}^{-2}\mathrm{s}^{-1} & \text{laboratory vacuum} \end{cases}$$

This means that if for example we create a superposition with $\Delta x \sim 10$ Å, much less that the size of the object, then the decoherence time

$$\tau \equiv \frac{1}{\Lambda(\Delta x)^2} \simeq \begin{cases} 10^{17}\ \mathrm{s} & \text{normal pressure} & \Rightarrow & \begin{cases} \text{there is no hope to see} \\ \text{quantum interference} \end{cases} \\ \\ 1\ \mathrm{s} & \text{laboratory vacuum} & \Rightarrow & \text{it can be done} \end{cases}$$

The conclusion is

- Because of decoherence effects, quantum superposition cannot be seen for macroscopic objects.
- It is possible to observe such superposition, i.e. interference effects, for elementary particles, atoms, large molecule if a sufficiently high vacuum is created. This is done in laboratories, and it is a currently ugly hot topic in research.

3.4 Solving The Joos-Zeh Equation

The master equation is

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}\left[H, \rho(t)\right] - F\left(q, \textstyle\sum_i q_i\right)\rho(t)$$

In the position representation for a free particle one obtain

$$\frac{\partial \rho(x, x', t)}{\partial t} = -\frac{i}{2m}\left(\frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial x^2}\right)\rho(x, x', t) - \Lambda(x - x')^2 \rho(x, x', t)$$

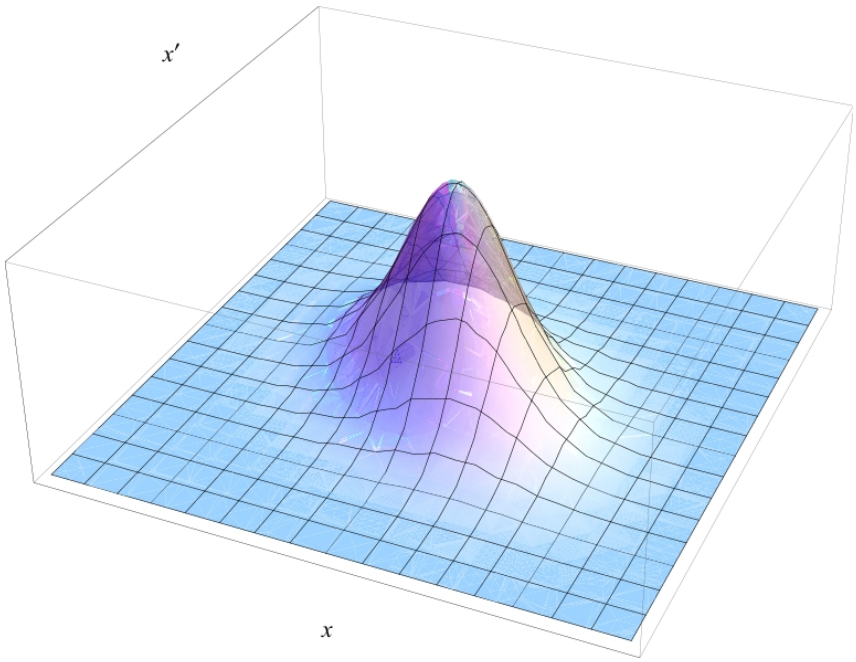
For the initial state we consider valid the gaussian ansatz, so we have

$$\rho(x,x',t) = \exp\left[-A(t)(x-x')^2 + iB(t)(x-x')(x+x') - C(t)(x+x')^2 - D(t)\right]$$

where A, B, C, D are time dependent real coefficient. They are real-valued functions, since ρ is hermitian. They have a precise physical meaning. Putting this ρ in the master equation one obtain

$$\begin{cases} \dot{A} = \dfrac{4}{m}AB + \Lambda \\ \dot{B} = \dfrac{2}{m}B^2 - \dfrac{8}{m}AC \\ \dot{C} = \dfrac{4}{m}BC \\ e^{-D} = 2\sqrt{\dfrac{C}{\pi}} \end{cases}$$

This is a set of coupled ordinary differential equations, which can be straightforwardly solved. Consider the representation of the gaussian state ρ on the (x, x') plane.



On this two dimensional gaussian we can consider two half height width:

- The width of the gaussian in the off-diagonal direction, parallel to bisector $x = -x'$. This quantity is the coherence length

$$l(t) = \frac{1}{\sqrt{8A(t)}}$$

- The width along the diagonal direction, i.e. $x = x'$. The density matrix represents the probability distribution $P(x,t) \equiv \rho(x,x,t)$ of finding the particle at position x at time t. This is the ensemble width

$$\Delta x(t) = \frac{1}{8C(t)}$$

In a similar, but less intuitive way, one can find out that the spread $\Delta p(t)$ of the momentum distribution is

$$\Delta p(t) = \sqrt{2\left[A(t) + \frac{B^2(t)}{4C(t)}\right]}$$

from which the following uncertainty relation follows

$$\Delta x(t)\Delta p(t) = \frac{1}{2}\sqrt{\frac{A(t)}{C(t)} + \frac{B^2(t)}{4C(t)}}$$

This relation ensures that the trace is conserved for any time.

Example Consider as initial state a gaussian one

$$\psi(x,0) = \left(\frac{1}{2\pi b^2}\right)^{1/4} \exp\left[-\frac{x^2}{4b^2}\right] \quad \Rightarrow \quad \rho(x,x',0) = \sqrt{\frac{1}{2\pi b^2}} \exp\left[-\frac{x^2 + x'^2}{4b^2}\right]$$

This state in terms of

$$\rho(x,x',t) = \exp\left[-A(t)(x-x')^2 + iB(t)(x-x')(x+x') - C(t)(x+x')^2 - D(t)\right]$$

has

$$\begin{cases} A(0) = C(0) = \dfrac{1}{8b^2} \\ \\ B(0) = D(0) = 0 \end{cases}$$

With relatively easy calculations one can find for coherence length

$$l(t) = \frac{1}{2}\sqrt{\frac{3t^2 + 8\Lambda b^2 t^3 + 12m^2 b^4}{2\Lambda t^3 + 3m^2 b^2 + 4\Lambda^2 b^2 t^4 + 24\Lambda m^2 b^4 t}}$$

where the dominant contribution for t sufficiently high is $4\Lambda^2 b^2 t^4$, so for large times one have

$$l(t) \simeq \frac{1}{\sqrt{2\Lambda t}}$$

This quantity is independent from parameter b. Instead for small times one have

$$l(t) \simeq b(1 - 4\Lambda b^2 t)$$

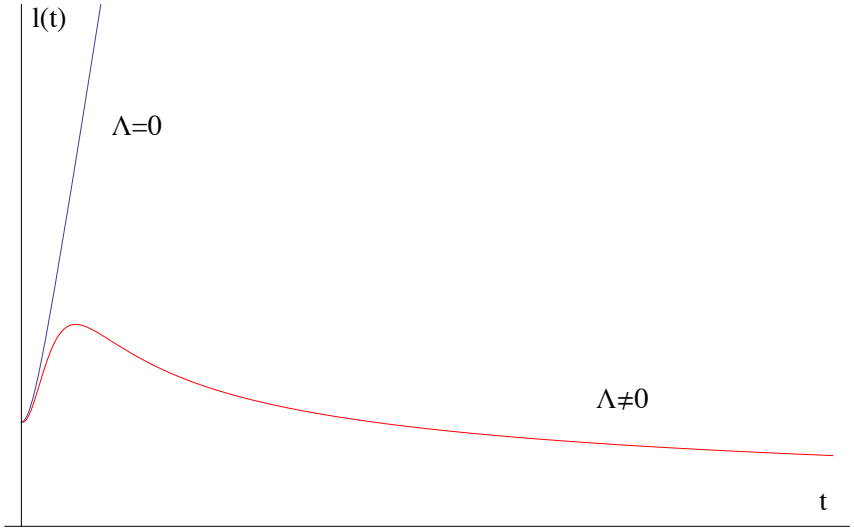
who depends from b. If there is no decoherence, i.e. $\Lambda = 0$, one have

$$l(t) = \frac{1}{2}\sqrt{\frac{t^2 + 4m^2b^4}{m^2b^2}}$$

In this case $l(t)$ goes from a constant shape for small times to

$$l(t) = \frac{1}{2mb}t$$

for large times.



As we expected, the coherence length decreases in time. Decoherence kills the interference terms. On the other hand for ensemble width one obtain

$$\Delta x(t) = \frac{1}{2}\sqrt{\frac{t^2}{m^2b^2} + \frac{8\Lambda t^3}{3m^2} + 4b^2}$$

The dominant contribution for t sufficiently large is the only dependent from Λ. Therefore for large times we have

$$\Delta x(t) \simeq \sqrt{\frac{2\Lambda t^3}{3m^2}}$$

Notice that in this limit $\Delta x(t)$ is independent from parameter b, as previously $l(t)$ in the same limit. For small times instead we have

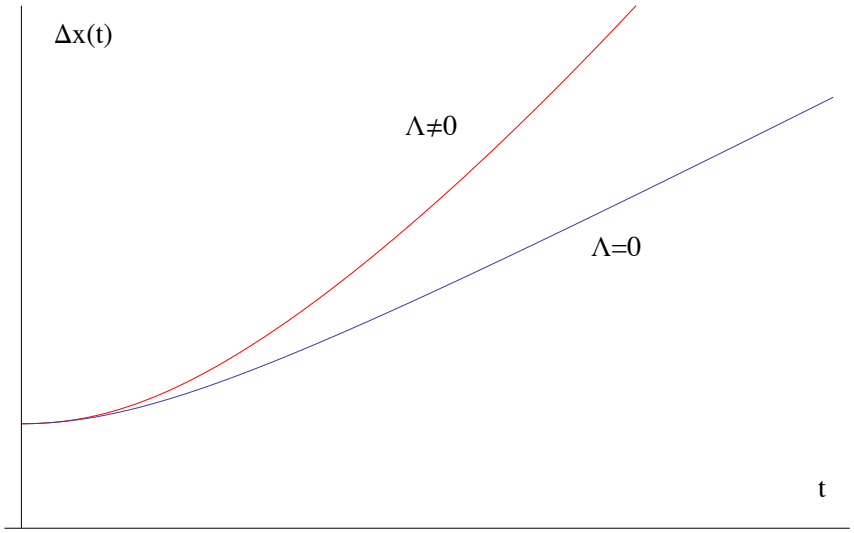
$$\Delta x(t) \simeq 2b + \frac{t^2}{2m^2b^2}$$

who depends from b. As above we can consider the case without decoherence, i.e. $\Lambda = 0$. In this case for large times we have

$$\Delta x(t) \simeq \frac{t}{2mb}$$

and for small times we obtain the same result as in the case with decoherence

$$\Delta x(t) \simeq 2b + \frac{t^2}{2m^2b^2}$$

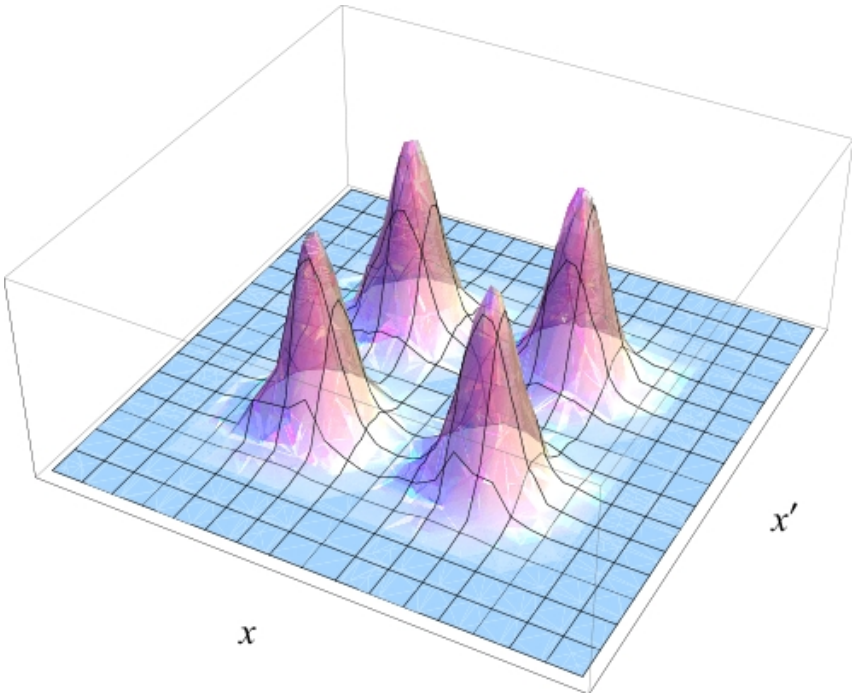


As is shown in above figure, there is a faster increase in the ensemble width than in the environment-free case. This is due to the fact that collisions with bath particles increase the randomlicity in position of the brownian particle.

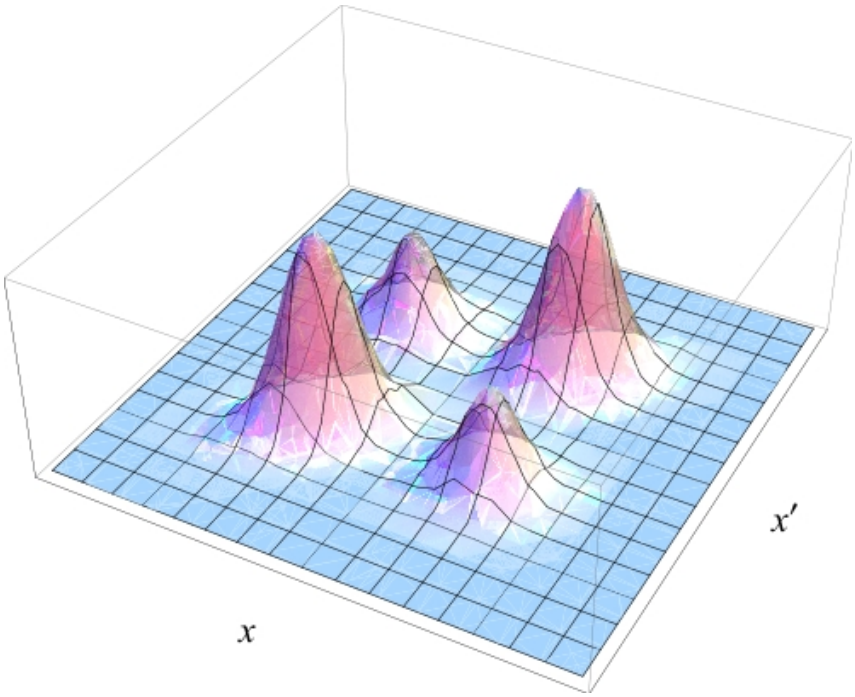
Example Consider as initial state two gaussian states

$$\psi(x,0) = \frac{1}{\sqrt{N}}\left\{\exp\left[-\frac{(x-x_0)^2}{4b^2}\right] + \exp\left[-\frac{(x+x_0)^2}{4b^2}\right]\right\}$$

where N is the normalization constant. The correspondent $\rho(x,x',0)$ is the sum of four gaussian terms, so we can use the previous ansatz and the linearity of the Lindblad evolution to write the solution. The graphical outcome is for $t = 0$



And after some time we obtain



The off-diagonal elements are killed. The diagonal elements are squeezed toward the diagonal.

3.5 Increase Of Energy

Let consider the time evolution of the energy E as expectation value of the hamiltonian H in the long wave-length limit

$$\begin{aligned}\frac{d}{dt}E &= \frac{d}{dt}\langle H\rangle \\ &= \mathrm{Tr}\left[\frac{d}{dt}(H\rho)\right] \\ &= \mathrm{Tr}\left[\frac{dH}{dt}\rho + H\frac{d\rho}{dt}\right] \\ &= \mathrm{Tr}\left[H\frac{d\rho}{dt}\right]\end{aligned}$$

Using the form of the master equation in this limit, i.e.

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}[H,\rho] - \frac{\Lambda}{2}[q,[q,\rho]]$$

we obtain with ciclicity property of the trace

$$\frac{d}{dt}E = -\frac{i}{\hbar}\mathrm{Tr}\big[[H,H]\rho\big] - \frac{\Lambda}{2}\mathrm{Tr}\big[[q,[q,H]]\rho\big]$$

For a isolated system we have the conservation of energy, i.e. $\Delta E = 0$. In this case we have

$$\begin{cases}[H,H] = 0 \\ \\ [q,[q,H]] = -\dfrac{\hbar^2}{m}\end{cases}$$

So we obtain

$$\frac{d}{dt}E = \frac{\Lambda\hbar^2}{2m}$$

This is a non-zero quantity. Therefore there is an increase of energy in time. The result is obtained because we do not consider the recoil of particles in the scattering process and therefore we do not consider a dissipative term in the dynamic. This is not a physical situation because the temperature will rise indefinitely. The Joos-Zeh model is therefore a model without the dissipative term and an infinite temperature. For consider the dissipation we have to add a term

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}[H,\rho] - \gamma\frac{2m}{\beta\hbar^2}[q,[q,\rho]] - \gamma\frac{\beta}{2m}[p,[p,\rho]] - \frac{i}{\hbar}\gamma[q,\{p,\rho\}]$$

where γ is the friction coefficient. This new equation give us as time evolution of the energy

$$E(t) = \left(E_0 - \frac{1}{\beta}\right)e^{-4\gamma t} + \frac{1}{\beta}$$

where $1/\beta$ is due to the equipartition theorem.

3.6 Decoherence Does Not Solve The Measurement Problem

As we shown in previous sections, the overall evolution is unitary. In particular linear, so there is no collapse.

Consider the following dynamic

$$\frac{d\psi_t}{dt} = \left[-\frac{i}{\hbar} H + \sqrt{\lambda} \hat{q} \omega_t \right] \psi_t$$

where H is the effective hamiltonian of the system, $\hat{q}$ is the position operator and ω_t indicates a white noise. Therefore this dynamic describes a system coupled to a noisy environment through position. This is a linear equation, therefore there are superpositions. However the equation for the correspondent statistical operator is

$$\frac{d\rho_t}{dt} = -\frac{i}{\hbar} [H, \rho_t] - \frac{\lambda}{2} [q, [q, \rho_t]]$$

This is the Joos-Zeh equation. From it we can compute that the off-diagonal elements are killed by decoherence.

The true meaning of decoherence can be interpreted only within the **framework of standard quantum mechanics**. If one makes a measurement, than interference can not be observed. Which is what happens in real experiments. But then this assumes the validity of the standard theory, with all the problems we know of.

Appendix A

Hilbert space and linear operators

Hilbert space

A Hilbert space is a scalar product space which is complete in the metric arising from the scalar product.

Linear manifold

A subset $\mathcal{S}$ of $\mathcal{H}$ is a linear manifold if

$$a\left|f\right\rangle + b\left|g\right\rangle \in \mathcal{S} \qquad \begin{cases} \forall \left|f\right\rangle, \left|g\right\rangle \in \mathcal{S} \\ \forall a, b \in \mathbb{C} \end{cases}$$

Hilbert subspace

$\mathcal{S}$ is a Hilbert linear subspace of $\mathcal{H}$ if and only if $\mathcal{S}$ is a linear manifold closed with respect to the topology of $\mathcal{H}$.

Linear operators

An operator $\mathcal{L}$ is linear if its domain $\mathcal{D}(\mathcal{L})$ is a linear manifold and it acts on the domain linearly:

$$\begin{cases} \forall \left|\phi\right\rangle, \left|\psi\right\rangle \in \mathcal{D}(\mathcal{L}) \\ \\ \forall a, b \in \mathbb{C} \end{cases} \quad \rightarrow \quad \begin{cases} a\left|\phi\right\rangle + b\left|\psi\right\rangle \in \mathcal{D}(\mathcal{L}) \\ \\ \mathcal{L}\left(a\left|\phi\right\rangle + b\left|\psi\right\rangle\right) = a\mathcal{L}\left|\phi\right\rangle + b\mathcal{L}\left|\psi\right\rangle \end{cases}$$

For a linear operator also its range is a linear manifold. Its norm is defined as

$$||\mathcal{L}|| \equiv \sup_{|\chi\rangle \neq 0} \frac{||\mathcal{L}\left|\chi\right\rangle||}{||\left|\chi\right\rangle||}$$

Adjoint operator

For each densely defined linear operator $\mathcal{L}$ one can define its adjoint operator $\mathcal{L}^\dagger$. The domain of $\mathcal{L}^\dagger$ is the linear manifold built from vectors $|\chi\rangle \in \mathcal{H}$ for which exists a vector $|\tilde{\chi}\rangle$ such that

$$\forall \left|\phi\right\rangle \in \mathcal{D}(\mathcal{L}) \quad \rightarrow \quad \langle\tilde{\chi}, \phi\rangle = \langle\chi, \mathcal{L}\phi\rangle$$

Therefore $|\tilde{\chi}\rangle = \mathcal{L}^\dagger |\chi\rangle$. $\mathcal{L}^\dagger$ is a linear operator.

Hermitian operator

A linear operator $\mathcal{L}$ is hermitian if its adjoint operator $\mathcal{L}^\dagger$ coincides with $\mathcal{L}$ on domain of $\mathcal{L}$. This is not equivalent to $\mathcal{L} = \mathcal{L}^\dagger$ everywhere but just in $\mathcal{D}(\mathcal{L})$.

Self-adjoint operator

A linear operator $\mathcal{L}$ is self-adjoint if coincides everywhere with its adjoint operator $\mathcal{L}^\dagger$.

Bounded operator

A linear operator $\mathcal{L}$ is bounded if and only if

$$\exists\, \gamma \geq 0 \quad \text{that} \quad ||\mathcal{L}\,|\chi\rangle\,|| \leq ||\,|\chi\rangle\,|| \quad \forall\, |\chi\rangle \in \mathcal{H}$$

If $\mathcal{L}$ is a linear bounded operator then it is also continuous and vice versa a continuous one is also bounded.

Eigenvalues of a bounded linear operator

$\lambda \in \mathbb{C}$ is a eigenvalue of the bounded linear operator $\mathcal{L}$ if and only if

$$\begin{cases} \exists\, |\chi\rangle \neq 0 \in \mathcal{H} \\ |\chi\rangle \neq 0 \end{cases} \qquad \mathcal{L}\,|\chi\rangle = \lambda\,|\chi\rangle$$

The corresponding $|\chi\rangle$ is called eigenvector corresponding to the eigenvalue λ of $\mathcal{L}$. For different eigenvalues correspond different eigenvectors that are mutually orthonormal.

Specter of a bounded self-adjoint operator

The specter $\Omega(\mathcal{L})$ of a bounded self-adjoint operator $\mathcal{L}$ is such that

$$\Omega(\mathcal{L}) \subseteq \big[-||\mathcal{L}||, ||\mathcal{L}||\big] \subseteq \mathbb{R}$$

Positive operator

A bounded linear operator $\mathcal{L}$ is positive if

$$\langle\chi|\mathcal{L}\chi\rangle \geq 0 \quad \forall\, |\chi\rangle \in \mathcal{H}$$

If an operator is positive then it is also self-adjoint.

Trace of a positive operator

Consider a positive operator $\mathcal{L}$ and a complete orthonormal set $\{\, |\phi_n\rangle \,\}$. The trace of $\mathcal{L}$ is defined as

$$\mathrm{Tr}\,[\mathcal{L}] = \sum_n \langle\phi_n|\mathcal{L}\phi_n\rangle$$

The trace of a positive operator is positive and do not depends on the chosen complete orthonormal set.

Trace class operator

A bounded operator $\mathcal{L}$ is a trace class operator if

$$\mathrm{Tr}\left[\sqrt{\mathcal{L}^2}\right] < +\infty$$

or equivalently if exists at least a complete orthonormal set $\{\, |\phi_n\rangle \,\}$ that

$$\sum_n ||\mathcal{L}\,|\phi_n\rangle\,|| < +\infty$$

Appendix B

Complete Positivity

The complete positivity is a more restrictive condition that the simply positivity.
Suppose there is a system S associated to the Hilbert space $\mathcal{H}$ and we coupling it with a second system A. A can be a copy of S or any other k dimensional system. To A is associated an Hilbert space isomorphic to $\mathbb{C}^k$. The total Hilbert space is $\mathcal{H}_{\mathrm{TOT}} \equiv \mathcal{H} \otimes \mathbb{C}^k$. Consider a linear map Λ that maps statistical operators of S in statistical operators of S

$$\Lambda : \ \rho \in \mathrm{T}(\mathcal{H}) \ \rightarrow \ \rho' \equiv \Lambda[\rho] \in \mathrm{T}(\mathcal{H})$$

The extended map from $\mathrm{T}(\mathcal{H}_{\mathrm{TOT}})$ to $\mathrm{T}(\mathcal{H}_{\mathrm{TOT}})$ using the identity map id_k for the A system is

$$\Lambda \otimes \mathrm{id}_k : \ \rho_{S+A} \in \mathrm{T}(\mathcal{H}_{\mathrm{TOT}}) \ \rightarrow \ \rho'_{S+A} \equiv (\Lambda \otimes \mathrm{id}_k)\left[\rho_{S+A}\right] \in \mathrm{T}(\mathcal{H}_{\mathrm{TOT}})$$

That map leaves unchanged the system A. If the initial state of the two systems is separable, i.e. $\rho_{S+A} = \rho \otimes \rho_A$ the map acts as following

$$(\Lambda \otimes \mathrm{id}_k)\left[\rho_{S+A}\right] = \Lambda[\rho] \otimes \mathrm{id}_k[\rho_A] = \Lambda[\rho] \otimes \rho_A$$

Instead if the initial state is an entangled one we can not write it in this form: $\rho_{S+A} \neq \rho \otimes \rho_A$. The total map $(\Lambda \otimes \mathrm{id}_k)$ however acts, but not separately on the two statistical operators.

The map $\Lambda : \rho \rightarrow \Lambda[\rho]$ is called k-positive map if $(\Lambda \otimes \mathrm{id}_k)$ is a positive map.

If Λ is k-positive for each $k \in \mathbb{N}$ the map Λ is called completely positive.

Not all positive maps are completely positive.

Example Consider the transposition map T

$$T : \ \rho \ \rightarrow \ \rho^{\top} = T[\rho]$$

This map is a positive map, in fact the eigenvalues remain unchanged. T map acts as

$$T\left|k\right\rangle\left\langle i\right| = \left|i\right\rangle\left\langle k\right|$$

We want to verify if $(T \otimes \mathrm{id}_2)$ is a positive map, i.e. if T is 2-positive. Consider the entangled state $|\psi_+\rangle$ and its associated statistical operator ρ_+

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle\otimes|0\rangle+|1\rangle\otimes|1\rangle\big) \rightarrow \rho_+ = \frac{1}{2}\big(|0\rangle\,|0\rangle\,\langle 0|\,\langle 0|+|0\rangle\,|0\rangle\,\langle 1|\,\langle 1|+|1\rangle\,|1\rangle\,\langle 0|\,\langle 0|+|1\rangle\,|1\rangle\,\langle 1|\,\langle 1|\big)$$

The representation of this statistical operator on the basis $\{\, |0\rangle \otimes |0\rangle\,, |0\rangle \otimes |1\rangle\,, |1\rangle \otimes |0\rangle\,, |1\rangle \otimes |1\rangle\,\}$ is

$$\rho_+ = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

Acting on it with the composed map $(T \otimes \mathrm{id}_2)$ we obtain

$$(T \otimes \mathrm{id}_2)[\rho_+] = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This matrix is not positive, therefore the composed map $T \otimes \mathrm{id}_2$ is not positive, i.e. T for sure is not a completely positive map.

Index