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**Quantum decoherence.**

A work on the quantum measurement problem.

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# Resumen general.

La mecánica cuántica es una de las teorías científicas más exitosas de la historia. Desde que se consolidó el formalismo matemático que rige sus leyes, ni un solo experimento ha conseguido poner en duda su capacidad predictiva y sus aplicaciones y hallazgos han sido múltiples, yendo desde la nanotecnología y ciencia de materiales hasta la física de partículas. A pesar ello, la mecánica cuántica es tal vez una de las teorías científicas menos intuitivas que han existido y, aún habiéndose formulado hace casi un siglo, presenta algunas peculiaridades que la hacen difícil de interpretar a día de hoy. Así pues, una de las predicciones más chocantes de la mecánica cuántica es la de que existen sistemas físicos en la naturaleza que se encuentran en una superposición de estados, esto es, la energía, posición o momento lineal de una partícula podrían tomar varios valores distintos en un mismo instante, contradiciendo así la experiencia cotidiana de la física clásica. Tal dicotomía ha sido expuesta en el presente trabajo como una consecuencia directa del enunciado matemático de los postulados de la mecánica cuántica y se han recogido algunas de las explicaciones que, a lo largo de los años, los físicos han tratado de dar a este problema a través de las llamadas interpretaciones de la mecánica cuántica. Más concretamente, en el primer capítulo de este proyecto se ha estudiado cómo la interpretación de mundos paralelos de Hugh Everett permite, junto a una descripción de la mecánica cuántica basada en operadores densidad, tratar de entender por qué resulta imposible medir estados superpuestos como una consecuencia de la interacción entre el sistema medido y su entorno, lo que podría explicar la transformación de estos estados en mezclas estadísticas de estados clásicamente interpretables (decoherencia).

Con el fin de poder justificar la emergencia de la decoherencia en los sistemas que interactúan con su entorno, en el segundo capítulo se desarrolla el formalismo matemático de las ecuaciones maestras, que generalizan la ecuación de Schrödinger a sistemas no aislados. En concreto, se ha desarrollado una derivación de la ecuación de Redfield basada en las aproximaciones de Born y Markov, con un significado físico claro, al tiempo que se ha expuesto una demostración axiomática de la ecuación de Lindblad basada en mapeos CPT en la que se ha tratado de identificar los puntos en los que dichas aproximaciones cobran relevancia. A partir de estas ecuaciones se ha podido describir la evolución temporal de dos sistemas físicos en interacción con un entorno de radiación: Un oscilador armónico y un sistema de dos niveles. En ambos casos, la decoherencia aparece de forma natural para cualquier condición inicial del problema, quedando así justificada la emergencia de estados clásicamente interpretables a partir de estados cuánticos superpuestos. También se ha añadido una breve discusión sobre la validez de las aproximaciones de Born y Markov, así como sobre su necesidad para poder evitar el problema computacional que supone resolver la evolución exacta del estado de un sistema en interacción con su entorno. Este problema ha sido expuesto para un caso particular en el que se estudia la interacción de un sistema de dos niveles con un entorno de osciladores mediante acoplamientos de tipo Jaynes-Cummings. Se recoge además en este capítulo una discusión sobre el panorama actual en la determinación de la base propia del

operador densidad una vez ha ocurrido la decoherencia (pointer basis), problema que adquiere una gran relevancia en la modelización de medidas mediante ecuaciones maestras pero que, sin embargo, ha sido resuelto únicamente para ciertos casos particulares.

Una vez se ha demostrado que la decoherencia es una consecuencia directa de la interacción de los sistemas con sus entornos, queda por ver qué papel juega la medida en este contexto. Así pues, el tercer capítulo del proyecto abre con una definición del concepto de POVM (positive operator valued measurement), que permite generalizar los postulados de la medida a casos en los que se realizan medidas imperfectas (no proyectivas) sobre un sistema y que se ha justificado atendiendo a las condiciones del llamado teorema de Choi-Kraus, que se emplea previamente en la deducción axiomática de la ecuación de Lindblad. Mediante el uso de este formalismo es posible deducir la forma que debería tener una ecuación maestra describiendo una medida continua de tipo POVM y, a partir de un modelo sencillo de medida sobre un sistema de dos niveles, se deduce la forma de una ecuación maestra de tipo Lindblad escrita en términos de observables físicos describiendo la medida. A partir de la misma se ha generalizado el resultado a una ecuación para describir cualquier proceso de medida y se han discutido algunas de sus propiedades. Así, se han analizado los efectos de calentamiento que se derivan de la aplicación de dicha ecuación, la existencia de distintas soluciones según sea el grado de perfección de la medida POVM, el comportamiento del tiempo de decoherencia y se ha establecido un procedimiento para la determinación de la pointer basis en el proceso, que, de acuerdo a los postulados, debería coincidir con la base propia del observable medido. Por último, se ha demostrado matemáticamente que dicha ecuación maestra puede obtenerse de forma independiente al formalismo de los POVM si se emplea un modelo de interacción adecuado para describir la medida, concretamente, se ha probado que para casos en los que el entorno del sistema medido y este interaccionan mediante un hamiltoniano proporcional al producto tensorial del observable medido y un observable del entorno, la aplicación de la ecuación de Redfield dará lugar a la ecuación para modelizar medidas si este último observable toma valores descorrelacionados estadísticamente en tiempos diferentes.

Con todo esto, el trabajo presentado a continuación pretende no solo ser un buen punto de partida para adentrarse en el estudio de la decoherencia, los sistemas cuánticos abiertos y las ecuaciones maestras, sino mostrar también cómo los postulados de la mecánica cuántica concernientes a la medida pueden, en cierta manera, ser entendidos como consecuencias del formalismo matemático empleado en estas áreas.

# Objectives

The objectives of this project are several and their achievement has been organized in three different chapters. In the first one, It has been tried to explain what the measurement problem is and how decoherence partially solves it, explaining why we are only able to measure non-superposed states. In the second chapter it is shown how, indeed, decoherence emerges naturally when considering the interaction between a system and its environment, thus giving a justification to Von Neumann's irreversible reduction process. With these first two chapters, moreover, a mathematical framework based on master equations and CPT maps is established, which is used in the last chapter to achieve the ultimate goal of being able to describe the evolution of the accessible states of a quantum system on which a measurement is performed without having to resort to the measurement postulates.

*Los objetivos de este proyecto son varios y su consecución se ha organizado en tres capítulos distintos. En el primero se ha tratado de explicar en qué consiste el problema de la medida y cómo la decoherencia lo resuelve parcialmente, explicando por qué tan solo somos capaces de medir estados no superpuestos. En el segundo capítulo se demuestra cómo, en efecto, la decoherencia emerge de forma natural cuando se considera la interacción entre un sistema y su entorno, dando una justificación así al proceso de reducción irreversible de Von Neumann. Con estos dos primeros capítulos, además, se consigue establecer un marco matemático basado en las ecuaciones maestras y los mapas CPT que, en el tercer capítulo, se emplea para lograr el objetivo final de poder describir la evolución de los estados accesibles de un sistema cuántico sobre el que se realiza una medición sin tener que recurrir a los postulados de la medida.*

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# Chapter 1

## Introduction.

According to quantum mechanics, there are systems in nature that are in a superposition of states that does not fit with our everyday experience. Throughout this first chapter, the six postulates of quantum mechanics are reviewed in order to analyze this dichotomy and its different interpretations. It is in this context that an approach to the postulates in terms of the density matrix shows to be useful, allowing us to explain the transition between the quantum superposition and the classical world through the Von Neumann irreversible reduction process and decoherence.

*De acuerdo con la mecánica cuántica, existen sistemas en la naturaleza que se encuentran en una superposición de estados que no termina de encajar con nuestra experiencia cotidiana. A lo largo de este primer capítulo, se revisan los seis postulados de la mecánica cuántica con tal de analizar esta dicotomía y sus distintas interpretaciones. Es en este contexto que un planteamiento de los postulados en términos de la matriz densidad muestra una mayor utilidad, permitiendo explicar la transición entre la superposición cuántica y el mundo clásico a través del proceso de reducción irreversible de Von Neumann y la decoherencia.*

### 1.1 The postulates of quantum mechanics.

To be able to understand the problems which led to the concept of decoherence and the concept itself, it is convenient to review the so-called *quantum mechanics postulates*, which constitute the starting point of the quantum theory and all its interpretations. These postulates, which are set forth in the form presented in [1], will be stated and discussed below.

#### 1. First postulate.

*Every physical system has a quantum state that evolves in time, which is mathematically defined by a vector of a Hilbert space,  $|\psi(t)\rangle \in \mathcal{H}$ .*

One of the first things one has to notice when studying quantum mechanics is the big difference between what is called the *quantum state* of a system and the classical state one is used to handle. The last one is defined as the set of positions and linear momentums of all the particles of the system, which is well defined in both a mathematical and physical sense. Nevertheless, even when this first postulate gives a solid mathematical vision of what a *quantum state* is, this cannot be directly measured or identified with any known empirical entity. It



is just a mathematical object which contains all the useful information about a physical system, and, as a consequence of this first postulate, any linear combination of quantum states will also be a possible quantum state of the system since they form a Hilbert vector space  $\mathcal{H}$ .

## 2. Second postulate.

*Every measurable quantity  $\mathcal{A}$  of a system whose states are vectors of a Hilbert space  $\mathcal{H}$  is mathematically defined by an observable  $\mathcal{A}$  acting on it.<sup>1</sup>*

This postulate gives a solid mathematical definition of what a measurable quantity is. In quantum mechanics, the position and momentum of a particle do not define its state, they are, as we will now see, a consequence of it.

## 3. Third postulate.

*Once the quantity  $\mathcal{A}$  is measured, the obtained value will always be one of the eigenvalues of the observable that defines it.*

The third postulate requires physical quantities to be represented by diagonalizable operators with real eigenvalues (no physical quantity can have a non-real value), which is insured by the second postulate since all observables are defined hermitian. Apart of this, there is a remarkable fact in this postulate which is related to the so-called *quantum measurement problem*. Specifically, this postulate is implicitly assuming the fact that we will never be able to measure, for example, two different positions for the same particle. Even when this may seem obvious, the truth is that, as we anticipated with first postulate, the quantum state of a system can be a linear combination of different states which could be associated to different positions at the same time, so it doesn't look so wild to consider that a superposition of measurements would also be possible.

## 4. Fourth postulate.

*If the quantity  $\mathcal{A}$  is defined by an observable  $\mathcal{A}$  of a discrete spectrum, when it is measured over a system whose state is  $|\psi(t)\rangle \in \mathcal{H}$ , the probability of measuring the discrete eigenvalue  $a_n$  at time  $t_0$  is given by:*

$$\mathcal{P}(a_n) = \sum_{i=1}^{g_n} |\langle \psi(t_0) | a_n^i \rangle|^2,$$

*where  $\{|a_n^i\rangle\}_{i=1}^{g_n}$  is a basis of the eigenspace of  $\mathcal{A}$  associated to the eigenvalue  $a_n$  and  $g_n$  is its degree of degeneracy.*

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<sup>1</sup>This statement has to be understood carefully since time is a measurable quantity of any physical system but cannot be associated with any operator acting on the Hilbert space of states of the system [2]. Anyways, this is not a problem since any other magnitude (energy, position and momentum) can be described this way. Time will always be treated as a parameter of the problems, not as a measurable quantity.

The fourth postulate can be expressed in a more general form including the cases when an observable has a continuum spectrum or a combination of a continuum and a discrete spectrum. The generalization is trivial since one just has to change the discrete summation above by an integral or a combination of both. Anyway, the important fact here is that according to this postulate, the quantum state of a system could be interpreted just like a mathematical tool to calculate probabilities of having a specific result, so a superposition of states wouldn't necessary be interpreted as a physical superposition of positions, energies or momentums, depending on the measured quantity. This would apparently solve the problematic with postulate 3, nevertheless, double slit experiment on electrons and other observations have shown that superposition of states has indeed a physical manifestation, so the quantum state is not just a mathematical representation of our uncertainty about measurable outcomes, it does indeed affect physical reality. Why can't we then measure any superposition of energies, positions or momentums?

### 5. Fifth postulate.

*If the quantity  $\mathcal{A}$  is measured at time “ $t$ ” and the eigenvalue  $a$  is obtained, then the quantum state just after the measurement is given by:*

$$|\psi(t')\rangle = \frac{\hat{P}_a|\psi(t)\rangle}{\sqrt{\langle\psi(t)|\hat{P}_a|\psi(t)\rangle}},$$

*where  $\hat{P}_a$  represents the projector operator over the eigenspace of the observable  $\mathcal{A}$  associated to the eigenvalue  $a$ .*

This quantum mechanics postulate is, by far, the most controversial one. One of the main reasons is that it is not well defined what *measuring* means in physical terms. Is the ground measuring the photons arriving from the sun when they collide with its atoms? Maybe should the measure be made by a conscience? In that case, how would this be defined? A known example that exposes this problematic is the thought experiment of Wigner's friend. If some scientist makes a measurement over a system, the quantum state of such system will become the one predicted by this postulate, but if some other scientist opens the door of the laboratory where the first one was making a measurement, the quantum state of the global system of the laboratory will be the one which is determined by this postulate, so which state has been modified by postulate 5? In addition to this, we have already highlighted the problematic of the non existence of superposed measure results, which now can be understood because of the reduction of the quantum state once we measure over the system. Anyway, this reduction still requires an explanation since it was historically imposed to be able to predict experimental results, but it was not deduced. Indeed, there is no reason to believe that this postulate is a real fundamental law of nature since it breaks with the continuum and unitary evolution of states given by the next postulate.

## 6. Sixth postulate.

The quantum state of a system evolves in time according to the Schrödinger equation:

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle,$$

where  $\hat{H}$  is the hamiltonian of the system.

The sixth postulate provides a mathematical equation that perfectly describes the time evolution of the quantum state of a system. Since this equation is linear and, in consonance with the first postulate, any linear combination of solutions to the equation will also be a solution, we arrive to the already mentioned *superposition of states* that has no classical analogy.

This set of postulates, that are amazingly useful to make calculations and predict experimental results, show then some ambiguities concerning the concepts of *measurement* and *superposition* that are usually englobed in the concept of what is called *the measurement problem*. Postulates five and six describe the evolution of the quantum state of a system in two very different ways depending on whether a measure is carried out or not, but this, of course, needs a deeper explanation. This situation has carried scientific community to manage what are known as the *interpretations of quantum mechanics*.

According to [3], the first interpretation that tried to handle with the measurement problem is the so-called *Copenhagen interpretation*, which considers that the quantum theory is not universal and there exists a boundary between the classic and quantum worlds that invalidates quantum theory in the classical domain. This explains why we can't see any superposition effects in our daily classical experience and why, since our measurement machines are classical, we need to accept fifth postulate as an ad hoc process to model measurements. This interpretation gives a definition of a measurement as an interaction with a classical device, but it doesn't allow us to understand if there is any physical mechanism which causes the collapse and the "boundary" between the quantum and classic world is not clear at all.

Other interpretation, purposed later by Hugh Everett, is the so-called *Many worlds interpretation* [4]. According to it, quantum theory is a general theory that could be applicable to any physical system, including the entire universe. For this interpretation, a measurement is an interaction between quantum systems, so, once the interaction happens, the global system has many possible accessible states. What many worlds interpretation stands is that every single one of this possible states exists in superposition with the rest in different universes, according to Schrödinger equation. This discards the need of the fifth postulate, nevertheless, such consideration still requires an explanation. Why do we perceive just one of the many superposed states?

The answer to this question is not completely clear to this day, since there is not even a consensus on what is the correct interpretation of quantum mechanics. The truth is, however, that quantum mechanics itself provides some ways to understand why it would never be possible for us to see any superposed states if we dispense with the postulates concerning measurement and consider that the entire universe evolves according Schrödinger equation. To understand how, let's briefly revise an important mathematical concept: *The density operator*.

## 1.2 The density operator.

In many circumstances, the quantum state of a system is not completely known and one has to consider a set of possible states for the system  $\{|\psi_i\rangle\}_{i=1}^N$ , every one of which has a probability  $p_i$  of being the real one. This is known as a *mixture of states* and it's necessary to describe many situations in quantum mechanics. If one wanted to solve a quantum problem with a mixed state, the problem should be solved for each state of the set and the results should be averaged with the probabilities  $p_i$ . An illustrative example is the calculation of the expectation value of an observable  $\mathcal{A}$ . As we know, the expectation value in one of the states of the set is given by  $\langle\psi_i|\mathcal{A}|\psi_i\rangle$ , so taking the average over all the states of the set we get:

$$\langle\mathcal{A}\rangle = \sum_{i=1}^N p_i \langle\psi_i|\mathcal{A}|\psi_i\rangle. \quad (1.1)$$

As this is a little complicated, it is natural to find some way to write this in a more compact form. Indeed, this can be achieved by defining the *density operator*  $\rho$  as follows:

$$\rho = \sum_{i=1}^N p_i |\psi_i\rangle \langle\psi_i|, \quad (1.2)$$

so it can be checked that the result of equation (1.1) is exactly equal to:

$$\langle\mathcal{A}\rangle = \text{Tr}[\rho\mathcal{A}]. \quad (1.3)$$

This is obviously a more compact and simple way to write the result. Furthermore, if one considers the definition (1.2) and takes into account that  $\sum_{i=1}^N p_i = 1$ , it can be shown that the density operator also satisfies the following relations:

$$\rho = \rho^\dagger, \quad (1.4) \quad \text{Tr}[\rho] = 1, \quad (1.5) \quad \text{Tr}[\rho^2] \leq 1, \quad (1.6) \quad \langle u|\rho|u\rangle \geq 0, \forall |u\rangle \in \mathcal{H}. \quad (1.7)$$

In (1.6), the equality stands iff  $\rho$  describes a *pure state*, this is, if  $N = 1$ . The density operator, nevertheless, is not just a mathematical tool with interesting properties that simplify the notation. In fact, this operator contains all the possible information one can have about a quantum system since it includes all its possible states and the probabilities of those being its real ones. Quantum mechanics can indeed be reformulated in terms of it by imposing the compliance of the postulates of quantum mechanics, what drives to the set of equations:

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}[\hat{H}, \rho], \quad (1.8) \quad \rho' = \frac{\hat{P}\rho\hat{P}}{\text{Tr}[\rho\hat{P}]}, \quad (1.9) \quad \mathcal{P} = \text{Tr}[\rho\hat{P}], \quad (1.10)$$

where  $\hat{H}$  is the hamiltonian of the system described by  $\rho$ ,  $\rho'$  is the density operator after a measurement,  $\mathcal{P}$  is the probability of that measurement being taken and  $\hat{P}$  is the projector operator of the eigenspace of the measured observable associated to the measured eigenvalue.

A quantum mechanics approach based on this density operator will allow a study on how the set of possible states of a system evolves in time. This will have a clear advantage over a single state approach, not just for being more realistic, but for allowing us to know which kind of state will a system potentially have, for example, after a measurement.

### 1.3 Decoherence and pointer basis

To clarify the last consideration, let's now consider an illustrative example. Suppose that a two levels system is prepared in the following superposed state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle, \quad (1.11)$$

where  $|0\rangle$  and  $|1\rangle$  form an orthonormal basis of the Hilbert space of the system. If the definition of the density operator is applied, it can be calculated for this pure state that:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 0| + \frac{1}{2}|0\rangle\langle 1| + \frac{1}{2}|1\rangle\langle 1|. \quad (1.12)$$

This density operator cannot be interpreted in a probabilistic way as a representation of a mixed state of  $|0\rangle$  and  $|1\rangle$  since some non-diagonal elements have appeared. Nevertheless, what would happen if a measurement was made over the system?. As we know from postulates four and five, the resulting state of the measurement will be  $|0\rangle$  or  $|1\rangle$ , both of them with probability  $1/2$ . This corresponds to a mixed state described by the density operator:

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \quad (1.13)$$

which, in opposition to the one in (1.12), can be easily interpreted in a probabilistic way as mixed state of  $|0\rangle$  and  $|1\rangle$ . In addition, this is a mixture of non-superposed states, this is, superposition effects are absent and the density operator is what someone would classically expect. Despite this, quantum mechanics postulates consider measurements as sudden processes and, as equation (1.9) yields, when the measurement is done, the density operator instantly collapses to  $|0\rangle\langle 0|$  or  $|1\rangle\langle 1|$  without passing through (1.13). This is why Von Neumann introduced the so-called *irreversible reduction process* [3] which stands that before one gets the result of the measurement, the density operator is reduced to an appropriate mixed state density operator constituted by non-superposed states like the one in (1.13).

The Von Neumann irreversible reduction process explains why superposition effects vanish when we measure over a quantum system since the only possible candidates appearing in (1.13) are not superposed states, but it still requires an explanation since it's just an *ad hoc* process. To understand how it happens, it has to be remembered that a measurement can be interpreted as an interaction between two quantum systems: the studied one and the environment in which the detector/measurement apparatus is found. From this point of view, it seems clear that the irreversible reduction process should be deduced as a consequence of a detailed study of the interaction between the system and its environment, as we had already highlighted. This process, as can be seen from (1.12) and (1.13), is closely related to a fading of the non-diagonal elements of the density operator when it is expressed in a particular vector base of the Hilbert space of the system. As diagonal and non-diagonal elements of density operator are usually called *populations* and *coherences*, this process is called **decoherence** and the vector basis in which it takes place has been called in literature as **pointer basis**. Our current purpose is then to be able to infer decoherence as a consequence of the environment-system interaction.

# Chapter 2

## Quantum master equations.

Once the concepts of the measurement problem and decoherence have been explained, it remains to be shown that the interaction between a measured system and its environment really causes this effect and that, moreover, it does so in a sufficiently small time for us not to notice it. The key to achieve this will be the study of the time evolution of the density operator associated with the system on which the measurement is made. However, as we are considering that this system is not isolated, we will not be able to use the Schrödinger equation to analyze its evolution, but we will have to use an equation that describes the time evolution of the density operator of the required subsystem interacting with its environment, this is, a **master equation**. Throughout this chapter, two ways of constructing a master equation for the system are presented, pointing out the equivalences and differences between the two, as well as between the results they lead to. Later, the equations are applied to describe the evolution of a harmonic oscillator and a two-level system interacting with their environments, demonstrating how decoherence naturally emerges in these systems. Finally, the use of master equations and the approximations involved are justified, as well as the main current knowledge about the pointer basis concept and its calculation is exposed.

*Una vez expuesto el concepto del problema de la medida y la decoherencia, queda por demostrar que la interacción entre un sistema medido y su entorno provoca realmente este efecto y que, además, lo hace en un tiempo lo suficientemente pequeño como para que no lo notemos. La clave para conseguirlo será el estudio de la evolución temporal del operador densidad asociado al sistema sobre el que se realiza la medida. Sin embargo, como estamos considerando que este sistema no está aislado, no podremos utilizar la ecuación de Schrödinger para analizar su evolución, sino que tendremos que emplear una ecuación que describa la evolución temporal del operador densidad del subsistema requerido que interacciona con su entorno, es decir, una **ecuación maestra**. A lo largo de este capítulo se exponen dos maneras de construir una ecuación maestra para el sistema, señalando las equivalencias y diferencias entre ambas, así como entre los resultados a los que conducen. Más adelante, las ecuaciones se aplican para describir la evolución de un oscilador armónico y un sistema de dos niveles que interactúan con sus entornos, demostrando cómo la decoherencia aparece de forma natural en estos sistemas. Finalmente, se justifica el uso de las ecuaciones maestras y las aproximaciones que conllevan, así como también se exponen los principales conocimientos actuales sobre el concepto de pointer basis y su cálculo.*

## 2.1 General derivation of Lindblad equation

One of the most extended ways to derive a master equation which describes the time evolution of the density operator of an interacting system is based in physical arguments and approximations. Those considerations allow a rewrite of the evolution equation of the composed system (1.8) only in terms of the desired interacting subsystem density operator. This derivation will be analyzed in 2.2, but before, a more general way to proceed usually preferred by quantum information specialists has been developed, which will allow us to take a broader point of view of some important concepts.

With this in mind, we can start by posing the problem of finding the density operator  $\rho(t)$  of a system once the initial condition  $\rho(t_0)$  is given. A natural way of establishing a relation between this two objects is to define an application from the set of all possible density operators of the system, which would be defined by conditions (1.4,1.5,1.6,1.7). This sets can't define a vector space since some linear combinations of density matrices won't give a density matrix (for example, trace could result to be different from one). Nevertheless, this set belongs to a Banach space usually called **Fock-Liouville space** we will denote as  $\mathcal{B}(\mathcal{H})$  which is defined by a set of bounded linear operators and an internal product. Operators in  $\mathcal{B}(\mathcal{H})$  will be denoted as  $|\phi\rangle\rangle$  and the internal product between them is defined by:

$$\langle\langle\phi|\varphi\rangle\rangle = Tr[\phi^\dagger\varphi].$$

Inequation (1.5) can then be written as  $\langle\langle\rho|\rho\rangle\rangle \leq 1$ . As we are not interested in carrying out an exhaustive analysis on Fock-Liouville spaces, we won't get into details about the conditions of Banach spaces but just accept the preceding and apply it as a useful mathematical tool. Once this is clear, we can try to find a linear map  $\Omega_t$  to relate the initial condition  $\rho(t_0)$  to the density matrix at time  $t$  as follows:

$$\begin{aligned} \Omega_t : \mathcal{B}(\mathcal{H}) &\rightarrow \mathcal{B}(\mathcal{H}) \\ \Omega_t(\rho(t_0)) &= \rho(t) \end{aligned}$$

As the map  $\Omega_t$  is expected to transform density operators into density operators, we will force it to be **completely positive** and to satisfy the **trace preservation** condition:

$$Tr[\Omega_t(\rho)] = Tr[\rho]. \quad (2.1)$$

It is important to highlight that it is said that a map  $\Omega$  is **positive** iff:

$$\forall \rho \in \mathcal{B}(\mathcal{H}) / \rho \geq 0 \implies \Omega(\rho) \geq 0, \quad (2.2)$$

and **completely positive** iff  $\forall n \in \mathbb{N}$ ,  $\Omega(\rho) \otimes \mathbb{1}_n$  is positive. (The notation  $\rho, \Omega(\rho) \geq 0$  is used to denote positive-defined matrices, which can be defined for our interests as those of positive

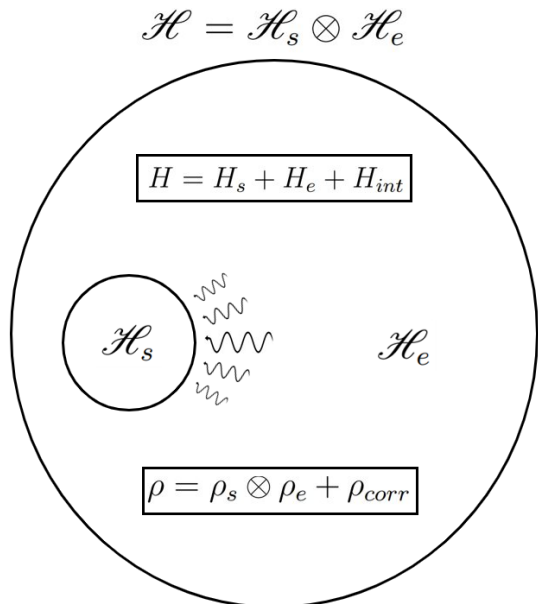


Figure 2.1: General scheme of the subsystem-environment interaction. Since the subsystem interacts with its environment, it evolves according to a master equation.

eigenvalues). With (2.1) we are forcing the trace of the density operator to be preserved by the map, so if (1.5) is initially satisfied, it will be satisfied at any time. If this condition is not satisfied, then it is no longer possible to talk about a density operator. In the other hand, the completely positive condition ensures that the eigenvalues of the density operator will never be negative according to (1.7), furthermore, ensuring that  $\Omega_t$  is not just a positive map but a completely positive one allows us to affirm that this will be satisfied not just by  $\rho$ , but by any other density matrix representing a composed system containing the system which state is represented by  $\rho$ . This, however, is only true if there is a **weak correlation between the studied subsystem and the environment**, which is the so-called **Born approximation**. To understand this a little better, let's imagine we are treating a subsystem-environment composed system which density operator is  $\rho_{total}$ . In the most general possible case, this density operator will be written in terms of the density operator of the subsystem and its environment as follows:

$$\rho_{total} = \rho_s \otimes \rho_e + \rho_{correlation},$$

where  $s$  and  $e$  stand for subsystem and environment respectively. This operator is defined over a Hilbert space  $\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_e$ , so if we call  $d$  the dimension of the Hilbert space of the environment states  $\mathcal{H}_e$  and  $\Omega_t$  is the map that describes the evolution of  $\rho_s$ , then we can apply the operator  $\Omega_t \otimes \mathbb{1}_d$  over  $\rho_{total}$  to obtain:

$$(\Omega_t \otimes \mathbb{1}_d) \rho_{total} = \Omega_t \rho_s \otimes \rho_e + [(\Omega_t \otimes \mathbb{1}_d) \rho_{correlation}].$$

When the interaction between the subsystem and its environment is not negligible, the density operator of the environment and the one which describes the correlation will evolve in time, so the right side of the equation would not have to correspond to the evolved state, which implies that  $(\Omega_t \otimes \mathbb{1}_d)$  doesn't describe the evolution of  $\rho_{total}$ . This implies that in the case of strong interaction, ensuring that  $\Omega_t$  is a complete positive map won't imply that  $\rho_{total}$  preserves positivity. Nevertheless, if the environment is not affected by the subsystem and there is no correlation, the last equation makes sense since:

$$(\Omega_t \otimes \mathbb{1}_d) \rho_{total} = \Omega_t \rho_s \otimes \rho_e,$$

and the right hand side of the equation corresponds to what we would expect to be the evolution of the system under this assumptions. The conclusion is that under Born approximation,  $(\mathbb{1}_d \otimes \Omega_t)$  is the time evolution map of the composed system, so ensuring that  $\Omega_t$  is completely positive will ensure that the density operator of the composed system will preserve positivity. This set of conditions over  $\Omega_t$  define what is called a **CPT map** (completely positive trace preserving map), which will be the key to find the time evolution of the density operator. This will be given by:

$$\left( \frac{d\rho}{dt} \right)_{t_0} = \lim_{t \rightarrow t_0} \frac{\rho(t) - \rho(t_0)}{t - t_0}. \quad (2.3)$$

Now, using the map  $\Omega_t$  and defining  $\Delta t = t - t_0$  we arrive to:

$$\left( \frac{d\rho}{dt} \right)_{t_0} = \lim_{\Delta t \rightarrow 0} \frac{\Omega_{t_0 + \Delta t} \rho(t_0) - \rho(t_0)}{\Delta t}. \quad (2.4)$$

To develop the right hand side of (2.4) the **Choi-Krauss theorem** below this paragraph will be used (the proof of this theorem can be found in [5], in which I have based the following reasoning).



**Theorem:** A linear map  $\Omega : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$  is completely positive and trace preserving  $\iff \left( \exists \{V_i\}_{i=0}^{d^2-1} \subset \mathcal{B}(\mathcal{H}) / \Omega(\rho) = \sum_{i=0}^{d^2-1} V_i^\dagger \rho V_i \wedge \sum_{l=0}^{d^2-1} V_l V_l^\dagger = \mathbb{1}_{\mathcal{H}} \right)$ .  
With  $d = \dim(\mathcal{H})$

According to Choi-Kraus theorem, the map  $\Omega_t$  admits the mentioned decomposition, which will be assumed in the following. Nevertheless, since the map has been considered to depend on the initial condition  $\rho(t_0)$ , the so-called *Kraus operators*,  $V_i$ , will also depend on it. This complicates the developing of (2.4) since some time integral operators appear, so here the **Markov approximation** is considered. This consists of assuming that  $\Omega_t$  does not depend on the previous state of the system that has to be evolved, so it does not take into account the history of the state from  $t_0$  to  $t$ . The approximation owes its name to the russian mathematician *Andréi Markov*, who studied stochastic processes in which future values of a random variables do not depend on its past history. This is very important to consider since some real situations cannot be described by Markovian processes, which indeed has a lot to do with decoherence (It has been proven that in certain circumstances non-Markovianity can produce sudden creations of coherences, this is, the contrary effect to decoherence [6][7]). Nevertheless, Markovian processes describe a very wide range of physical systems and will allow us to study decoherence in a first approximation (for a detailed discussion of the concept of Markovianity, the reader is referred to [8]).

There is only one remaining step we have to make to be able to find the master equation we are looking for, specifically, we will use the Fock-Liouville space to develop the following calculations and we need to choose an adequate basis of the space, which will be used to expand the Kraus operators. Let's then take  $\{F_i\}_{i=1}^{d^2}$  basis of  $\mathcal{B}(\mathcal{H})$ . In the Fock-Liouville space, this operators will satisfy the orthonormality condition and close relation, which are written:

$$\langle\langle F_i | F_j \rangle\rangle = Tr[F_i^\dagger F_j] = \delta_{ij}, \quad \sum_{i=1}^{d^2} |F_i\rangle\rangle \langle\langle F_i| = \mathbb{1}_{d^2}.$$

In particular, let's take  $F_{d^2} = \frac{1}{\sqrt{d}} \mathbb{1}_{\mathcal{H}}$ . One can see that, by construction,  $\langle\langle F_{d^2} | F_{d^2} \rangle\rangle = 1$  and, for the orthonormality condition to be satisfied, it will be necessary that  $Tr[F_i] = 0, \forall i \neq d^2$ . As the map  $\Omega_t$  we are looking for depends on time, the Krauss operators  $V_l$  will also do, so we can expand them in the previous basis using closure relation as follows:

$$|V_l(t)\rangle\rangle = \sum_{i=1}^{d^2} \langle\langle F_i | V_l(t) \rangle\rangle |F_i\rangle\rangle \implies \langle\langle V_l(t) | = \sum_{i=1}^{d^2} \langle\langle V_l(t) | F_i \rangle\rangle \langle\langle F_i |.$$

As we are considering our map  $\Omega_t$  to be completely positive and trace preserving, by Choi-Kraus theorem we have:

$$\Omega_t(\rho) = \sum_{l=0}^{d^2-1} V_l^\dagger(t) \rho V_l(t) = \sum_{l=0}^{d^2-1} \left( \sum_{i=1}^{d^2} \langle\langle V_l(t) | F_i \rangle\rangle F_i^\dagger \right) \rho \left( \sum_{j=1}^{d^2} \langle\langle F_j | V_l(t) \rangle\rangle F_j \right) = \sum_{i=1}^{d^2} \sum_{j=1}^{d^2} C_{ij}(t) F_i^\dagger \rho F_j,$$

where we have defined  $C_{ij}(t) = \sum_{l=0}^{d^2-1} \langle\langle F_j | V_l(t) \rangle\rangle \langle\langle V_l(t) | F_i \rangle\rangle$ . Going back to equation (2.4) we find:

$$\left( \frac{d\rho}{dt} \right)_{t_0} = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left( \sum_{i=1}^{d^2} \sum_{j=1}^{d^2} C_{ij}(t_0 + \Delta t) F_i^\dagger \rho(t_0) F_j - \rho(t_0) \right).$$

Separating the terms with  $i, j = d^2$  we get:

$$\begin{aligned} \left(\frac{d\rho}{dt}\right)_{t_0} = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} & \left( \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} C_{ij}(t_0 + \Delta t) F_i^\dagger \rho(t_0) F_j + \sum_{j=1}^{d^2-1} C_{d^2 j}(t_0 + \Delta t) F_{d^2}^\dagger \rho(t_0) F_j + \right. \\ & \left. + \sum_{i=1}^{d^2-1} C_{i d^2}(t_0 + \Delta t) F_j^\dagger \rho(t_0) F_{d^2} + C_{d^2 d^2}(t_0 + \Delta t) F_{d^2}^\dagger \rho(t_0) F_{d^2} - \rho(t_0) \right), \end{aligned}$$

so, as we have chosen  $F_{d^2}$  to be proportional to identity, this trivially reduces to:

$$\begin{aligned} \left(\frac{d\rho}{dt}\right)_{t_0} = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} & \left( \sum_{i=2}^{d^2-1} \sum_{j=2}^{d^2-1} C_{ij}(t_0 + \Delta t) F_i^\dagger \rho(t_0) F_j + \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} C_{d^2 j}(t_0 + \Delta t) \rho(t_0) F_j + \right. \\ & \left. + \frac{1}{\sqrt{d}} \sum_{i=1}^{d^2-1} C_{i d^2}(t_0 + \Delta t) F_i^\dagger \rho(t_0) + \frac{C_{d^2 d^2}(t_0 + \Delta t)}{d} \rho(t_0) - \rho(t_0) \right). \end{aligned}$$

If we now define the following:

$$g_{ij} = \lim_{\Delta t \rightarrow 0} \frac{C_{ij}(t_0 + \Delta t)}{\Delta t}, \forall (i, j) \neq (d^2, d^2), \quad (2.5) \quad g_{d^2 d^2} = \lim_{\Delta t \rightarrow 0} \frac{C_{d^2 d^2}(t_0 + \Delta t) - d}{\Delta t}, \quad (2.6)$$

it can be seen from the definition of  $C_{ij}(t)$  that  $g_{ij} = g_{ji}^*$ , this is,  $g_{ij}$  are the elements of a hermitian matrix. Applying this to the last equation we get:

$$\left(\frac{d\rho}{dt}\right)_{t_0} = \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} g_{d^2 j} \rho(t_0) F_j + \frac{1}{\sqrt{d}} \sum_{i=1}^{d^2-1} g_{i d^2} F_i^\dagger \rho(t_0) + \frac{g_{d^2 d^2}}{d} \rho(t_0).$$

To write this in a more compact form, we define  $F = \frac{1}{\sqrt{d}} \sum_{i=1}^{d^2-1} g_{i d^2} F_i^\dagger$ , so applying that  $\mathbf{g}$  is an hermitian matrix, we can easily see that  $F^\dagger = \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} g_{d^2 j} F_j$  and, substituting, we get:

$$\left(\frac{d\rho}{dt}\right)_{t_0} = \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + \rho(t_0) F^\dagger + F \rho(t_0) + \frac{g_{d^2 d^2}}{d} \rho(t_0).$$

A step further can be made to separate  $F$  in two parts  $G$  and  $H$ . Specifically, we can define:

$$G = \frac{F + F^\dagger}{2}, \quad H = \frac{F^\dagger - F}{2i},$$

so  $H$  and  $G$  are trivially hermitian and:  $F = G - iH \iff F^\dagger = G + iH$ . This drives us to the following equation:

$$\left(\frac{d\rho}{dt}\right)_{t_0} = \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + \{G, \rho(t_0)\} - i[H, \rho(t_0)] + \frac{g_{d^2 d^2}}{d} \rho(t_0),$$

so if one defines  $J = G + \frac{g_{d^2 d^2}}{2d}$  then:

$$\left(\frac{d\rho}{dt}\right)_{t_0} = \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + \{J, \rho(t_0)\} - i[H, \rho(t_0)]. \quad (2.7)$$

The last step will be to impose that  $\frac{d}{dt}Tr[\rho] = 0 \iff Tr[\frac{d\rho}{dt}] = 0$ . By doing so, one gets:

$$\begin{aligned} Tr\left[\left(\frac{d\rho}{dt}\right)_{t_0}\right] &= Tr\left[\sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + \{J, \rho(t_0)\} - i[H, \rho(t_0)]\right] = \\ &= Tr\left[\sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + J\rho(t_0) + \rho(t_0)J - iH\rho(t_0) + i\rho(t_0)H\right]. \end{aligned}$$

By linearity and cyclic property of trace, this reduces to:

$$Tr\left[\left(\frac{d\rho}{dt}\right)_{t_0}\right] = Tr\left[\sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_i^\dagger \rho(t_0) F_j + 2J\rho(t_0)\right] = 0,$$

so, as this stands for any possible density matrix, we conclude:

$$J = -\frac{1}{2} \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} F_j F_i^\dagger,$$

what we can insert in (2.7) to get:

$$\left(\frac{d\rho}{dt}\right)_{t_0} = -i[H, \rho(t_0)] + \sum_{i=1}^{d^2-1} \sum_{j=1}^{d^2-1} g_{ij} \left(F_i^\dagger \rho(t_0) F_j - \frac{1}{2}\{F_j F_i^\dagger, \rho(t_0)\}\right).$$

Finally, as  $\mathbf{g}$  is hermitian and therefore diagonalizable, we can find a new basis of operators  $F_i \rightarrow L_i^\dagger$  such that:

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_{k=1}^{d^2-1} \Gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\}\right), \quad (2.8)$$

where, for simplicity, we have called  $g_{kk} = \Gamma_k$  and suppressed the specification that  $\rho$  and its derivative are evaluated in a certain same time  $t_0$ .

Equation (2.8) is known as **Gorini–Kossakowski–Sudarshan–Lindblad equation** in honor to their ideators. This equation, as has been exposed, constitutes a very general description of a markovian time-evolving process of a system which is not correlated to its environment. As we have proved,  $H$  represents a hermitian operator,  $\Gamma_k$  are real coefficients (which can also be proven to be positive) and  $L_k$  are some operators acting on the Hilbert space of the states of the interacting subsystem, which mixed state is mathematically defined by  $\rho$ . The operators  $L_k$  are usually called the *Lindblad jump operators* and describe the interaction between the subsystem and the environment. Indeed, if we make them zero, we will get back an equation with the form of (1.8), what makes us think that the  $H$  appearing in (2.8) is clearly related to the hamiltonian of the subsystem. As we will see, Lindblad equation is not the only possible master equation for a system that interacts with its environment, but according to the previous derivation, whenever an interaction can be described through (2.8), the trace and positiveness of  $\rho$  will be preserved.

## 2.2 A physical approach. Redfield equation.

As we had anticipated, a master equation can be derived from a physical microscopic study of the dynamics of the composed subsystem-environment quantum system, which is what we are going to do now. With this purpose, let's take  $s$  and  $e$  to denote the subsystem and the environment, respectively, and let's consider the total hamiltonian:

$$H = H_s + H_e + H_{int}. \quad (2.9)$$

As we know, the Hilbert space of the complete system will be  $\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_e$  and the density operator describing its state will be  $\rho = \rho_s \otimes \rho_e + \rho_{corr}$ . As we are considering that the entire system is isolated, we can now apply (1.8) to describe the evolution of its density operator:

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H, \rho(t)]. \quad (2.10)$$

If we now write this in terms of the interaction picture, this is, if we define in the total system:

$$\tilde{\mathcal{A}} = e^{\frac{i}{\hbar}(H_e+H_s)t} \mathcal{A} e^{-\frac{i}{\hbar}(H_s+H_e)t}, \quad (2.11)$$

it can be shown through some algebra that:

$$\frac{d\tilde{\rho}}{dt} = \frac{1}{i\hbar} [\tilde{H}_{int}, \tilde{\rho}(t)]. \quad (2.12)$$

Integrating this equation and assuming  $t_0 = 0$  for simplicity:

$$\tilde{\rho}(t) = \tilde{\rho}(0) + \frac{1}{i\hbar} \int_0^t [\tilde{H}_{int}(\tau), \tilde{\rho}(\tau)] d\tau. \quad (2.13)$$

By iterating this equation, one arrives to:

$$\tilde{\rho}(t) = \tilde{\rho}(0) + \frac{1}{i\hbar} \int_0^t \left[ \tilde{H}_{int}(\tau), \tilde{\rho}(0) + \frac{1}{i\hbar} \int_0^\tau [\tilde{H}_{int}(\tau'), \tilde{\rho}(\tau')] d\tau' \right] d\tau. \quad (2.14)$$

Derivating again with respect to time we will get, by applying Leibniz rule:

$$\frac{d\tilde{\rho}}{dt} = \frac{1}{i\hbar} [\tilde{H}_{int}(t), \tilde{\rho}(0)] + \frac{1}{(i\hbar)^2} \left[ \tilde{H}_{int}(t), \int_0^t [\tilde{H}_{int}(\tau), \tilde{\rho}(\tau)] d\tau \right]. \quad (2.15)$$

Taking now the trace over the environment:

$$Tr_e \left[ \frac{d\tilde{\rho}}{dt} \right] = \frac{1}{i\hbar} Tr_e [\tilde{H}_{int}(t), \tilde{\rho}(0)] + \frac{1}{(i\hbar)^2} Tr_e \left[ \tilde{H}_{int}(t), \int_0^t [\tilde{H}_{int}(\tau), \tilde{\rho}(\tau)] d\tau \right],$$

which can be simplified if we now assume that there is no correlation at  $t = 0$ . This makes sense, for example, if the subsystem and the environment were not interacting before that instant. That implies that  $\rho(0) = \rho_s(0) \otimes \rho_e(0)$ . It can be shown that this also implies  $\tilde{\rho}(0) = \tilde{\rho}_s(0) \otimes \tilde{\rho}_e(0)$ , where the tilde notation is related to the interaction picture of each of the systems  $s$  and  $e$ , defined by relation (2.11) by cancelling  $H_e$  and  $H_s$  respectively. We can write then:

$$\left[ \tilde{H}_{int}(t), \tilde{\rho}(0) \right] = \left[ \tilde{H}_{int}(t), \tilde{\rho}_s(0) \otimes \tilde{\rho}_e(0) \right],$$

so if we now expand the interaction hamiltonian as follows:

$$\tilde{H}_{int}(t) = \hbar \sum_i \tilde{S}_i \otimes \tilde{E}_i, \quad (2.16)$$

where the possible number of terms in the sum is not fixed, then we get:

$$\left[ \tilde{H}_{int}(t), \tilde{\rho}(0) \right] = \hbar \sum_i \left( \tilde{S}_i \tilde{\rho}_S(0) \otimes \tilde{E}_i \tilde{\rho}_e(0) - \tilde{\rho}_S(0) \tilde{S}_i \otimes \tilde{\rho}_e(0) \tilde{E}_i \right).$$

Now, if the trace over the environment is calculated, by the cyclic property of the trace one gets:

$$Tr_e \left[ \tilde{H}_{int}(t), \tilde{\rho}(0) \right] = \hbar \sum_i \left( \tilde{S}_i \tilde{\rho}_S(0) - \tilde{\rho}_S(0) \tilde{S}_i \right) Tr_e \left[ \tilde{E}_i \tilde{\rho}_e(0) \right].$$

Without generality loss, it can be considered that  $Tr_e \left[ \tilde{E}_i \tilde{\rho}_e(0) \right] = 0$ . This is due to the fact that this only affects the origin of energies of the system, but not its time evolution. It is then concluded:

$$Tr_e \left[ \frac{d\tilde{\rho}}{dt} \right] = \frac{1}{(i\hbar)^2} Tr_e \left[ \tilde{H}_{int}(t), \int_0^t \left[ \tilde{H}_{int}(\tau), \tilde{\rho}(\tau) \right] d\tau \right].$$

One can now assume that the initial state of the environment is preserved and that correlation is zero for any time  $t > 0$ , so it can be written:

$$\tilde{\rho}(t) = \tilde{\rho}_s(t) \otimes \tilde{\rho}_e(0).$$

This assumption is the **Born approximation** we had already commented in the previous section. Under this consideration, it is trivial to see that:

$$Tr_e [\tilde{\rho}(t)] = \tilde{\rho}_s(t) Tr_e [\tilde{\rho}_e(0)] = \tilde{\rho}_s(t),$$

so, as trace and time derivative commute, we can finally write:

$$\frac{d\tilde{\rho}_s}{dt} = \frac{1}{(i\hbar)^2} Tr_e \left[ \tilde{H}_{int}(t), \int_0^t \left[ \tilde{H}_{int}(\tau), \tilde{\rho}_s(\tau) \otimes \tilde{\rho}_e(0) \right] d\tau \right].$$

We can also introduce here the **Markov approximation** by imposing that  $\tilde{\rho}_s(\tau) \simeq \tilde{\rho}_s(t)$ , this is, we assume that the final state does not depend on its history, which should be integrated from  $t = 0$  to  $t$  (This is also known as *the first Markov approximation* [8]). Substituting the expansion of the interaction hamiltonian, the equation takes the form:

$$\frac{d\tilde{\rho}_s}{dt} = -\frac{1}{(\hbar)^2} Tr_e \left[ \hbar \sum_i \tilde{S}_i(t) \otimes \tilde{E}_i(t), \int_0^t \left[ \hbar \sum_j \tilde{S}_j(\tau) \otimes \tilde{E}_j(\tau), \tilde{\rho}_s(t) \otimes \tilde{\rho}_e(0) \right] d\tau \right],$$

this is:

$$\frac{d\tilde{\rho}_s}{dt} = -\sum_i \sum_j \int_0^t Tr_e \left[ \tilde{S}_i(t) \tilde{E}_i(t), \left[ \tilde{S}_j(\tau) \tilde{E}_j(\tau), \tilde{\rho}_s(t) \tilde{\rho}_e(0) \right] \right] d\tau,$$

where the tensor product symbol has been suppressed by simplicity. If the commutators are expanded and it is taken into account that:

$$\langle \tilde{E}_i(t) \tilde{E}_j(\tau) \rangle_e = Tr_e \left[ \tilde{\rho}_e \tilde{E}_i(t) \tilde{E}_j(\tau) \right], \quad (2.17)$$

$$\langle \tilde{E}_j(\tau) \tilde{E}_i(t) \rangle_e = Tr_e \left[ \tilde{\rho}_e \tilde{E}_j(\tau) \tilde{E}_i(t) \right], \quad (2.18)$$

then we finally conclude:

$$\begin{aligned} \frac{d\tilde{\rho}_s}{dt} = & - \sum_i \sum_j \int_0^t \left\{ \left( \tilde{S}_i(t) \tilde{S}_j(\tau) \tilde{\rho}_s(t) - \tilde{S}_j(\tau) \tilde{\rho}_s(t) \tilde{S}_i(t) \right) \langle \tilde{E}_i(t) \tilde{E}_j(\tau) \rangle_e + \right. \\ & \left. + \left( \tilde{\rho}_s(t) \tilde{S}_j(\tau) \tilde{S}_i(t) - \tilde{S}_i(t) \tilde{\rho}_s(t) \tilde{S}_j(\tau) \right) \langle \tilde{E}_j(\tau) \tilde{E}_i(t) \rangle_e \right\} d\tau. \end{aligned} \quad (2.19)$$

This equation tells us how the density operator of the subsystem we are studying evolves in time under the Born and Markov approximations. Nevertheless, this equation does not fit, at least written like this, with the form of the general Lindblad equation (2.8). This apparent contradiction is due to the fact that we still haven't forced all the conditions we assumed to deduce Lindblad equation. Indeed, (2.19) is what's known as the **Redfield equation**<sup>1</sup>, which, as it's known, doesn't guarantee that the evolution of the density operator preserves its positivity [9]. To arrive to a Lindblad equation form, we will need to force this condition, which can be done through the imposition of the **secular approximation**. This is also known as the **rotating wave approximation** and it consists in only considering resonant terms in the integrals in (2.19) when a certain decomposition of the coupling operators in (2.16) in terms of the *eigenoperators* of  $H_{int}$  is taken [10]. If one does so, equation (2.8) would be recovered.

Even when this equation doesn't insure the positivity of the evolution of the density operator, it can perfectly describe some extensively studied systems we will now see and, of course, will give account of the effects of decoherence we are interested in. In addition, this approach has the advantage of allowing us to construct master equations from accessible physical information such as the Hamiltonians of the systems, which is not the case with the approach used to prove the Lindblad equation.

## 2.3 The harmonic oscillator.

One of the systems that Redfield equation describes really well is the case of a harmonic oscillator immersed in an optical cavity in interaction with a thermal bath of radiation. In this section, we will develop (2.19) to arrive to a master equation for the subsystem of the cavity and, after giving a numerical solution to the equation, we will try to analyze the effect of decoherence. Some mathematical steps have been outlined to arrive to the master equation, but the reader can find a more detailed developing of the calculations in [11].

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<sup>1</sup>Depending on the bibliographic reference, the Redfield equation is written in one way or another. According to [5], equation (2.19) is a Redfield equation when the upper limit of the integral is extended to infinity (*second Markov approximation* [8]).

The mathematical description of the system is based on the quantization of the electromagnetic field, which leads to the following photonic hamiltonians:

$$H_s = \hbar\omega_s a^\dagger a, \quad H_e = \sum_j \hbar\omega_j r_j^\dagger r_j.$$

A way to model the interaction hamiltonian from these expressions is to consider a set of complex coefficients  $k_j$  such that:

$$H_{int} = \sum_j \hbar \left( k_j^* a r_j^\dagger + k_j a^\dagger r_j \right).$$

If one defines:

$$\begin{aligned} S_1 &= a, & E_1 &= \sum_j k_j^* r_j^\dagger, \\ S_2 &= a^\dagger, & E_2 &= \sum_j k_j r_j, \end{aligned}$$

then the definition of the interaction picture can be used to see that  $\tilde{H}_{int}$  has the form of (2.16). Developing the calculations according to (2.11) one gets, for  $S_1(t)$ :

$$\begin{aligned} \tilde{S}_1(t) &= e^{\frac{i}{\hbar}H_s t} a e^{-\frac{i}{\hbar}H_s t} = e^{i\omega_s a^\dagger t} a e^{-i\omega_s a^\dagger t} \implies \\ \tilde{S}_1(t) |n\rangle &= e^{i\omega_s a^\dagger t} a e^{-i\omega_s t} |n\rangle = e^{i\omega_s a^\dagger t} \sqrt{n} e^{-i\omega_s t} |n-1\rangle = \\ &= e^{i\omega_s(n-1)t} \sqrt{n} e^{-i\omega_s t} |n-1\rangle = e^{-i\omega_s t} \sqrt{n} |n-1\rangle = e^{-i\omega_s t} a |n\rangle, \end{aligned}$$

where  $\{|n\rangle\}_{n=0}^\infty$  is the eigenbasis of  $H_s$ . By comparing the first and last terms it is deduced that  $\tilde{S}_1(t) = e^{-i\omega_s t} a$ . If one proceeds analogously for the rest of the operators it is concluded that:

$$\begin{aligned} \tilde{S}_1(t) &= a e^{-i\omega_s t}, & \tilde{E}_1(t) &= \sum_j k_j^* r_j^\dagger e^{i\omega_j t}, \\ \tilde{S}_2(t) &= a^\dagger e^{i\omega_s t}, & \tilde{E}_2(t) &= \sum_j k_j r_j e^{-i\omega_j t}. \end{aligned}$$

The last ingredient we need to evaluate (2.19) is the initial condition for the density operator of the environment  $\tilde{\rho}_e$ , which we need to calculate the *correlation functions* (2.17) and (2.18). As we are considering the environment to be in thermal equilibrium, we can apply the Boltzmann expression for the canonical ensemble to conclude:

$$\tilde{\rho}_e = \frac{e^{-\beta H_e}}{\text{Tr}_e [e^{-\beta H_e}]} = \frac{\prod_j e^{-\beta \hbar \omega_j r_j^\dagger r_j}}{\text{Tr}_e [e^{-\beta H_e}]},$$

where  $\beta = \frac{1}{k_B T}$ . To compute the denominator, we proceed as follows:

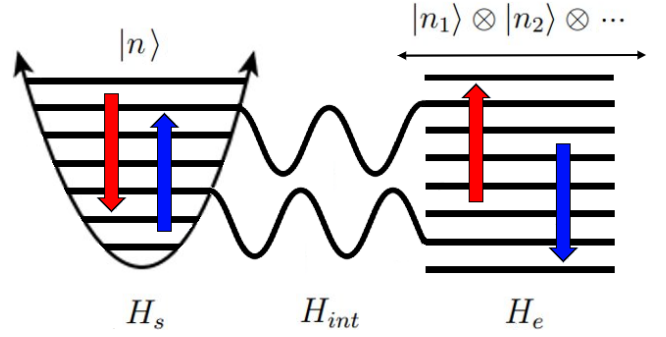


Figure 2.2: Scheme of the interaction between the harmonic oscillator and its radiation environment. Both systems experiment different transitions represented by colored arrows.

$$\begin{aligned}
Tr_e [e^{-\beta H_e}] &= Tr_e \left[ \prod_j e^{-\beta \hbar \omega_j r_j^\dagger r_j} \right] = \sum_{n_1, n_2, \dots} \langle n_1 | \otimes \langle n_2 | \otimes \dots \prod_j e^{-\beta \hbar \omega_j r_j^\dagger r_j} \dots | n_2 \rangle \otimes | n_1 \rangle = \\
&= \sum_{n_1, n_2, \dots} \langle n_1 | e^{-\beta \hbar \omega_1 r_1^\dagger r_1} | n_1 \rangle \langle n_2 | e^{-\beta \hbar \omega_2 r_2^\dagger r_2} | n_2 \rangle \dots = \left( \sum_{n_1} \langle n_1 | e^{-\beta \hbar \omega_1 r_1^\dagger r_1} | n_1 \rangle \right) \left( \sum_{n_2} \langle n_2 | e^{-\beta \hbar \omega_2 r_2^\dagger r_2} | n_2 \rangle \right) \dots = \\
&= \prod_j \left( \sum_{n_j} \langle n_j | e^{-\beta \hbar \omega_j r_j^\dagger r_j} | n_j \rangle \right) = \prod_j \sum_{n_j} e^{-\beta \hbar \omega_j n_j} = \prod_j \frac{1}{1 - e^{-\beta \hbar \omega_j}}.
\end{aligned}$$

Substituting this into the expression of  $\tilde{\rho}_e$  we get:

$$\tilde{\rho}_e = \prod_j (1 - e^{-\beta \hbar \omega_j}) e^{-\beta \hbar \omega_j r_j^\dagger r_j},$$

so if we finally substitute this results in (2.17), (2.18) and (2.19), we can, after a lot of algebra and some estimations, arrive to:

$$\frac{d\rho_s}{dt} = -i\omega'_c [a^\dagger a, \rho_s] + \kappa (2a\rho_s a^\dagger - a^\dagger a\rho - \rho a^\dagger a) + 2\kappa\tilde{n}(a\rho_s a^\dagger + a^\dagger \rho_s a - a^\dagger a\rho_s - \rho_s a a^\dagger), \quad (2.20)$$

where  $\omega'_c$ ,  $\kappa$  and  $\tilde{n}$  are some constants which are defined in terms of integrals through the calculations. To be precise,  $\omega'_c$  is related to the frequency of the harmonic oscillator inside the cavity,  $\tilde{n}$  is the average number of photons of the environment, which follow a bosonic distribution at its temperature, and  $\kappa$  parameterizes the strength of the interaction. If we rearrange the terms in (2.20) we get:

$$\frac{d\rho_s}{dt} = -i\omega'_c [a^\dagger a, \rho_s] + 2\kappa \left( a\rho_s a^\dagger - \frac{1}{2} \{a^\dagger a, \rho_s\} \right) + 2\kappa\tilde{n} [a^\dagger, [\rho_s, a]]. \quad (2.21)$$

This equation doesn't have the form of the Lindblad equation since a double-commutator term has appeared, what is a typical thing when working with Redfield equation. It can be noticed that this dissipative term is the only one associated to the number of photons of the bath  $\tilde{n}$ , so it will be related to stimulated transitions and absorptions by the harmonic oscillator. In the other hand, the first term will give account of spontaneous transitions and decays (this can be qualitatively seen by projecting the equation onto the eigenbasis of  $H_s$ ). To see how the density operator evolves in time, this equation must be solved, what has been done for the particular case of initial condition:

$$\rho_s(0) = \begin{pmatrix} 2/3 & -1/2 \\ -1/2 & 1/3 \end{pmatrix}, \quad (2.22)$$

with  $\omega'_c = 20 \text{ rad/s}$ ,  $\tilde{n} = 3$  and  $\kappa = 2 \text{ rad/s}$  (This values have been taken for numerical purposes, but they obviously do not reproduce any real physical situation). It must be specified that equation (2.22) is referred to the eigenbasis of  $H_s$ ,  $\{|n\rangle\}_{n=0}^\infty$ . As this defines an infinite-dimensional Hilbert space, the problem can't be analytically solved as a system of differential equations, so a program has been developed to solve it numerically. The results for the time evolution of the elements of the density operator are shown below 2.3:



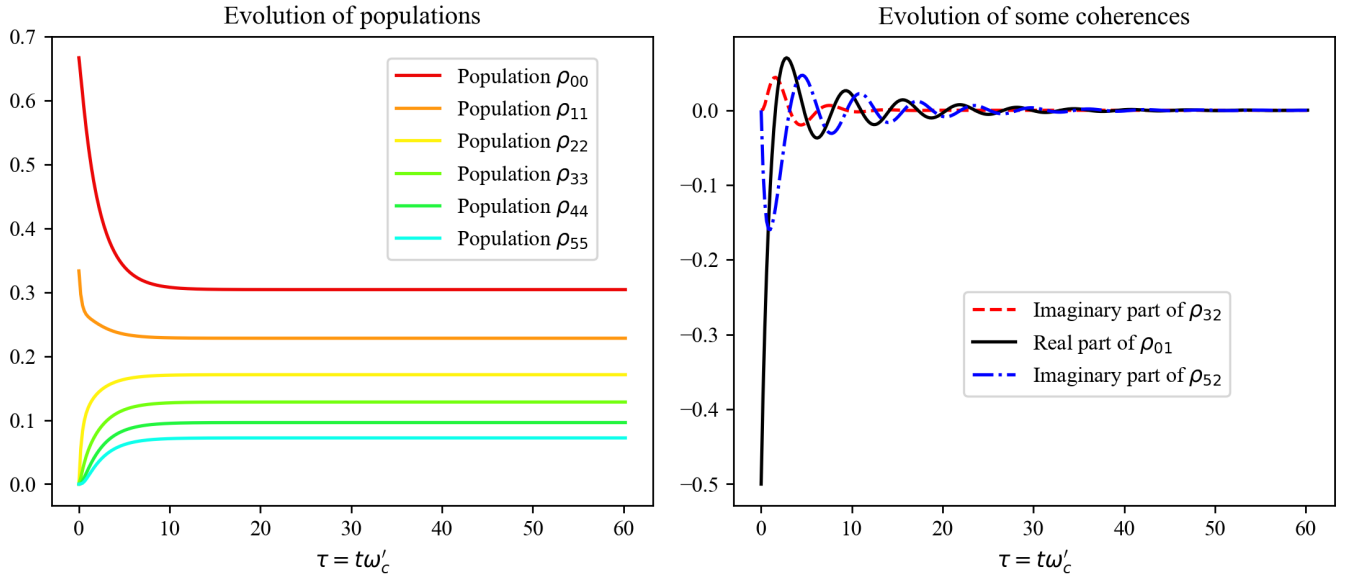


Figure 2.3: Temporal evolution of the harmonic oscillator state. Only a few representative populations and coherences have been represented for clarity.

This solutions confirm our initial intuition about decoherence emerging from subsystem-environment interaction, which we have modeled through the use of a master equation, in this case, a Redfield equation that has shown to preserve positivity. Emergence of decoherence is clear since both real and imaginary parts of coherences vanish for  $\tau \simeq 50$ , what additionally indicates that we have used the pointer basis of the system (eigenstates of  $H_s$ ) to represent the density matrix. Another fact that has to be explained is that decoherence takes a really big time to be completed since it depends on the value of  $\kappa$ , which has been chosen very low for numerical purposes but is not a realistic value. In general, decoherence time is, in this system, of the order of  $t \simeq 1/\kappa$ , so it is obvious that a real situation should be described by a very high value of  $\kappa$  and decoherence would rapidly emerge.

It may also be interesting to notice that after decoherence has taken place, the system reaches an equilibrium state in which, as can be deduced from the graphs,  $\frac{d\rho_{ij}}{dt} = 0, \forall i, j$ . This is something one would expect for a system which is interacting with a thermal bath, and it can be used to try to find an analytical solution for the density operator in such equilibrium state, what would help to verify the validity of the numerical solution. With this purpose, we can rearrange the terms in (2.20) to arrive to:

$$\begin{aligned} \frac{d\rho_s}{dt} &= -(i\omega'_c + \kappa + 2\kappa\tilde{n})N\rho_s + (i\omega'_c - \kappa)\rho_s N + 2\kappa(\tilde{n} + 1)a\rho_s a^\dagger + 2\kappa\tilde{n}a^\dagger\rho_s a - 2\kappa\tilde{n}\rho_s a a^\dagger \\ \implies \frac{d\rho_{mm}}{dt} &= -\rho_{mm}(C_1 m + C_2) + \rho_{(m+1)(m+1)}C_3(m+1) + \rho_{(m-1)(m-1)}C_2 m, \end{aligned}$$

where  $C_1 = (4\tilde{n} + 2)\kappa$ ,  $C_2 = 2\tilde{n}\kappa$  and  $C_3 = 2\kappa(\tilde{n} + 1)$ , so forcing the condition of equilibrium  $\frac{d\rho_s}{dt} = 0$  we arrive to a set of equations that, by iteration, yield the solution:

$$\begin{aligned} \rho_{11} &= \frac{C_2}{C_3}\rho_{00} = \gamma_1\rho_{00}. \\ \rho_{22} &= \frac{1}{2C_3}[\gamma_1(C_1 + C_2) - C_2]\rho_{00} = \gamma_2\rho_{00}. \\ \rho_{33} &= \frac{1}{3C_3}[\gamma_2(2C_1 + C_2) - 2C_2\gamma_1]\rho_{00} = \gamma_3\rho_{00}. \end{aligned}$$

$$\begin{aligned}\rho_{44} &= \frac{1}{4C_3} [\gamma_3(3C_1 + C_2) - 3C_2\gamma_2] \rho_{00} = \gamma_4\rho_{00}. \\ \rho_{55} &= \frac{1}{5C_3} [\gamma_4(4C_1 + C_2) - 4C_2\gamma_3] \rho_{00} = \gamma_5\rho_{00}.\end{aligned}$$

If we take into account that  $\text{Tr}[\rho] = 1$  and define  $\gamma_0 = 1$ , then trivially  $\rho_{kk} = \gamma_k / (\sum_k \gamma_k)$  in the equilibrium state. In fact, it can be shown by induction that in the general case  $\gamma_k = \left(\frac{\tilde{n}}{\tilde{n}+1}\right)^k$  and since  $\tilde{n}$  is the number of photons in thermal equilibrium, then they will be distributed according to bosonic statistics as  $\tilde{n} = 1/(e^{\beta\hbar\omega'_c} - 1)$ , so  $\gamma_k = e^{-k\beta\hbar\omega'_c}$  and  $\rho_{kk}(t)$  is asymptotically described by *Boltzmann's distribution*, **independently of the initial state**. Since one can find a solution for  $\frac{d\rho}{dt} = 0$  in many master equations, the initial state independence of the asymptotic behavior is very common in these systems. In fact, although this is not the case of the harmonic oscillator just studied, it has been proven that all systems evolving according to the Lindblad equation (2.8) are transformed under a *contractive mapping* [10]. If we make the exact calculations for this problem we will arrive to a set of values for the gamma coefficients we can compare with the numerical values obtained by programming to check the validity of the developed code. The results are more than satisfactory:

Exact value	Numerical value	Relative error
$\gamma_1 = 3/4$	$\gamma_1 = 0.75$	0%
$\gamma_2 = 9/16$	$\gamma_2 = 0.5625$	0%
$\gamma_3 = 27/64$	$\gamma_3 = 0.4218750$	0%
$\gamma_4 = 81/256$	$\gamma_4 = 0.31640625$	0%
$\gamma_5 = 81/320$	$\gamma_5 = 0.23730469$	6.25%

## 2.4 The two levels system.

Other interesting system we can study is the case of a two levels one interacting with the radiation field of its environment, which will be treated as a thermal bath. To derive the master equation describing this process, the same steps of the last example have to be followed, but now taking the hamiltonians:

$$H_s = \frac{1}{2}\hbar\omega_A\sigma_z, \quad H_e = \sum_{\vec{k},\lambda} \hbar\omega_{\vec{k}} r_{\vec{k}\lambda}^\dagger r_{\vec{k}\lambda},$$

$$H_{int} = \sum_{\vec{k},\lambda} \hbar(\kappa_{\vec{k},\lambda}^* r_{\vec{k}\lambda}^\dagger \sigma_- + \kappa_{\vec{k},\lambda} r_{\vec{k}\lambda} \sigma_+).$$

The entire derivation of the master equation from (2.19) can also be found in [11], so it's proved that the density operator evolves in time according to:

$$\frac{d\rho_s}{dt} = -i\frac{1}{2}\omega'_A [\sigma_z, \rho_s] + \frac{\gamma}{2}(\tilde{n}+1)(2\sigma_- \rho_s \sigma_+ - \sigma_+ \sigma_- \rho_s - \rho_s \sigma_+ \sigma_-) + \frac{\gamma}{2}\tilde{n}(2\sigma_+ \rho_s \sigma_- - \sigma_- \sigma_+ \rho_s - \rho_s \sigma_- \sigma_+),$$

where  $\omega'_A$  is related to the frequency of the system  $\omega_A$ ,  $\tilde{n}$  is the number of photons of the radiation environment and  $\gamma$  is a positive constant of the system. This equation, even when derived from

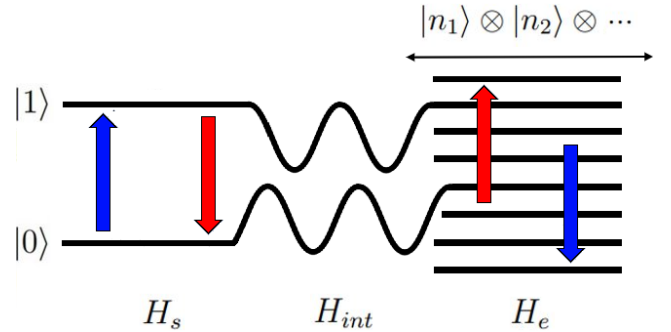


Figure 2.4: Scheme of the interaction between the two levels system and its harmonic oscillators environment. Both systems experiment different transitions represented by colored arrows.

(2.19), can be written in the form (2.8) as follows:

$$\frac{d\rho_s}{dt} = -i\frac{1}{2}\omega'_A [\sigma_z, \rho_s] + \gamma(\tilde{n}+1) \left( \sigma_- \rho_s \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_-, \rho_s \} \right) + \gamma\tilde{n} \left( \sigma_+ \rho_s \sigma_- - \frac{1}{2} \{ \sigma_- \sigma_+, \rho_s \} \right), \quad (2.23)$$

where the Lindblad jump operators are then  $\sigma_-$  and  $\sigma_+$ . This equation, in opposition of that of the harmonic oscillator, can be exactly solved since we are not dealing with an infinite dimensional Hilbert space. If the equation is projected onto the eigenbasis of  $\sigma_z$ , one gets:

$$\frac{d\rho_{00}}{dt} = \gamma(\tilde{n}+1)\rho_{11} - \gamma\tilde{n}\rho_{00}, \quad \frac{d\rho_{11}}{dt} = -\gamma(\tilde{n}+1)\rho_{11} + \gamma\tilde{n}\rho_{00}, \quad (2.24)$$

$$\frac{d\rho_{10}}{dt} = \rho_{10}(-i\omega'_A - \tilde{n}\gamma - \frac{\gamma}{2}), \quad \frac{d\rho_{01}}{dt} = \rho_{01}(i\omega'_A - \tilde{n}\gamma - \frac{\gamma}{2}). \quad (2.25)$$

By observing this equations, it can be noticed that the first parenthesis in (2.23), the one associated with the jump operator  $\sigma_-$ , is related to a decay from  $|1\rangle \rightarrow |0\rangle$ , which is not only stimulated by the photons of the bath but also spontaneous since for  $\tilde{n} = 0$  it still plays an important role. In the other hand, the second parenthesis describes stimulated transitions from  $|0\rangle \rightarrow |1\rangle$ . To solve the system of differential equations, one has to notice that equations (2.24) are related by the condition of the trace,  $\rho_{00} + \rho_{11} = 1$ , so once one of the diagonal elements is calculated, the other one will be given by this relation. In addition, as we know the density matrix is hermitian, once we know one of the coherences we will know the other by calculating its complex conjugate. Solution to (2.25) is trivial and we have, in terms of the initial condition:

$$\rho_{01}(t) = \rho_{10}(0)e^{-(\gamma(\tilde{n}+\frac{1}{2}))t}e^{i\omega'_A t} \quad \rho_{01}(t), = \rho_{10}(0)e^{-(\gamma(\tilde{n}+\frac{1}{2}))t}e^{-i\omega'_A t}. \quad (2.26)$$

Now, applying the Laplace transform method on (2.24) drives to the solutions:

$$\rho_{00}(t) = \frac{\tilde{n}+1}{2\tilde{n}+1} + \left( \rho_{00}(0) - \frac{\tilde{n}+1}{2\tilde{n}+1} \right) e^{-(1+2\tilde{n})\gamma t},$$

$$\rho_{11}(t) = \frac{\gamma\tilde{n}}{\gamma(2\tilde{n}+1)} + \left( \rho_{11}(0) - \frac{\gamma\tilde{n}}{\gamma(2\tilde{n}+1)} \right) e^{-(1+2\tilde{n})\gamma t}. \quad (2.27)$$

Since  $\gamma$  and  $\tilde{n}$  are positive, it is clear from (2.26) that coherences vanish with time, so decoherence is also reproduced by this model. In this case, it takes place in the chosen eigenbasis of  $\sigma_z$ , which means that the kets  $|0\rangle$ ,  $|1\rangle$  constitute the pointer basis of the interaction. It can also be noticed that the asymptotic values of populations, as we expected according to the discussion in 2.3, are independent of the initial condition of the problem. If we give numerical values to the problem, we can find a particular solution for  $\omega'_A = 10 \text{ rad/s}$ ,  $\gamma = 3 \text{ rad/s}$ ,  $\tilde{n} = 2$  and the initial condition:

$$\rho_0 = \begin{pmatrix} 2/3 & -1/2 \\ -1/2 & 1/3 \end{pmatrix}.$$

The results are represented in figure 2.5:

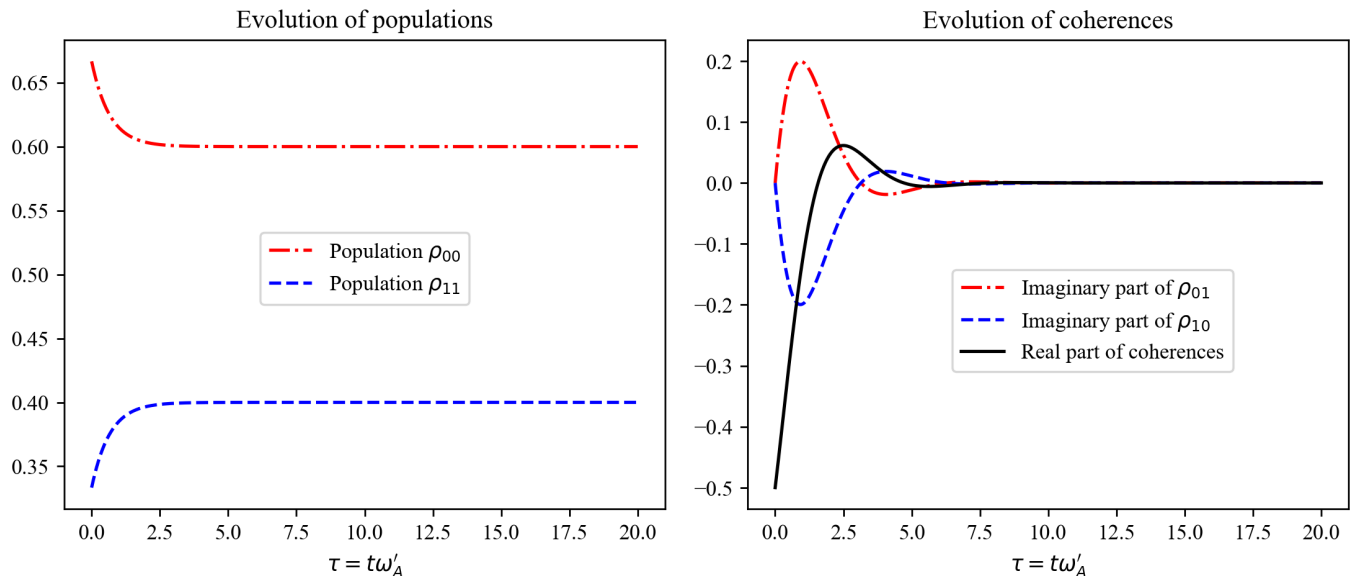


Figure 2.5: Temporal evolution of the two levels system state.

Similar to what happened in the harmonic oscillator example, decoherence is reached for a very late instant  $\tau \simeq 10$ , what is explained by the low value given to  $\gamma$ , which, as can be seen from the analytical solutions, is the decay rate of the system. This implies the decoherence time is of the order of  $t \simeq 1/\gamma$  so, again, a realistic interaction should be modelled by a greater value of said parameter. Both in this case and the one of the harmonic oscillator (figures 2.7, 2.5) the imaginary part of coherences is initially induced by the interaction, which is very typical of this interacting systems, nevertheless, as can be seen, this does not affect the final emergence of decoherence.

## 2.5 A discussion of the approximations. The Jaynes Cummings model.

Until now, we have solved some master equations which can be obtained under the Born and Markov approximations, nevertheless, it remains to be explained why such approximations allow us to describe those systems. The key to understand this question lays on two important parameters: The correlation time of the system ( $\tau_c$ ) and its characteristic evolution time ( $\Delta T$ ). The first one,  $\tau_c$ , can be defined as the time the composed system takes to loss the possible initial correlation of the interacting subsystems, that, as we have already said, will always be zero if those were not interacting before the initial time. If it is small enough in comparison to the time interval we are studying, the Born approximation will not be too coarse. The second one,  $\Delta T$ , is defined as the time it takes to the reduced density matrix  $\rho_s$  appearing in (2.19) to experiment a notorious change that would modify the corresponding integral value. Of course, if the time interval in which we are studying such evolution is much smaller than  $\Delta T$ , the Markov approximation will be justified. It has been shown [12] that this two time scales have orders of magnitude related by:

$$\Delta T \simeq \frac{\hbar^2}{\tau_c (H_{int})^2},$$

so the calculation of one of them will give us the order of magnitude of the other. In fact, the evaluation of  $\tau_c$  can be done calculating the value of  $\tau$  which would convert equations (2.17) and

(2.18) into Dirac deltas, what would drive to a Markovian equation without necessarily imposing  $\tilde{\rho}_s(\tau) \simeq \tilde{\rho}_s(t)$  previously (this fact reveals that Markovianity is also related to the neglecting of short time correlations between the interacting subsystems, which is the reason why sometimes Born approximation is also called Born-Markov approximation). In [11], it has been shown that for the system treated in 2.3, this approximation allows an estimation of the correlation time given by  $\tau_c \simeq \hbar/k_B T$  (where  $T$  stands for temperature). Therefore  $\Delta T \simeq \hbar k_B T / \langle H_{int} \rangle^2$ . Now, if we estimate  $\langle H_{int} \rangle \simeq \hbar \sqrt{\tilde{n}} \kappa$ , we will get, for the numerical resolution that has been carried:  $T \simeq 10^{11} s$ , so the condition  $\tau_c \ll \Delta t \ll T$  is fulfilled (here  $\Delta t$  is the length of the interval in which we have studied the evolution of the system, in our case, of the order of seconds).

Even when this estimation seems to be imprecise, the truth is that there does not exist any other way to check the validity of the approximations. Indeed, even for the most simple cases of subsystems that interact with their environments, a numerical solution of the exact dynamics of the composed system cannot be achieved to be compared with the solution of the master equation in which the approximations have been considered. This is due to the fact that if one tried to solve the Von Neumann equation (1.8) and, by applying the trace over the environment states, obtain the density operator  $\rho_s$ , the basis of the Hilbert space of the composed system would be so large that no numerical calculation would be feasible (Master equations, beyond being a way to obtain an analytical expression for  $\rho_s$  evolution, are precisely a way to solve this computational problem). To show this, a simplified version of the problem treated in 2.4 has been considered. In particular, a two levels system has been supposed to be interacting with a set of harmonic oscillators according to the **Jaynes-Cummings model**. The last one is a simplified mathematical model that was originally developed to describe the interaction between a two levels atom and the electromagnetic field. In particular, if one imposes some considerations just like the rotating-wave approximation, it can be shown that such interaction is defined by the hamiltonians:

$$H_s = \frac{1}{2} \hbar \omega_A \sigma_z, \quad H_e = \hbar \omega_c a^\dagger a, \quad H_{int} = \hbar \Omega (a \sigma_+ + a^\dagger \sigma_-).$$

If we wanted to use this model to verify the validity of the approximations made in 2.4, an environment of  $N \gg 1$  harmonic oscillators should be simulated, so we would have to take:

$$H_s = \frac{1}{2} \hbar \omega_A \sigma_z, \quad H_e = \sum_{j=1}^N \hbar \omega_c^{(j)} a_j^\dagger a_j, \quad H_{int} = \sum_{j=1}^N \hbar \Omega_j (a_j \sigma_+ + a_j^\dagger \sigma_-).$$

Since the Hilbert space basis of the composed system is equal to the set:

$$\{|+, n_1, n_2, \dots, n_N\rangle, |-, n_1, n_2, \dots, n_N\rangle\}_{n_1, n_2, \dots, n_N},$$

then it is easy to see that if  $n_1, n_2, \dots, n_N \leq s$ , then the dimension of the Hilbert space is  $d \simeq 2(s+1)^N$ . The problem for  $N = 1$  has been numerically solved to get an approximation of the upper limit  $s$ . It has been considered that  $\omega_A = 2 rad/s$ ,  $\omega_c = 3 rad/s$ ,  $\Omega = 4 rad/s$ , and the initial condition is:

$$\rho_0 = \begin{pmatrix} 1/9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 5/9 & i/3 \\ 0 & 0 & -i/3 & 1/3 \end{pmatrix}.$$

The obtained solutions are represented below:

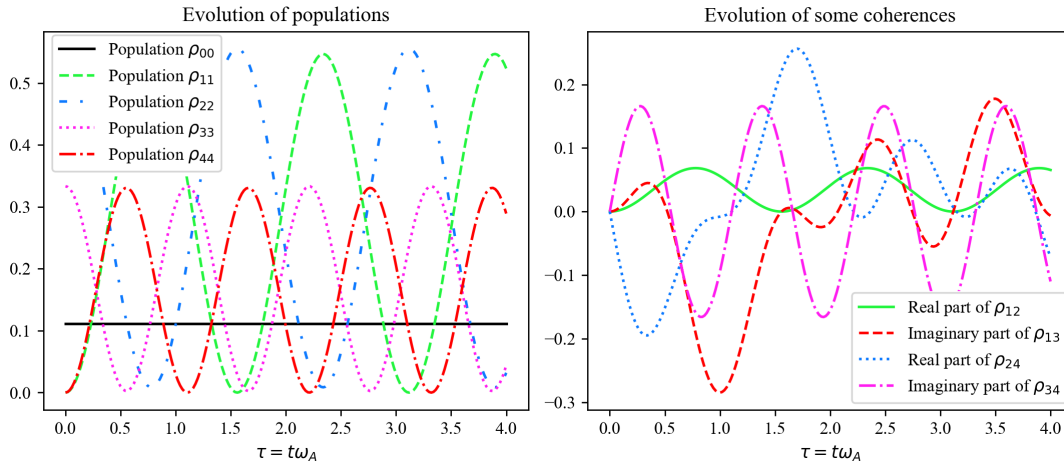


Figure 2.6: Time evolution of the composed system state

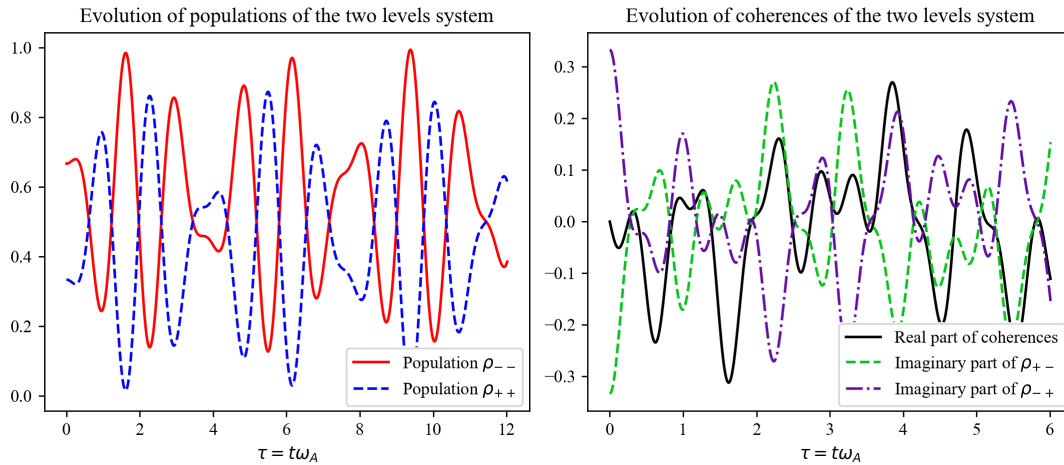


Figure 2.7: Time evolution of the two levels atom state

This set of solutions show many interesting behaviours we had not seen before. The populations of the composed system appearing in figure 2.6 don't go to an equilibrium state but periodically oscillate forever and no new populations are generated, but initially null coherences start growing and oscillating. This kind of behaviour is a consequence of the unitary character of Von Neumann equation, which is also related to some problems concerning entropy conservation [13]. In the other hand, once the trace over environment states has been calculated, the populations and coherences of the two levels system do not reach an equilibrium state, which proves the obvious fact that including just one harmonic oscillator is not enough to simulate an environment (condition  $N \gg 1$  must be satisfied). To calculate this results, 12 dimension matrices were used, which, according to how the basis has been ordered, implies that  $s = 5$ . If we consider a bigger amount of harmonic oscillators, for example  $N = 50$ , what is still very low, and consider that  $s \simeq 5$ , then the dimensions of the matrices would blow up to  $d \simeq 10^{39}$ , which is obviously not computable.

## 2.6 Determination of the pointer basis.

So far, we have seen how the Redfield equation can be used to describe the interaction between some microscopic systems and their environments under the Born-Markov approximation, reducing the corresponding equations to a Lindblad form in some circumstances. According to the previous section, these approximations are in fact the only way to deal with this type of problems, which can be solved analytically, at least, when the corresponding Hilbert spaces have finite dimension. The latter is of great relevance as far as the determination of the aforementioned pointer basis is concerned. Indeed, if the analytical solution of a master equation is found, the determination of the pointer basis of the system, i.e., the set of its possible states after interaction, can be computed by simply diagonalizing the corresponding result  $\rho_s(t)$ , which will be constant for large times. But what happens when there's no analytical solution?

Many authors have worked to give an answer to this question, obtaining some interesting results for specific mathematical models. According to [14], for the cases in which the subsystem hamiltonian  $H_s$  is neglected or co-diagonal with the interaction one  $H_{int}$ , it has been shown that the pointer basis will emerge as the eigenbasis of what's called as *the pointer observable*,  $\Lambda$ , such that:

$$[H_s + H_{int}, \Lambda] = 0.$$

In the other hand, as it is pointed out in [15], some models involving harmonic oscillators have shown the pointer basis to be constituted by *coherent states*. For weak interactions, the eigenstates of  $H_s$  have also shown to be the ones which constitute the pointer basis, but there's not a final answer yet, so much so that it's not even completely clear how the pointer basis depends on the initial state  $\rho_s(0)$  of the problem.

A very interesting case which illustrates how surprising can the calculation of the pointer basis be, is the interaction between a moving particle and a harmonic oscillators environment, described by a *Caldeira-Leggett hamiltonian* which has the form:

$$H = \frac{p^2}{2m} + \sum_{j=1}^N \frac{P_j^2}{2M_j} + \frac{M_j^2 \Omega_j^2}{2} \left( X_j - \frac{S_j x}{M_j \Omega_j^2} \right)^2. \quad (2.28)$$

It has been shown in [16] that the corresponding master equation results in the pointer basis being that of linear momenta. This is kinda suprising since the interaction term couples the environmental freedom degrees with the position of the moving particle and, in many situations, the coupling observables are precisely the pointer ones (see 3.4).

The problem of determining the pointer basis not only depends on the kind of master equation one is trying to solve, but it's also related to the specific problem and even to the corresponding initial condition. This makes it a very hard problem that, as we have exposed, has only been solved for reduced cases and concrete conditions. Nevertheless, it is important to highlight that a general solution of this problem would be very interesting in order to achieve a better understanding of the measurement problem. Indeed, if given a master equation and an initial condition one was able to predict the pointer basis, it would be very easy to check if a mathematical model to describe a measurement would diagonalize or not into the orthonormal eigensatetes of the measured quantity.

# Chapter 3

## The measuring process.

Until now, the general formalism of master equations has been exposed and discussed, allowing us to show that when a system interacts with a macroscopic environment, decoherence emerges. This decoherence, which converts the quantum superposition of states into a classically interpretable statistical mixture of the same, allows us to understand the frontier between classic and quantum worlds, but it has just been applied to some particular systems in which measurement has not been modelled. Throughout this chapter we will therefore focus on the mathematical description of the measurement processes in quantum mechanics, looking at how they relate to decoherence and the measurement problem. The formalism of POVM's has been exposed and applied to find a master equation describing a measurement over a two levels system, which is generalized to find a master equation describing any measurement over an observable. The same equation is derived independently of the measure postulates from a physical approach and its main properties are discussed.

*Hasta ahora se ha expuesto y discutido el formalismo general de las ecuaciones maestras, que nos ha permitido demostrar cómo la decoherencia emerge de forma natural en un sistema cuando este interactúa con su entorno macroscópico. Esta decoherencia, que convierte la superposición cuántica de estados en una mezcla estadística clásicamente interpretable de los mismos, nos permite entender la frontera entre los mundos clásico y cuántico, pero sólo se ha aplicado a algunos sistemas particulares en los que no se ha modelizado ninguna medida. Por este motivo, a lo largo de este capítulo nos centraremos en la descripción matemática de los procesos de medición en la mecánica cuántica, viendo cómo se relacionan con la decoherencia y el problema de la medida. El formalismo de los POVM se ha expuesto y aplicado para encontrar una ecuación maestra que describa una medida sobre un sistema de dos niveles, que se generaliza para encontrar una ecuación maestra que describa cualquier medición sobre un observable. La misma ecuación se deriva independientemente de los postulados de medida desde un enfoque físico y se discuten sus principales propiedades.*

### 3.1 Positive operator-valued measurement.

According to the fifth postulate of quantum mechanics, once a measurement is done, the state of the system collapses under a transformation of the form (1.9). This corresponds to an ideal measurement, usually called in literature as *Von Neumann measurement*, in which all the possible information of an observable is obtained. The truth is, however, that in many practical cases this is not what happens and a mathematical model to describe some kind of imperfect measurements has



to be applied. A very extended way to generalize equation (1.9) to more complex measurements is by considering the transformation:

$$\rho'_i = \frac{\hat{A}_i \rho \hat{A}_i^\dagger}{\text{Tr}[\hat{A}_i \rho \hat{A}_i^\dagger]}, \quad (3.1)$$

where  $\hat{A}_i$  is an operator which accounts for a certain measurement. It is trivial to see that (1.9) can be deduced as a particular case of this equation when  $\hat{A}_i$  is a projector operator, but does (3.1) match the form of a CPT map, according to Choi-Kraus theorem? It is in this context that the **positive operator-valued measurement** (POVM) appears. In mathematical terms, a POVM is defined as a set of **hermitian** and **positive-defined** operators  $\{\hat{\pi}_m\}$  such that the completeness relation  $\sum_m \hat{\pi}_m = \mathbb{1}$  is satisfied. Since any positive-defined hermitian matrix admits a decomposition of square matrices as  $\hat{\pi}_m = \hat{A}_m^\dagger \hat{A}_m$ , we can impose the operators in (3.1) to factorize a POVM this way, so  $\sum_i \hat{A}_i^\dagger \hat{A}_i = \mathbb{1}$  and the conditions of Choi-Kraus theorem would be satisfied. This ensures that (3.1) is a valid equation to model a generalized measurement, but it's not all. As in (1.10), (1.9), the denominator of (3.1) can be interpreted as the probability of obtaining the outcome associated to the index  $i$ , so it turns out that, by applying the cyclic property of trace:

$$P(i) = \text{Tr}[\hat{A}_i \rho \hat{A}_i^\dagger] = \text{Tr}[\hat{A}_i^\dagger \hat{A}_i \rho] = \text{Tr}[\hat{\pi}_i \rho], \quad (3.2)$$

so  $\hat{\pi}_i$  is indeed a relevant operator for the calculation of probabilities. This can be applied for the general case in which the outcome of the measurement is not known and an average over all the POVM elements has to be carried, so (3.1) is transformed into:

$$\rho' = \sum_i P(i) \frac{\hat{A}_i \rho \hat{A}_i^\dagger}{\text{Tr}[\hat{A}_i \rho \hat{A}_i^\dagger]} = \sum_i \hat{A}_i \rho \hat{A}_i^\dagger, \quad (3.3)$$

which, of course, still defines a CPT map. The formalism of POVM is thus a very intuitive generalization of the measurement postulates that will allow us to make some interesting calculations.

## 3.2 Measurement master equations.

The formalism of POVM can be used to deduce the form of a master equation modelling a measurement process. In particular, we can consider a very simple model to find this kind of equation through the concept of *continuous measurement*. In general, a continuous measurement can be defined as any measurement that takes place in a finite period of time, so the mathematical modelling of the process can be very different from one source to another. According to [17], this can be defined by a set of random instantaneous measurements which are taken over the system with an average rate we can call  $R$ , so the probability of a measurement taking place in a time interval  $\Delta t$  can be calculated as  $P = R\Delta t$  (Obviously, this is only valid if  $\Delta t \simeq 0$  so that  $0 \leq P \leq 1$ , so the following reasoning is based in such consideration). According to the previous section, a density matrix  $\rho(t)$  will be, after a time interval  $\Delta t$ , the one predicted by (3.3) with probability  $R\Delta t$ , while, in the opposite case, it will evolve according to (1.9). In mathematical terms:

$$\rho(t + \Delta t) = \sum_i \hat{A}_i \rho(t) \hat{A}_i^\dagger, \quad \text{with probability } P = R\Delta t.$$

$$\rho(t + \Delta t) = \rho(t) - \frac{i}{\hbar} [H, \rho(t)] \Delta t, \quad \text{with probability } P = 1 - R\Delta t.$$

It is interesting to highlight that the second equation constitutes a Markovian form since the path of evolution of  $\rho(t)$  has been removed and the final state only depends on the preceding instant. Averaging both results and applying the definition of the derivative of an operator, it is easy to arrive to the equation presented in [17]:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] + R \left[ \sum_i \hat{A}_i \rho \hat{A}_i^\dagger - \rho \right]. \quad (3.4)$$

It can be shown that, since Kraus operators  $\hat{A}_i$  satisfy the completeness relation, equation (3.4) is a Lindblad-like one in which Kraus operators are the Lindblad jump operators of the system. Since we are not worrying about the interaction between the system and the measuring environment but only applying the POVM model, the dissipative term in the right hand side of the equation is not related, in principle, to any physical observable of the system. A first step to find that relation can be made by considering the particular case of a two levels system exposed in [17], where it is assumed one is dealing with a POVM constituted by the generalized measurement operators:

$$\hat{\pi}_0 = p |+\rangle \langle +| + (1-p) |-\rangle \langle -|, \quad \hat{\pi}_1 = p |-\rangle \langle -| + (1-p) |+\rangle \langle +|, \quad (3.5)$$

where  $0 < p < 1/2$  is a parameter which models the imprecision degree of the measurement, so if it was null, a Von Neumann measurement would be reproduced, and, if it was equal to one half, no information would be obtained of such measurement. As the factorization of the elements of a POVM in Kraus operators is not unique, we can take:

$$\hat{A}_0 = \hat{A}_0^\dagger = \sqrt{p} |+\rangle \langle +| + \sqrt{(1-p)} |-\rangle \langle -|, \quad \hat{A}_1 = \hat{A}_1^\dagger = \sqrt{p} |-\rangle \langle -| + \sqrt{(1-p)} |+\rangle \langle +|. \quad (3.6)$$

For simplicity, we can take the hamiltonian of the measured system to be  $H = \frac{\hbar}{2} \Omega \sigma_z$  and we can then consider we are measuring the value of the observable  $\sigma_x$ , so  $|-\rangle, |+\rangle$  would be its eigenvectors. By applying some algebra it can be shown that equation (3.4) yields:

$$\frac{d\rho}{dt} = -\frac{i\Omega}{2} [\sigma_z, \rho] - \frac{\gamma}{2} [\sigma_x, [\sigma_x, \rho]], \quad (3.7)$$

with  $\gamma = \frac{R}{2} (\sqrt{p} - \sqrt{1-p})^2 > 0$ , the characteristic decay rate of the system. This equation, contrary to (3.4), is written in terms of quantum observables of the system, but the connection between the equations is not clear in principle. Nevertheless, there's a very interesting thing to notice here, in particular, equation (3.7) has the form of a Lindblad equation with just one hermitian jump operator. In fact, if one imposes  $L_k = L_k^\dagger$  in (2.8) and considers just one term into the summation, the resulting equation is:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] - \frac{\Gamma}{2} [L, [L, \rho]], \quad (3.8)$$

where the factor  $\hbar$  has been introduced. The similarity of (3.7) and (3.8) is now obvious. Furthermore, the POVM that carried us to equation (3.7) models a measurement over  $\sigma_x$ , which is precisely the operator that appeared in the dissipative term of (3.7), and since (3.8) is just a particular case of the Lindblad equation for hermitian operator, it seems like, somehow, choosing the jump operators in Lindblad equation to be physical observables of the system would derive into an equation describing the monitoring of the system via continuous measurements over such observables. Such idea has led equation (3.8) to become one of the master equations for describing

continuous measurements par excellence, what has been reinforced by other examinations, like the one concerning stochastic processes that can be found in [18]. For now, let's assume this intuition and discuss some interesting properties of the equation.

### 3.3 Measurement master equations properties.

#### Measurement heating effects.

The fact that (3.8) is much simpler than Lindblad equation will allow us to find a mathematical equation to describe the variation of energy in the measured system. Let's consider a time independent hamiltonian, such that:

$$\langle H \rangle = Tr [H\rho] \implies \frac{d\langle H \rangle}{dt} = Tr \left[ H \frac{d\rho}{dt} \right].$$

If we now consider a measurement of  $L$  over the system and we assume equation (3.8) to model it, we can write, as it is done in [19]:

$$\frac{d\langle H \rangle}{dt} = -\frac{i}{\hbar} Tr [H[H, \rho]] - \frac{\Gamma}{2} Tr [H [L, [L, \rho]]], \quad (3.9)$$

and, since  $Tr[A[B, C]] = Tr[[A, B], C]$ , the last equation is reduced to:

$$\frac{d\langle H \rangle}{dt} = -\frac{\Gamma}{2} Tr [[H, L][L, \rho]]. \quad (3.10)$$

If equation (3.8) truly describes a measurement over a system, the last equation gives the exact value of power that the measurement develops over it. The equation implies that, in general, when the measured quantity does not commute with the hamiltonian of the system, an energy variation is produced, what is due to the fact that the measured system is not isolated. We can now consider the particular case of a measurement of the  $x$  position of a free particle by imposing  $H = \frac{P^2}{2m}$  and  $L = X$ , what gives, since  $[X, P] = i\hbar$ :

$$\frac{d\langle H \rangle}{dt} = \frac{\hbar^2}{2m} \Gamma. \quad (3.11)$$

This equation shows that when the measurement is done, the energy of the particle is increased at a constant rate in time, which is kinda interesting since this result is totally independent of the measuring device one applies to make the measurement. Nevertheless, this can be understood in terms of Heisenberg's uncertainty principle since a measurement over the position of a particle will be directly related to a decrease in the value of  $\Delta x$ , so  $\Delta p$  and, therefore, the mean value of its energy, will increase. In a very similar way, it can be shown for equation (3.7) that heating effects are given by:

$$\frac{d\langle H \rangle}{dt} = 4\Omega\gamma\hbar\Re_e\{\rho_{+-}(t)\}, \quad (3.12)$$

and since equation (3.7) has been analytically solved for a general initial condition (see appendix 3.5), the explicit form of (3.12) can be given as follows:

$$\frac{d\langle H \rangle}{dt} = 4\Omega\gamma\hbar e^{-2\gamma t} \Re_e\{\rho_{+-}(0)\}, \quad (3.13)$$

so we see that, in this case, the system is losing or gaining energy depending, exclusively, on the sign of the real part of coherences at initial time, effect that vanishes in a time  $t \simeq \frac{1}{\gamma}$ .

### Weak and strong measurements

Another interesting fact that yields from the analytical solution of (3.7) is that we can distinguish three different situations which will allow us to talk about different kind of measurements. As we have anticipated, when  $p = 0$ , we will have a perfect Von Neumann measurement, so we would expect decoherence to happen faster in processes of lower values of  $p$ . In the other hand, for  $p = 1/2$  it is trivial to see that  $\gamma = 0$  and hence the evolution of the system is unitary, so no decoherence effects appear. This would intuitively carry us to think that two regimes of weak and strong measurement would result from solving (3.7) depending on how close or far away we are from these values, nevertheless this differential equations system has three possible solutions depending on the relation between  $\gamma$  and  $\Omega$ , showing some very interesting behaviours that go against the above intuition. To see how this happens, the solution has been represented for the particular case of  $\Omega = 10 \text{ rad/s}$ ,  $R = 50 \text{ rad/s}$  and initial condition:

$$\rho_0 = \begin{pmatrix} 2/3 & -1/2 \\ -1/2 & 1/3 \end{pmatrix}.$$

The values of  $\Omega$  and  $R$  have been selected so that the three regimes are visible. The results are the following:

1.  $\gamma > \Omega$  (**Strong measurement regime**): The situation of strong measurement is the one in which the measurement is closer to a Von Neumann one. Mathematically, this corresponds to the situation in which  $\gamma > \Omega$ , this is, the dissipative term in (3.7) dominates over the unitary one. For the values we have given to the problem, this situation is achieved for  $0 \leq p < 0.1$ . Particularizing for  $p = 0$ , one obtains the following result:

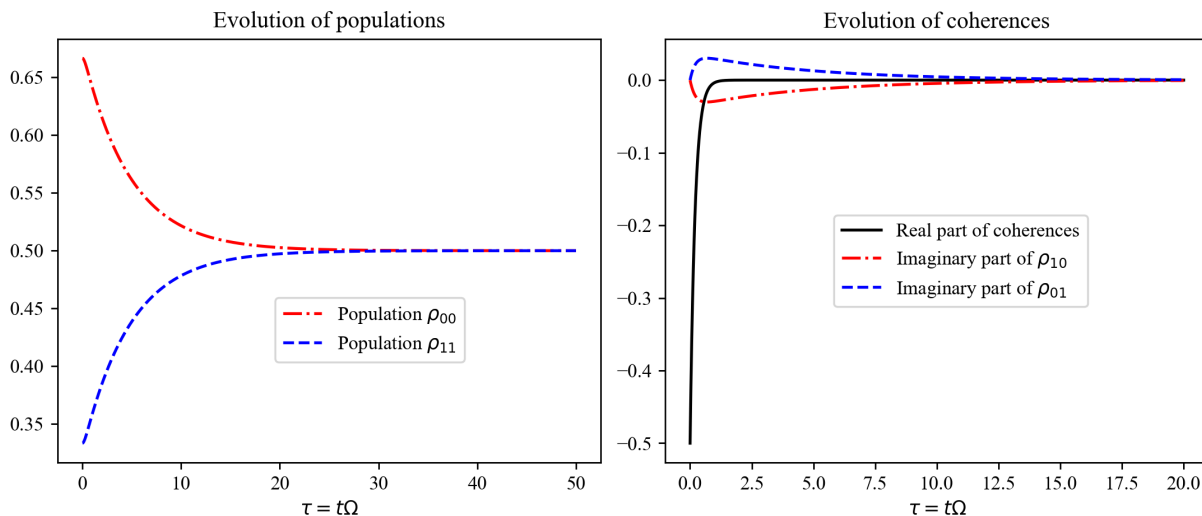


Figure 3.1: Evolution of the state of the system for a perfect measurement

The profile of these curves is trigonometric-hyperbolic in nature, faded by a decreasing exponential function. As it can be seen, decoherence has been completed as expected for times such that  $\tau \simeq 20$ , which is due to the fact that we have not chosen realistic values for the

parameters of the problem by numerical reasons.

2.  $\gamma = \Omega$  (**Resonant situation**): This situation has been called as the resonant one since a very shocking result emerges from it. The situation is only obtained for the value  $p = 0.1$ , so equation (3.7) yields the solutions of figure 3.2. The profile of these curves is linear in nature, faded by a decreasing exponential function. As it can be seen, the profile of coherences is much more bulged in this regime, but decoherence has been completed for  $\tau \simeq 10$  and populations have reached the equilibrium state in the half of the time it took in the strong measurement regime, which is a very outstanding fact since we are modelling a more imperfect measure. In a mathematical sense, the fact that the interaction parameter  $\gamma$  is smaller allows the system's own oscillations to develop more freely, but these tend, initially, to reduce the populations. This, when properly coordinated with the decay effect, produces this surprising effect whereby an imperfect measurement can bring the system more quickly to equilibrium.

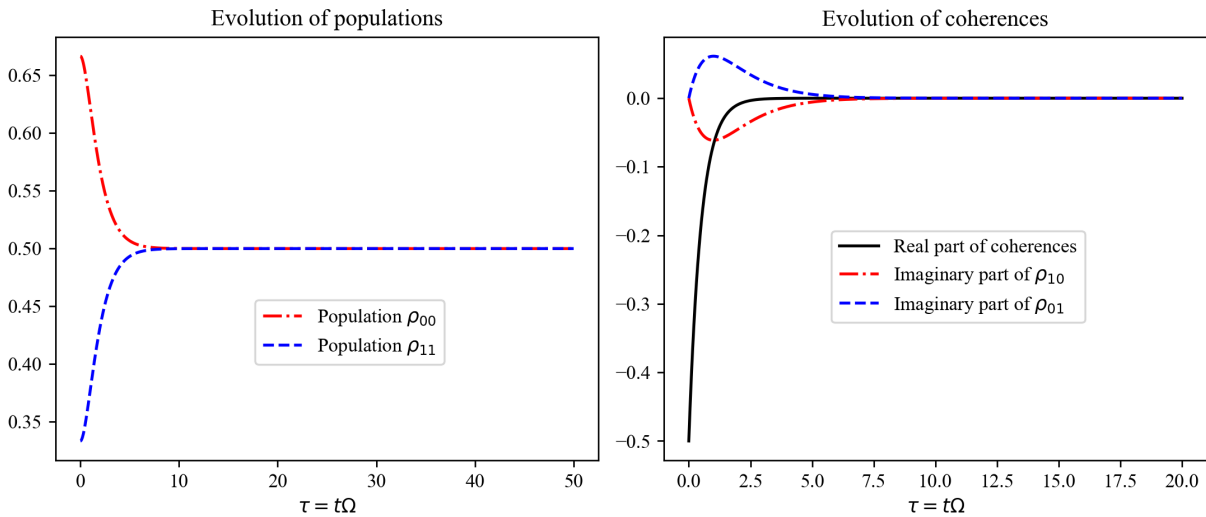


Figure 3.2: Evolution of the state of the system in the resonant situation.

3.  $\gamma < \Omega$  (**Weak measurement regime**): The weak measurement regime is the most similar one to a Von Neumann unitary evolution. For the particular case we are studying, this is obtained for  $0.1 < p \leq 0.5$ , so if we take  $p = 0.3$ , the equation yields the solutions of figure 3.3. The profile of these curves is trigonometric in nature, again, faded by a decreasing exponential function. Both decoherence and equilibrium state are now reached for larger times. Indeed, if one takes  $p$  very close to  $1/2$ , decoherence time can become arbitrary large, being infinity for  $p = 1/2$ . As it can be seen, the oscillations of the system tend, initially, to decrease populations, as it was highlighted for the discussion of the resonant case.

It is also interesting to highlight that, as anticipated, Lindblad form master equations are contractive mappings, so it is not surprising that the asymptotic behaviour in all three regimes is the same regardless of the initial state of the system. In particular, the master equation (3.7) leads the system to an equiprobable statistical mixture of the eigenstates of  $\sigma_x$ .

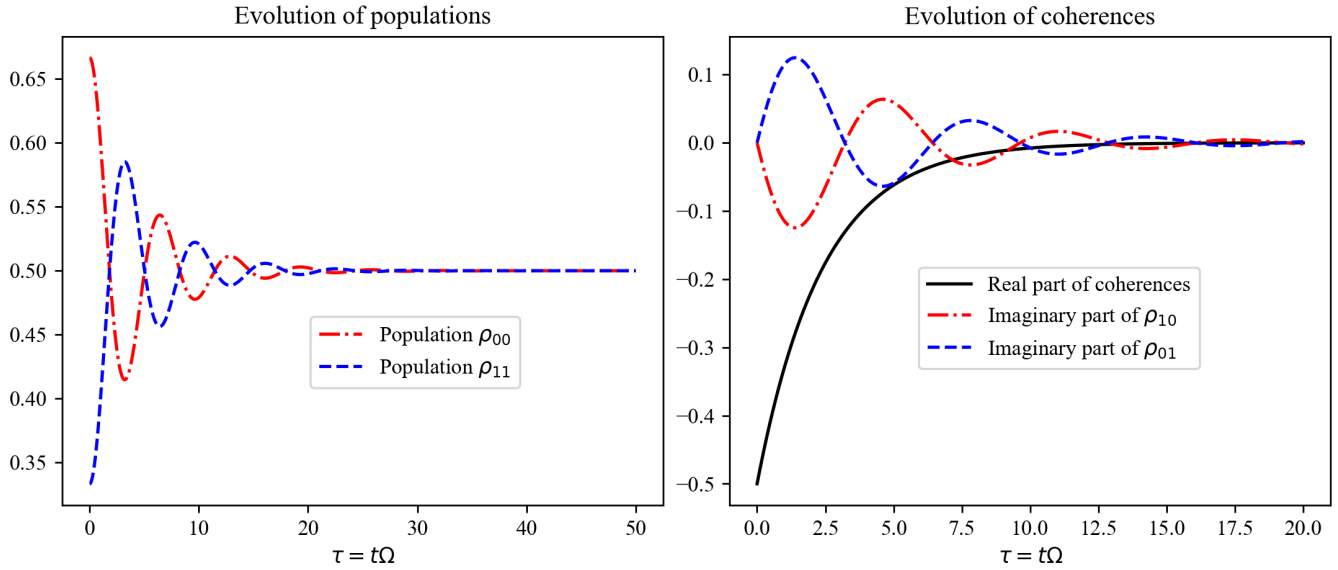


Figure 3.3: Evolution of the state of the system for a weak measurement modeled by  $p = 0.3$ .

For the sake of completeness, the problem has been solved for a whole set of values of the parameter  $p$  and, in each case, the time taken for the populations to reach the equilibrium state as well as the decoherence time have been calculated applying the criterion that the difference between the population/coherence value and its asymptotic one has to be less than  $10^{-6}$ . The results are shown in figure 3.4. For  $p > 0.35$ , time starts to increase and goes to infinity for  $p = 0.5$ , but this has not been computed for numerical reasons. As it can be seen, even for the weak measurement situation ( $0.1 < p \leq 0.5$ ) there are many values of  $p$  for which decoherence and equilibrium times are lower than for the perfect measurement situation  $p = 0$ . This is a very strange result that, as we highlighted in the previous discussion, can be intuitively understood as if the environment took advantage of the strongest oscillations of the system to bring it to decoherence faster, nevertheless, a more rigorous discussion can be made if we look at the analytical solution to the master equation (see 3.5). More specifically, it can be seen that if  $\rho_{00}(0) = 1/2$  and  $\mathcal{I}_m\{\rho_{01}\} = 0$ , populations will remain constant and coherences will decay, following a very typical behaviour. Nevertheless, in any other circumstance it can be seen that the terms that take the longest to decay, both in the expression of the coherences and in that of the populations, go as  $e^{-\gamma t}$  for  $\gamma < \Omega$  (weak measurement) and as  $e^{-(\gamma - \sqrt{\gamma^2 - \Omega^2})t}$  for  $\gamma > \Omega$  (strong measurement). This implies that, indeed, the decay rate can be bigger in the situation of weak measurements than in the strong measurements one.

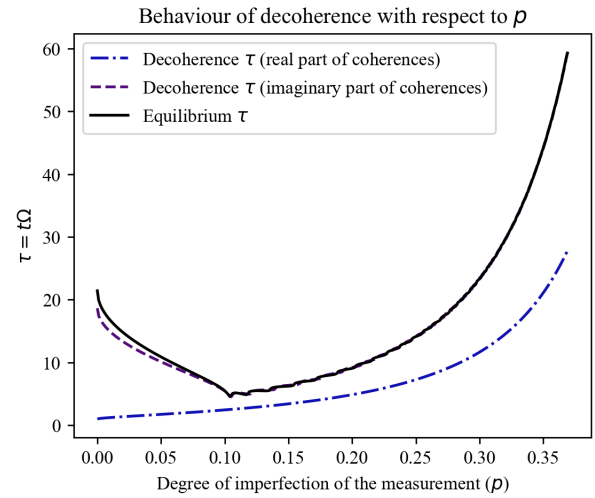


Figure 3.4: Representation of  $\tau$  values of decoherence and equilibrium with respect to  $p$ .

To understand this a little better, let's consider the values  $\gamma_1 < \Omega$  and  $\gamma_2 > \Omega$  and force the condition  $\gamma_1 > \gamma_2 - \sqrt{\gamma_2^2 - \Omega^2}$ . By doing so, one can finally conclude that this condition will be satisfied if:

$$\gamma_1 \in \left( \gamma_2 - \sqrt{\gamma_2^2 - \Omega^2}, \gamma_2 + \sqrt{\gamma_2^2 - \Omega^2} \right),$$

and since  $\gamma_1 < \gamma_2$ :

$$\gamma_1 \in \left( \gamma_2 - \sqrt{\gamma_2^2 - \Omega^2}, \gamma_2 \right).$$

For the particular case we have solved,  $\Omega = 10 \text{rad/s}$ ,  $\gamma_1 \in (0, 10)$  and  $\gamma_2 \in (10, 25)$ , so we can make a graphic representation of the values  $\gamma_1$ ,  $\gamma_2$  and identify the region of values for which this condition of anomaly is fulfilled, what has been done in figure 3.5. This representation shows that, indeed, for most of the pairs  $(\gamma_1, \gamma_2)$  the decay rate in the weak measurement region is higher than in the strong measurement one, what explains the fact that decoherence and equilibrium values of  $\tau$  can be lower for weak measurements. Nevertheless, this does not explain why those values show a decreasing behaviour in the strong measurement regime, but this is an immediate consequence of the behaviour of the decay rate  $\gamma - \sqrt{\gamma^2 - \Omega^2}$ . If we derive this expression with respect to  $\gamma$ , we obtain the result  $1 - \frac{\gamma}{\sqrt{\gamma^2 - \Omega^2}}$ , but since  $\gamma > \Omega > 0$ , this quantity is trivially negative and, therefore, **the decay rate decreases in the strong measurement regime when  $\gamma$  increases, or, equivalently, when  $p$  decreases.**

### The pointer basis in a measurement.

As it has been highlighted many times along this work, a master equation modelling a measurement should result in a decoherence process in the eigenbasis of the measured observable. If one takes equation (3.8) and projects it on the eigenbasis of the observable  $L$  for a situation in which a discrete spectrum hamiltonian is considered, the resulting equations are written:

$$\frac{d\rho_{ij}}{dt} = -\frac{\Gamma}{2}(l_i - l_j)^2 \rho_{ij} + \sum_k C_{ik} \rho_{kj} - \sum_k \rho_{ik} C_{kj}, \quad (3.14)$$

where  $l_i$  represents the eigenvalue of  $L$  associated to the eigenstate  $|l_i\rangle$  and  $C_{ik} = -\frac{i}{\hbar} \sum_\alpha E_\alpha \lambda_\alpha^{(k)} \lambda_\alpha^{(i)*}$ , being  $E_\alpha$  the eigenvalue of the hamiltonian associated to its eigenstate  $|E_\alpha\rangle$  and being the lambda coefficients defined by  $|l_k\rangle = \sum_\alpha \lambda_\alpha^{(k)} |E_\alpha\rangle$ . It is now trivial to see that the term associated to  $\Gamma$  is a dissipative one, which, when  $i \neq j$ , produces a decay we can identify with decoherence. In fact, if one divides both sides of (3.14) by  $\rho_{ij}$  and integrates, it will be shown that:

$$\rho_{ij} \propto e^{-\frac{\Gamma}{2}(l_i - l_j)^2 t} e^{\sum_k C_{ik} \int \frac{\rho_{kj}}{\rho_{ij}} dt - C_{kj} \int \frac{\rho_{ik}}{\rho_{ij}} dt}, \quad (3.15)$$

as  $\Gamma > 0$ , the first exponential tends to decrease the value of matrix elements when  $i \neq j$ , effect that disappears for diagonal terms, when the following equation holds:

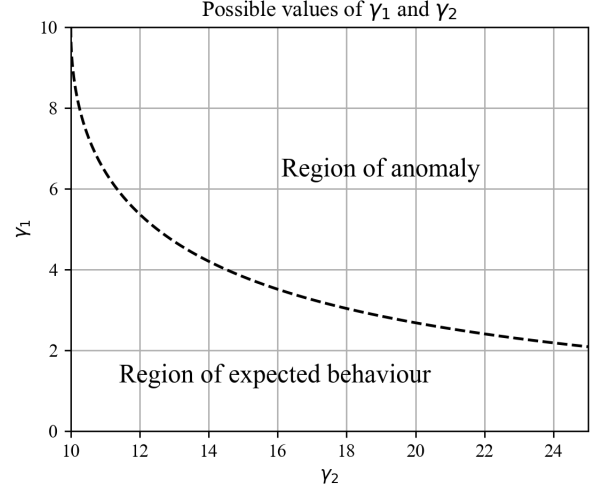


Figure 3.5: Possible values of the decay parameters  $\gamma_1$  and  $\gamma_2$ .

$$\rho_{ii}(t) \propto e^{2\text{Re}\{\sum_k C_{ik} \int \frac{\rho_{ki}}{\rho_{ii}} dt\}}. \quad (3.16)$$

Nevertheless, the fact that decoherence finally takes place will also depend on the value of the second exponential in (3.15), so it could happen that for certain hamiltonians and values of  $\Gamma$ , decoherence didn't take place. This, of course, wouldn't be consistent for real measurements with the Von Neumann's irreversible reduction process, nevertheless, it is precisely by this reason that we can intuit that real measurements will always be modelled by high values of  $\Gamma$ , such that the first exponential in (3.15) will *win the battle* to the second one. It has also been studied how to be able to discern if decoherence will or not emerge from equation (3.8), in fact, as this is a linear equation, the solution  $\rho(t) = Ve^{\lambda t}$  can be tested, what drives to the characteristic equation:

$$\det \left( \frac{i}{\hbar} [H, V] + \frac{\Gamma}{2} [L, [L, V]] + \lambda V \right) = 0. \quad (3.17)$$

Once this equation is solved for  $\lambda$ , the ‘‘eigenmatrices’’  $V$  will be potentially calculated, so the final solution could be expressed as:

$$\rho(t) = \sum_j c_j V_j e^{\lambda_j t}, \quad (3.18)$$

so, even when this family of functions should not necessarily be the general solution to the problem, the truth is that by the *solution structure theorem* we know that the asymptotic behaviour of the general solution would be governed by this exponentials, so decoherence should be identified in this particular solution. However, particularizing (3.17) for the simplest case of a two levels system yields the following fourth degree equation:

$$\lambda^4 + (\Gamma(l_1 - l_2)^2) \lambda^3 + \left( \frac{\Gamma^2(l_1 - l_2)^4}{4} + [(H_{11} - H_{22})^2 + 4|H_{12}|^2] \frac{1}{\hbar^2} \right) \lambda^2 + \left( \frac{2\Gamma(l_1 - l_2)^2 |H_{12}|^2}{\hbar^2} \right) \lambda = 0, \quad (3.19)$$

where  $H_{ij}$  are the hamiltonian matrix elements when written in the eigenbasis of  $L$ . This can easily be simplified to a third-degree equation after identifying  $\lambda = 0$  as a trivial solution, which is associated to the ‘‘eigenmatrix’’  $V = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ . This is consistent with decoherence since  $\lambda = 0$  implies that the respective term in (3.18) will remain constant in time. In addition, since all the coefficients appearing in (3.19) are strictly positive, then there's another real solution to the remaining third degree equation which would be associated to a decay since it must be negative. For example, if equation (3.19) is particularized for the problem (3.7) when  $\gamma > \Omega$ , the remaining eigenvalues are  $\lambda_1 = -2\gamma$ ,  $\lambda_2 = -\sqrt{\gamma^2 - \Omega^2} - \gamma$ ,  $\lambda_3 = \sqrt{\gamma^2 - \Omega^2} - \gamma$ , so all of them are negative and reproduce the results in 3.5 (the same happens for the resonant and weak measurement regimes). According to the previous reasoning, the asymptotic form of  $\rho$  would be proportional to the identity matrix, what is confirmed by the general solution it has been found. Nevertheless, even when we have seen that this equation will always have at least two real solutions ( $\lambda_0 = 0$  and  $\lambda_1 < 0$ ), it is still needed to show that the two remaining solutions will be consistent with decoherence, which requires the general solution to (3.19) to be found. Since it is very impractical to handle, this approach has not been found to be conclusive for the general problem of showing that the eigenbasis of  $L$  will be the pointer basis of the process.



### 3.4 An interaction model approach.

As was pointed out in the first pages of this project, one of our main interests, as far as the problem of measurement is concerned, is precisely the capability of modelling measurements from a physical approach based on physical interactions. In fact, since the POVM's formalism can be understood as a generalization of postulate 4, equation (3.4) cannot be used to try to prove that measurement postulates are prescindible to show the emergence of classicality, described by decoherence. It is thus our goal to find an interaction model to arrive to an equation of the form of (3.8) from the approach presented in 2.2. With this in mind, we can consider the time derivative of the density operator under the interaction picture, so it can be seen that:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H_s, \rho] + e^{-\frac{i}{\hbar}H_s t} \frac{d\tilde{\rho}}{dt} e^{\frac{i}{\hbar}H_s t}, \quad (3.20)$$

so, by forcing equation (3.8) to be satisfied, one gets:

$$-\frac{i}{\hbar} [H_s, \rho] + e^{-\frac{i}{\hbar}H_s t} \frac{d\tilde{\rho}}{dt} e^{\frac{i}{\hbar}H_s t} = -\frac{i}{\hbar} [H, \rho] - \frac{\Gamma}{2} [L, [L, \rho]], \quad (3.21)$$

where  $H$  is an hermitian operator, not necessary equal to the hamiltonian of the system  $H_s$  since equation (3.8) has been obtained by particularizing Lindblad's equation (2.8) (In particular, here  $H$  has been modified by a factor  $\hbar$ , but this is legit because it is a real value). Nevertheless, since  $H$  is not fixed and we are free to impose our model to yield  $H = H_s$ , we can write, under this assumption:

$$e^{-\frac{i}{\hbar}Ht} \frac{d\tilde{\rho}}{dt} e^{\frac{i}{\hbar}Ht} = -\frac{\Gamma}{2} [L, [L, \rho]] = -\frac{\Gamma}{2} (L^2\rho + \rho L^2 - 2L\rho L). \quad (3.22)$$

This equation constitutes a first relation between the measured observable  $L$ , the measurement strength  $\Gamma$  and the interaction model we are looking for. By using Redfield equation (2.18) for the particular case in which the interaction hamiltonian can be written as  $H_{int} = \hbar (S(t) \otimes E(t))$ , equation (3.22) can be written as:

$$S(t)\Lambda_1(t)\rho(t) + \rho(t)\Lambda_2(t)S(t) - \Lambda_1(t)\rho(t)S(t) - S(t)\rho(t)\Lambda_2(t) = \frac{\Gamma}{2} (L^2\rho + \rho L^2 - 2L\rho L), \quad (3.23)$$

where:

$$\Lambda_k(t) = \int_0^t \left( e^{\frac{i}{\hbar}H_s(\tau-t)} S(\tau) e^{\frac{i}{\hbar}H_s(t-\tau)} \right) \left[ \langle \tilde{E}(t) \tilde{E}(\tau) \rangle_e \delta_{k1} + \langle \tilde{E}(\tau) \tilde{E}(t) \rangle_e \delta_{k2} \right] d\tau, \quad (3.24)$$

The left side of (3.23) starts to get a very similar form to that of the right hand side. In fact, it is easy to see that if one imposes the condition  $\langle \tilde{E}(\tau) \tilde{E}(t) \rangle_e = C\delta(\tau - t)$ , then trivially  $\Lambda_1(t) = \Lambda_2(t) = CS(t)$  and therefore:

$$C (S(t)^2\rho + \rho S(t)^2 - 2S(t)\rho S(t)) = \frac{\Gamma}{2} (L^2\rho + \rho L^2 - 2L\rho L), \quad (3.25)$$

so it is now easy to identify that we can take  $S(t) = L$  and  $C = \Gamma/2$  so the equation holds and a first approximation to an interaction description of the measurement has been achieved. Indeed, we have demonstrated that if equation (3.8) certainly models a measurement, then it can be affirmed that a measurement over the observable  $L$  of a system can be described by an interaction hamiltonian  $H_{int} = \hbar L \otimes E$ , if the coupling observable of the environment  $E$  satisfies  $\langle \tilde{E}(\tau) \tilde{E}(t) \rangle_e \simeq \frac{\Gamma}{2} \delta(\tau - t)$ , with  $\Gamma > 0$ . It is also easy to prove in an analogous manner that the same measurement can be described by a more general interaction hamiltonian  $H_{int} = \hbar L \otimes \sum_{i=1}^N E_i$  if  $\sum_{i,j=1}^N \langle \tilde{E}_i(\tau) \tilde{E}_j(t) \rangle_e \simeq \frac{\Gamma}{2} \delta(\tau - t)$ , with  $\Gamma > 0$ .

### 3.5 Appendix. Analytical solution of (3.7)

In general:

$$\mathbb{R}_e\{\rho_{01}(t)\} = \mathbb{R}_e\{\rho_{01}(0)\}e^{-2\gamma t} \quad (3.26)$$

If  $\gamma > \Omega$ :

$$\begin{aligned} \rho_{00}(t) = & \rho_{00}(0) + \frac{\Omega \mathcal{I}_m\{\rho_{01}(0)\}}{\gamma + \sqrt{\gamma^2 - \Omega^2}} \left( e^{-(\gamma + \sqrt{\gamma^2 - \Omega^2})t} - 1 \right) + \\ & + \frac{2C}{\Omega} e^{-\gamma t} \left[ \gamma \sinh\left(\sqrt{\gamma^2 - \Omega^2}t\right) + \sqrt{\gamma^2 - \Omega^2} \left( \cosh\left(\sqrt{\gamma^2 - \Omega^2}t\right) - e^{\gamma t} \right) \right] \end{aligned} \quad (3.27)$$

$$\mathcal{I}_m\{\rho_{01}(t)\} = 2C e^{-\gamma t} \sinh\left(\sqrt{\gamma^2 - \Omega^2}t\right) + \mathcal{I}_m\{\rho_{01}(0)\} e^{-(\gamma + \sqrt{\gamma^2 - \Omega^2})t} \quad (3.28)$$

$$\text{where } C = \frac{\Omega(\rho_{00}(0) - 1/2)}{2\sqrt{\gamma^2 - \Omega^2}} + \frac{1}{2} \left( 1 - \frac{\gamma}{\sqrt{\gamma^2 - \Omega^2}} \right) \mathcal{I}_m\{\rho_{01}(0)\}$$

If  $\gamma = \Omega$ :

$$\begin{aligned} \rho_{00}(t) = & \rho_{00}(0) + \mathcal{I}_m\{\rho_{01}(0)\} (e^{-\gamma t} - 1) + \\ & + \left[ \rho_{00}(0) - \frac{1}{2} - \mathcal{I}_m\{\rho_{01}(0)\} \right] (e^{-\gamma t} (1 + \gamma t) - 1) \end{aligned} \quad (3.29)$$

$$\mathcal{I}_m\{\rho_{01}(t)\} = \mathcal{I}_m\{\rho_{01}(0)\} e^{-\gamma t} + \Omega \left[ \rho_{00}(0) - \frac{1}{2} - \mathcal{I}_m\{\rho_{01}(0)\} \right] t e^{-\gamma t} \quad (3.30)$$

If  $\gamma < \Omega$ :

$$\begin{aligned} \rho_{00}(t) = & \rho_{00}(0) - \frac{\gamma}{\Omega} \mathcal{I}_m\{\rho_{01}(0)\} - \\ & - C \frac{\sqrt{\Omega^2 - \gamma^2}}{\Omega} + \frac{C}{\Omega} e^{-\gamma t} \left[ \gamma \sin\left(\sqrt{\Omega^2 - \gamma^2}t\right) + \sqrt{\Omega^2 - \gamma^2} \cos\left(\sqrt{\Omega^2 - \gamma^2}t\right) \right] - \\ & - \frac{\mathcal{I}_m\{\rho_{00}(0)\}}{\Omega} e^{-\gamma t} \left[ \sqrt{\Omega^2 - \gamma^2} \sin\left(\sqrt{\Omega^2 - \gamma^2}t\right) - \gamma \cos\left(\sqrt{\Omega^2 - \gamma^2}t\right) \right] \end{aligned} \quad (3.31)$$

$$\mathcal{I}_m\{\rho_{01}(t)\} = \mathcal{I}_m\{\rho_{01}(0)\} e^{-\gamma t} \cos\left(\sqrt{\Omega^2 - \gamma^2}t\right) + C e^{-\gamma t} \sin\left(\sqrt{\Omega^2 - \gamma^2}t\right) \quad (3.32)$$

$$\text{where } C = \frac{1}{\sqrt{\Omega^2 - \gamma^2}} (\Omega(\rho_{00}(0) - 1/2) - \gamma \mathcal{I}_m\{\rho_{01}(0)\})$$

# Conclusions

We saw in the first pages of this work how the postulates of quantum mechanics, and more particularly those related to the measurement process, gave rise to certain interpretation problems concerning it that needed to be explained. With this work, we have been able to achieve a better understanding of the measurement problem, concluding some very interesting results we can now compile as follows:

1. An approach to quantum mechanics in terms of density operators allows to understand the transition between quantum superposition and the classical world as a consequence of Von Neumann's irreversible reduction process, which converts pure superposed states into classically interpretable mixed states.
2. Von Neumann's irreversible reduction process, beyond being an ad hoc process, is a consequence of decoherence, which has been proved to emerge when the interaction between a system and its environment is modeled by a master equation.
3. Redfield equation allows an adequate description of many physical systems in spite of not assuring the preservation of the positivity of the density operators, accounting also for different types of transitions and properties in the studied systems.
4. Master equations, beyond being a way to obtain an analytical expression for the time evolution of the state of a system that interacts with its environment, are precisely a way to solve the computational problem of simulating a macroscopic environment.
5. Measurement processes can be modeled by master equations according to the POVM formalism, but this equations can be derived, independently of any kind of generalized measurement formalism, from interaction models with certain properties, showing that the emergence of classicality can be explained avoiding postulate five.

In addition to this, we could also mention some other interesting results we have found like, for example, the fact that decoherence time does not necessarily increase for weaker measurements or the associated heating effects. Nevertheless, the previous conclusions constitute the most important results of this work, with which, I hope, the reader has built a broader point of view of the measurement problem and how it can be, as far as the emergence of classicality is concerned, partially solved by decoherence. However, some other questions such as the interpretation of the quantum state of a system or the final collapse of the wavefunction/splitting of the parallel universes have not been studied. These questions, of a notoriously greater complexity than the one discussed here, will have to be addressed in future projects in order to achieve a deeper understanding of the most fundamental concepts governing the functioning of the universe, of course, if this is possible at all...

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