

**Experimentally accessible measure to quantify the  
non-Markovian character of the dynamics of open  
quantum systems**

by

Humberto Triviño Navarro

Submitted to the Instituto de Física  
in partial fulfillment of the requirements for the degree of

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**Abstract**

We use the divisibility approach to describe non-Markovian dynamics (memory effects) in open quantum systems coupled to an environment (reservoir). Specifically, sufficient and necessary criteria were incorporated in the energy domain that play a relevant role in dynamics of the system. In this case, we adopt the Feshbach partition in the space of (Hilbert-Liouville). On the other hand, to investigate both Markovianity and non-Markovianity, we study the divisibility of the Wigner function propagator. For this, within the framework of path integrals, we carry out an analysis of non-classical paths in phase space. Furthermore, we have used tools of topology to propose theorems intimately related to measures of non-Markovianity that are experimentally accessible.

Thesis Supervisor: Leonardo A. Pachon  
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# Chapter 1

## Introduction

In the course of history, mankind has made multiple theoretical and experimental efforts to interpret and understand Nature and the behavior (dynamics) of the universe. However, this is not trivial and the answer to this or similar questions has been of utmost importance in the systematic construction of our current knowledge. These concerns and questions led to profound efforts of formalization and implementation of theoretical and experimental study methods, based on mathematical axiomatization, observation and extrapolation of natural phenomena and, therefore, on the generation of hypotheses, conjectures and their validation. In this case, mathematics and physics had to be consolidated, taking into account the issues of historical contexts and the imperative need to understand the dynamics immersed in everyday life and the universe. In fact, we could go back to the time of Aristotle, a disciple of Socrates. He was characterized for giving valuable contributions in different fields: logic, metaphysics, philosophy of science, aesthetics, rhetoric, physics, astronomy, biology, among other branches of knowledge . Aristotle established a basis for the systematic investigation of the mobile bodies. Later, Galileo in his book (Dialogues on two new sciences) stipulates that all falling objects move with the same acceleration regardless of the mass if and only if, the resistance of the air is negligible. Furthermore, he was one of the first scientists to propose the scientific method in the 16th century. During the Renaissance Nicolas Copernicus (mathematician, physicist, jurist, economist and astronomer) studied the first heliocentric theory of the solar system and in his

book (*De revolutionibus orbium coelestium*) generated the first notes of the modern astronomy. In 1543, it was decided to name (Copernicus) a visible lunar crater with the help of binoculars, located at Mare Isularum. Subsequently, Johannes Kepler (astronomer and mathematician) formalized the rules that describe the motion of the planets. He states that all planets move around the sun following elliptical orbits and establishes that the radius vector that joins a planet and the sun, sweeps in equal areas and, therefore, equal times. Furthermore, he proposes that for any planet, the square of its orbital period is directly proportional to the cube of the length of the semi-major axis of its elliptical orbit. Later, Isaac Newton-considered from Western thought as the father of classical physics-, developed the dynamical laws that bear his name. After the failure of classical mechanics to explain a series of microphysical phenomena that were observed in the late nineteenth and early twentieth centuries, the construction of a new theory, quantum mechanics, was necessary.

In the late XIX century, physics consisted essentially of classical mechanics, electromagnetic theory, and thermodynamics. Classical mechanics was used to predict the dynamics of material bodies. Electromagnetism gave an adequate framework for the study of radiation. Matter and radiation are described in terms of particles and waves, respectively. As for the interactions between matter and radiation, they were well explained by the Lorentz force or by thermodynamics. The overwhelming success of classical physics (classical mechanics, classical theory of electromagnetism, and thermodynamics) led people to believe that the definitive description of nature had been achieved. It seemed then that all the physical phenomena could be explained within the framework of the general theories of matter and radiation.

However, at the beginning of the XX century, classical physics, was seriously questioned by two great sources. In the first instance, the relativistic domain, Einstein's theory of relativity of 1905 showed that the validity of Newton's mechanics fails to very close speeds of light.

Otherwise, microscopic domain as soon as new experimental techniques were developed in order to probe the structures of the atomic and subatomic, it turned out that classical physics fails when trying to explain with them various phenomena mainly

blackbody radiation, photoelectric effect, atomic stability and atomic spectroscopy. Lord Rayleigh, Plank, Thomson, Hedrik Lorentz, Rayleigh – Jeans, Robert Andrews Millikans, Arthur Compton, Ernest Rutherford, Hans, Luis Broglie, Bohr took a step beyond classical physics.

That is, they gave to the birth and consolidation of quantum mechanics, demonstrating the impossibility of carrying out an experiment that can simultaneously measure two complementary variables with arbitrary precision. Subsequently, a branch of quantum mechanics emerged, called open quantum systems, in charge of studying the behavior of complex systems of many bodies (atoms, ions, molecules).

This line has made multiple advances in: statistical mechanics, biophysics, quantum optics, nuclear physics, solid state, particle physics, and quantum computing. In particular, an essential ingredient of any real dissipative real quantum system is the separation of a global quantum system into a subsystem, usually called the relevant part, and the environment (reservoir), called the irrelevant part and initially assumed to be in thermal equilibrium. The path integral formulation of quantum mechanics has played a fundamental role, relevant in some generalizations of quantum theory. However, several authors converge on the difficulty of understanding the behavior of a quantum system with many degrees of freedom strongly coupled to a thermal bath. On the other hand, the emergence of classical behavior within quantum mechanics is of fundamental importance. In fact, this problem is closely related to understanding the decoherence.

Now, despite advances in quantum theory, no general agreement on interpretation has yet been reached. In recent decades, a combination of advanced stochastic processes, algebraic structures (groups, semigroups, algebras, co-algebras), measurement theory, and quantum mechanics has emerged. Specifically, open quantum processes of a Markovian or non-Markovian nature (memory effects).

Currently, open quantum systems with memory, also known as non-Markovian open quantum systems, have been studied, for fundamental and applied reasons [BLPV16, WHX<sup>+</sup>19a]. From the fundamental point of view, the study of quantum systems that interact with structured environments (reservoir) presents considerable

difficulties a theoretical point of view [BLPV16, MKPM19, BLP09]. However, from an applied point of view in the field of biochemistry and technology [ABCasanM14, CM12], the path opens to new methods of decoherence control based on the manipulation and modification of environmental properties, such as its frequency spectrum [CasamMM17, DB17].

The theoretical formulation of the quantification of the degree of Markovianity of a quantum system has focused on two approaches. In the first instance, in Ref. [BLPV16] the trace distance,  $\mathcal{D}(\rho, \sigma) = \text{Tr} \sqrt{(\rho - \sigma)(\rho - \sigma)^\dagger}$ , where  $\rho$  and  $\sigma$  are density matrices. This mathematical expression guarantees that the system is Markovian if  $\frac{d}{dt} \mathcal{D}_{ij} < 0$ , for all  $t$ , otherwise, the system is said to have non-Markovian dynamics. This measure coincides with the entropy of Kolmogorov in the classical limit. However, in this case, it is necessary to optimize over all the states inherent in the open quantum system. This optimization implies the use of quantum tomography in the analysis of non-Markovianity, which is highly expensive experimentally [dVA17, EGNK08a].

On the other hand, the second approach corresponds to the criterion of divisibility of a family of traces of the density operator associated to the evolution of a quantum system in time [MKPM19], which is an alternative way to face the study of the dynamics of open quantum systems. The two versions are not equivalent [BLPV16, MKPM19], but they direct their attention to the study of the characteristic properties of non-Markovian dynamics, robust methods for the detection and quantification of correlations in the system-environment.

Now, the quantification of these cross-correlations, induced by the environment in the system, is intended to be addressed through the connection between the domain of time and the domain of the energy established by the spectroscopy. Specifically, we have introduced the principle of divisibility [MKPM19] into discrete or continuous varieties. Furthermore, this law of composition was introduced to analyze non-Markovianity in the Winger function, using the time evolution of a damped harmonic oscillator with a functional and comprehensive approach. Finally, the absorption-fluorescence spectra were calculated, this allowed for obtaining the spectral lines of the correlation function at two points and therefore characterizing the spectral line profiles as Lorentzian

(Markovian) or Gaussian (non-Markovian). Likewise, the fundamental principles of linear response theory were studied and the results were formalized through theorems or corollaries.

The Thesis is structured as follows. In Chapter 2, we show the main theoretical-experimental descriptions of open Markovian and non-Markovian quantum systems. Likewise, we exhibit the definitions of the divisibility principle (composition principle) and carry out an exhaustive study of functional analysis, generating connections between the spaces (Hilbert, Banach, Sobolev). In fact, we propose metrics based on those existing in the literature and the topology associated with each space is enhanced. Next, in Chapter 3, we show projection operators, reduced equations of motion, effective Hamiltonians, and introduced the principle of divisibility in open quantum systems. Specifically, we propose the sufficient and necessary criteria in the energy domain to compose in the time domain and, therefore, the analytical result is formalized through theorems and corollaries. We were defined a measure of the non-Markovian character in terms of a cross-correlation between the measured spectrum and a Markovian simulated spectrum. In chapter 4, we present the Wigner function in the classical trajectory space, taking into account the damped harmonic oscillator and the composition law is incorporated to discriminate a Markovian or non-Markovian analysis (memory effect). That is, if the extrapolations decline in the field of non-divisibility, it implies non-Markovianity in these processes. Concluding remarks are presented in Section 5.





# Chapter 2

## Markovian and non-Markovian open quantum systems

In this chapter, we will show the generalities of classical Markov processes, the fundamentals of open quantum systems (reservoir-system) and the extension of Markovianity to the quantum regime. We present the approaches and difficulties, existing in the description of the Markovian or non-Markovian dynamics. Further, we discuss the theoretical and experimental approaches to determine the degree of Markovianity. In this case, we highlight the advances in the experimental of non-Markovian dynamics. Likewise, we explain the importance of normed vector spaces (Hilbert, Banach,  $L^p$ ), which enable us to find relations between measurements of non-Markovianity and the underlying metric. In addition, we will show the generalities of the Linear Response Theory (LRT) and, the operators associated with the unit or non-unit dynamics, directly in the memory effects (non-Markovian open quantum systems).

### 2.1 Classical stochastic Markov process

A classical stochastic Markov process is a family of random variables  $X(t)$  such that the probability of occurring any event given the history, is only the probability of occurring that event given the previous one. If  $(X_i)_{i=1}^{n+1}$  denotes the set of ordered

events and  $P(\cdot|\cdot)$  the conditional probability, the previous condition can be written as:

$$P(X_{n+1}|X_n, X_{n-1}, \dots, X_1) = P(X_{n+1}|X_n). \quad (2.1)$$

The representation  $P(x_i, t_i|x_j, t_j)$  is used to denote the event  $x_i$  and the time  $t_i$  at which this event occurs. It can be easily demonstrated that for a classical Markov process, the conditional or transient probabilities obey the Chapman Kolmogorov equation (also known as the classical master equation)

$$P(x_2, t_2|x_0, t_0) = \sum_{x_1 \in X} P(x_2, t_2|x_1, t_1)P(x_1, t_1|x_0, t_0). \quad (2.2)$$

In fact, any process in which the transition probabilities satisfy the Chapman-Kolmogorov equation (CK) can be represented as a Markov process (Theorem 2.1 in Ref [RHP14]). The CK equation can be formulated through a differential equation, that is to say

$$\frac{\partial P(x, t|x', t')}{\partial t} = \mathcal{L}_t P(x, t|x', t'), \quad (2.3)$$

where  $\mathcal{L}_t$  is a linear operator [RH12]. Let  $\vec{P}(t)$  be the vector with  $i$ -th component equal to  $P(x_i, t)$  and  $T(t, t')$  the matrix with entries  $i, j$  equal to  $P(x_i, t_i|x_j, t_j)$ , then (2.2), can be written as

$$T(t_2, t_0) = T(t_2, t_1)T(t_1, t_0), \quad (2.4)$$

and the vector of total (or stochastic) probability, that is, the classical probability description of the state, changes as

$$\vec{P}(t) = T(t, t')\vec{P}(t'). \quad (2.5)$$

In this section, we have shown the generalities of the classical Markovian processes, taking into account the stochastic characterization and, therefore, their vector representations.

However, for a rigorous analysis it is necessary to formalize these criteria at the quantum level. In the next section we will deal with this aspect.

## 2.2 Quantum Markovian processes

The main objective of the theory of open quantum systems is to fully describe the various types of interactions of the system with its environment and its effect on the dynamics of the system of interest [BP<sup>+</sup>02, HH17]. Any quantum system is bound to be affected by its environment, and therefore the dynamic characteristics of open quantum systems are particularly important from a practical perspective. Due to the advent of quantum technologies, such as quantum communication [NC02] or quantum cryptography [SRH<sup>+</sup>21], a marked interest in the application of various techniques of open quantum systems is evident. Furthermore, in recent years, quantum systems, specifically, non-Markovian systems have been receiving much attention, as evidenced by the rapid growth in related literature [CZCK21, For18]. Indeed, the potential relevance of memory effects in the field of complex quantum systems and quantum information has led to intense study [SS15, SRH<sup>+</sup>21]. However, there are numerous outstanding questions still to be studied. In this case, fundamental questions such as the mathematical structure of non-Markovian quantum dynamics, the role of complexity in the appearance of memory effects or the relevance of non-Markovianity in the study of the border between classical and quantum aspects, as well as more applied issues such as the identification of environmental characteristics or the correlation between the system and the environment.

From a physical point of view, the non-local character of dynamics can, for example, induce apparent violations of the second law of thermodynamics [EGNK08b] or could redefine quantum phenomena [PTZB19]. In the context of photochemical systems, such as amino acids, proteins (rhodopsin, amphipathic), photosynthetic reaction centers, etc., the presence of non-Markovian dynamics is a rule [DB17, SHP21].

An extension of the classical definition in (2.1) of a Markovian process to the quantum regime is not direct [HLA20]. The main difference is that the sampling of a

set of quantum states depends on the way in which the measurement is performed. Therefore, the right side of (2.1) has no practical meaning for the quantum scenario: each time the system status is measured, the following sample result is disturbed.

However, as we have already seen in the previous section, a process which satisfies the CK equation is Markovian. We can find an analogous definitions of Markovian processes in quantum systems by introducing a non-commutative of the divisibility condition of CK (2.4). That is we want to have a map  $\hat{\varepsilon}$  that satisfies for  $t' < t$ ,  $t_0 < t_1 < t_2$

$$\hat{\rho}(t) = \hat{\varepsilon}_{(t,t')}[\hat{\rho}(t')], \quad (2.6)$$

$$\hat{\varepsilon}_{(t_2,t_0)} = \hat{\varepsilon}_{(t_2,t_1)}\hat{\varepsilon}_{(t_1,t_0)}. \quad (2.7)$$

Clearly, the map  $\hat{\varepsilon}$  has to take quantum states and produce valid quantum states as output. This special type of operator is known as a quantum channel and is the subject of the next section.

## 2.3 Quantum Channel

The conditions for the map  $\hat{\varepsilon}$  to be the general description of a quantum evolution are the following

- Linear:  $\hat{\varepsilon}(\lambda_1\hat{\rho}_1 + \lambda_2\hat{\rho}_2) = \hat{\varepsilon}(\lambda_1\hat{\rho}_1) + \hat{\varepsilon}(\lambda_2\hat{\rho}_2)$
- Trace preserving:  $\text{Tr}[\hat{\varepsilon}(\hat{\rho})] = \text{Tr}[\hat{\rho}]$
- Completely positive:  $\forall n \in \mathbb{N}$ , the map  $\varepsilon \otimes id_n$  is a positive map, i.e.,  $\varepsilon \otimes id_n(A^*, A) \geq 0$ ,  $\forall A \in \mathcal{B}(\mathcal{H})$

where,  $id_n$  is the dynamic map of identity and,  $\mathcal{B}$  is an algebra of a Hilbert space  $\mathcal{H}$ . For a detailed review of quantum channels the interested reader is referred to [CGLM14] and references therein. We will focus on Gaussian channels which are channels that just affect the second moments of the input states. This means that the Hamiltonian

of the reservoir, subsystem and interaction are almost quadratic expression in the mode operators.

## 2.4 Measures of non-Markovianity

In this section, we give a short description of popular measures used in the literature. As pointed out in Ref. [RHP14], we mention some difficulties arising when working with this measure.

### 2.4.1 BLP Measure

This is the measure proposed by Breuer, Laine and Pilo [LPB10]. The dynamics is Markovian if the distance decreases in time for any pair of states  $\rho_1$  and  $\rho_2$  we have

$$\|\rho_1(t_2) - \rho_2(t_2)\|_1 \leq \|\rho_1(t_1) - \rho_2(t_1)\|_1, \quad (2.8)$$

for all  $t_1 < t_2$ . It turns out that this statement is not always true. The reason rests on the fact that (2.8) is a property of positive maps, while quantum channels are completely positive implying that there may be cases where this previous Equation is satisfied although the dynamics is non-Markovian (see Theorem 3.4 and Sec. 3.4 in Ref. [RHP14]). On the other hand, their definition does work as a witness of non-Markovianity. This means that when (2.8) is not fulfilled we have a non-Markovian evolution. An experimental implementation of this witness can be found on Ref. [LLH<sup>+</sup>11].

### 2.4.2 RHP Measure

This measure was introduced by Rivas, Huelga and Plenio [RHP14]. It quantifies how the intermediate evolution deviates from being completely positive. They argue that by (time continuity) one has

$$\hat{\mathcal{E}}_{(t_2, t_0)} = \hat{\mathcal{E}}_{(t_2, t_1)} \hat{\mathcal{E}}_{(t_1, t_0)}, \quad (2.9)$$

and that the evolution is Markovian if the intermediate dynamics

$$\hat{\epsilon}_{(t_2,t_1)} = \hat{\epsilon}_{(t_2,t_0)}\hat{\epsilon}_{(t_1,t_0)}^{-1}. \quad (2.10)$$

The way they prove complete positivity is by means of the Choi–Jamiołkowski isomorphism [Jam72], a well-known tool in the quantum information community. Using this, they define

$$h(t) = \lim_{\epsilon \rightarrow 0^+} \frac{\|\hat{\epsilon} \otimes id[|\Psi\rangle\langle\Psi|]\| - 1}{\epsilon}, \quad (2.11)$$

where  $|\Psi\rangle$  is the maximally entangled state in  $\mathbb{C}^n$ . Also, noticing that  $h(t) \geq 0$ , with  $h(t) = 0$  if and only if  $\hat{\epsilon}(t + \epsilon, t)$  is CP [RHP14]. Therefore the integral

$$N_{RHP}^I = \int_0^\infty dt h(t), \quad (2.12)$$

can be taken as a measure of non-Markovianity, and as long  $h(t)$  decreases fast enough (this will not be always the case) will be finite.

### 2.4.3 SE Measure

Recently, Strasberg and Esposito [SE18] have used the Linear Response Theory (*LRT*) by quantifying the non-Markovian character through response functions. They have shown that *LRT* also provides a way to derive dynamic maps, but for initially correlated (and generally entangled) states. In this case, it is important to note that these maps are always invariable in translation time and allow a much simpler quantification of non-Markovianity compared to previous approaches. They have applied a theory to the Caldeira-Leggett model, for which the respective quantifier is valid beyond the linear response and can be expressed analytically. Furthermore, this measurement (*SE*) has allowed extrapolating that a classic Brownian particle coupled to an Ohmic bath can already exhibit non-Markovian behavior, a phenomenon related to the initial state preparation procedure. In this case, they have taken into account the fundamental properties of the Green propagators in the quantification of

the non-Markovian character (see Chap. VII in Ref. [Sch12] for detail). In operator form, the time-dependent Green's function (for time-independent  $\hat{H}$ ) is

$$\hat{G}(t) = \theta(t) \exp -\frac{i\hat{H}t}{\hbar} \quad (2.13)$$

The family  $\{\hat{G}(t)|t > 0\}$  satisfies

$$\hat{G}(t) = \hat{G}(t-s)\hat{G}(s) \quad \forall s \in [0, t], \quad (2.14)$$

a condition which is also called divisibility.

To introduce new non-Markovianity quantifiers within this approach, Strasberg and Esposito [SE18] quantify the distance between two functions  $m(t)$  and  $n(t)$ . However, [SE18] use the standard  $L_2$  scalar product  $\langle m, n \rangle = \int_{-\infty}^{\infty} m(t)n(t)dt$  and the induced norm  $\|m\| = \sqrt{\langle m, m \rangle}$ , where it is tacitly assumed that the integrals are converging. They then define the distance

$$\mathcal{D}(m, n) \equiv \sqrt{1 - \frac{|\langle m, n \rangle|^2}{\|m\|^2\|n\|^2}}. \quad (2.15)$$

By the Cauchy-Schwarz inequality,  $0 \leq \mathcal{D}(m, n) \leq 1$  and  $\mathcal{D}(\lambda m, \lambda n) = \mathcal{D}(m, n)$  for any  $\lambda \in \mathbb{C}$ ; i.e., the difference has the favorable properties that it is positive, bounded, and independent for any global scaling. By analogy with the Euclidean scalar product,  $\mathcal{D}(m, n) = |\sin(\phi)|$  can be seen quantifying the "angle"  $\phi$  between the two vectors  $m(t)$  and  $n(t)$ . In fact, we propose to place metrics in terms of others. This facilitates the respective study and, therefore, extends the study of measurements in different spaces ( $L^p$ , Sobolev). Most importantly for its applications, by Parseval's theorem, they can deduce that  $\mathcal{D}(m, n) = \mathcal{D}(\tilde{m}, \tilde{n})$ , where the right hand side is computed by using the  $L_2$  scalar product in Fourier space,  $\langle \mathcal{D}(\tilde{m}, \tilde{n}) \rangle = \int_{-\infty}^{\infty} [\frac{dw}{2\pi}] \tilde{m}(w)\tilde{n}^*(w)$ . Now, keep in mind the principle of divisibility in the  $LRT$ . Specifically, the susceptibility

$$\chi(t) = \chi(t-s)\chi_+^{-1}\chi(s). \quad (2.16)$$

Therefore, integrating in (2.16) over  $s$  from zero to  $t$  implies in Fourier space

$$-i \frac{d}{dw} \tilde{\chi}(w) = \tilde{\chi}(w) \chi_+^{-1} \tilde{\chi}(w). \quad (2.17)$$

Then, to measure violations of (2.17) as a consequence of the (assumed) divisibility property, they have proposed quantifier  $[\tilde{\chi}'(w) = \frac{d\tilde{\chi}(w)}{dw}]$

$$\mathcal{N}_{ij}^1 = \mathcal{D}[-i\tilde{\chi}'_{ij}, (\tilde{\chi}\chi_+^{-1}\tilde{\chi})_{ij}] \quad (2.18)$$

Furthermore, they introduced the skew-symmetric matrix  $(\chi_+)_{ij} = \frac{i}{\hbar} \langle [A_i, A_j] \rangle_\beta$ , where  $[A, B]$  denotes the commutator and  $\langle \dots \rangle_\beta$  represents an expectation value with respect to the global equilibrium,  $A_i$  are system observables. The expectation value of  $A_i$  at a later time  $t \geq t_0$  is then connected to the response function  $(\chi)_{ij} \equiv \frac{i}{\hbar} \theta(t) \langle [A_i(t), A_j] \rangle_\beta$  via Kubo formula [Pot09].

In conclusion, Strasberg and Esposito show that it is possible to quantify non-Markovianity in the linear response regime in a rigorous and simple way by means of the  $\mathcal{N}_{ij}^1$  representation.

Nevertheless, we know from the outset that the elements of the respective Hilbert complex space are functions. However, this does not completely generalize the situation. By existing fundamental principles in literature [Apo96], every Hilbert space is thus also a Banach space (but not vice versa). Now, a space of infinite dimension is the spaces  $L^p$ . These are functional spaces associated with measure spaces  $(X, \mathcal{B}, \mu)$ , where  $\mathcal{B}$  is a  $\sigma$ -associated subset algebra of  $X$  and  $\mu$  is an accounting additive measure in  $\mathcal{B}$ . Also, if  $p = 2$  these spaces are from Hilbert

$$\langle \mathcal{D}(\tilde{m}, \tilde{n}) \rangle = \int_X \overline{\tilde{m}(t)} \tilde{n}(t) d\mu(t). \quad (2.19)$$

In fact, the integral makes sense and note that applying Lebesgue Theory [Apo96] ensures that the space is complete. On the other hand, in general we must guarantee that the Hilbert spaces in size are separable. Also, Sobolev spaces are a special class



of Hilbert, defined as follows

$$W^{n,p}(\Omega) = \{f \in L^p(\Omega) | D^\alpha f \in L^p(\Omega) \quad \forall \alpha \in N^n : |\alpha| \leq n\} \subset L^p(\Omega) \quad (2.20)$$

In this case,  $\Omega$  is a domain contained in  $\mathbf{R}^n$  and  $D^\alpha f$  is a multi – index notation for partial derivatives. Now, the norm associated with the Sobolev space is defined  $\|\cdot\|_{L^p(\Omega)}$  in  $L^p$

$$\|f\|_{m,n,\Omega} = \left[ \sum_{|\alpha| \leq n} \|D^\alpha f\|_{L^p(\Omega)}^p \right]^{\frac{1}{p}}, \quad 1 \leq p \leq \infty, \quad (2.21)$$

On the other hand, the Sobolev spaces, with  $p = 2$  are naturally endowed with the Hilbert space structure just like the spaces  $L^2$ . That is to say,

$$H^n(\Omega) \equiv W^{(n,2)}(\Omega), \quad (2.22)$$

where, the inner product is defined in the space  $L^2$

$$(\tilde{m}, \tilde{n})_{H^n(\Omega)} = \sum_{|\alpha| \leq n} (D^\alpha \tilde{m}, D^\alpha \tilde{n})_{L^2(\Omega)}. \quad (2.23)$$

Therefore, we indicate that there is a connection between several spaces (Hilbert,  $L^p$ , Sobolev) by associating each of them with a norm. Therefore, in the (2.15) can be generalized to different spaces.

## 2.5 Experimental measurements

In this section, we present a description of the main experiments that have been performed to quantify non-Markovian dynamics in open quantum systems. In this case, a description is made of the different advances in this area of knowledge, taking into account recent works in the literature [MKPM19, dLSWS+20a, WHX+19b]. In Ref. [MKPM19] it is that the classical domain, it is well known that divisibility does not imply that a stochastic process is Markovian. However, for quantum processes,

divisibility is often considered synonymous with Markovianity. They have shown that fully positive divisible (PD) quantum processes can still involve non-Markovian temporal correlations, which they then fully classify using the newly developed tensorial process formalism, which generalizes the theory of stochastic processes to the quantum domain.

In general, they have generated a complete feature of temporal correlations in Markovian that can be hidden in a divisible process, as well as a clear connection and delineation between Markovianity and CP divisibility. In addition, they return to the basic variables, existing in the literature. Such as:

**Definition 1.** (*CP divisibility*). A quantum dynamical process of a system on an interval  $[0, \mathcal{T}]$  is CP divisible if (i) the dynamical map from  $r$  to  $t$  acting on the system of interest can be broken up at  $s$  such that

$$\hat{\varepsilon}_{t:r} = \hat{\varepsilon}_{t:s} \circ \hat{\varepsilon}_{s:r}, \forall \mathcal{T} \geq t \geq s \geq r \geq 0, \quad (2.24)$$

and (ii) each map  $\hat{\varepsilon}_{x:y}$  is completely positive.

**Definition 2.** (*iCP divisibility*). A process is CP divisible by inversion (*iCP – divisible*) if for any two maps  $\hat{\varepsilon}_{s,0}, \hat{\varepsilon}_{t,0} \in \lambda_0$  with  $\mathcal{T} \geq t \geq s \geq 0$  the map

$$\hat{\varepsilon}_{t:s} := \hat{\Upsilon}_{t,0} \circ \hat{\Upsilon}_{s,0}^{-1} \quad (2.25)$$

is completely positive.

**Definition 3.** (*oCP divisibility*). A process is operationally CP–divisible (*oCP divisibility*), if for any  $\mathcal{T} \geq t \geq s \geq r \geq 0$

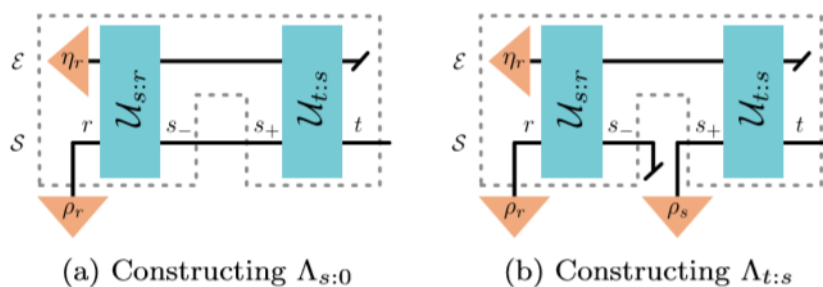
$$\hat{\Upsilon}_{t:r} := \hat{\Upsilon}_{t:s} \circ \hat{\Upsilon}_{s:r} \quad (2.26)$$

However,  $\hat{\varepsilon}_{t:s}[\eta_s] = \text{tr}_\varepsilon[\hat{U}_{t:s}(\eta_s \otimes \rho_s)]$ , where  $\rho_s$  is reduced state of the environment at time  $s$  and  $\hat{U} := \hat{U}_{t,s} x_s \hat{U}_{t,s}^\dagger = x_t$  is the unitary system– environment map. In general, a formal representation has been developed for the description of open Markovian or

non-Markovian processes.

Likewise, [MKPM19] present a tensor perspective to study Markovian or non-Markovian dynamics. Indeed, mathematically the process tensor  $T := T_{t,s,r}$  is an operator on Hilbert space  $\hat{H}_r \otimes \hat{H}_{s-} \otimes \hat{H}_{s+} \otimes \hat{H}_t$ . On the other hand, a quantum process is Markovian iff the Choi state of the corresponding process tensor has the form  $T^{Markov} = L_{t,r,s,r}$ . Specifically, as follows  $T = L_{t:s} \otimes L_{s:r} + \xi_{tsr}$ , where the matrix  $\xi$  contains all the non-Markovian tripartite correlation and satisfies  $\text{Tr}_{s-r}[\xi_{tsr}] = \text{Tr}_{ts+}[\xi_{tsr}] = 0$  which provides a full classification of non-Markovian temporal correlations that can be presented in oCP-divisible processes.

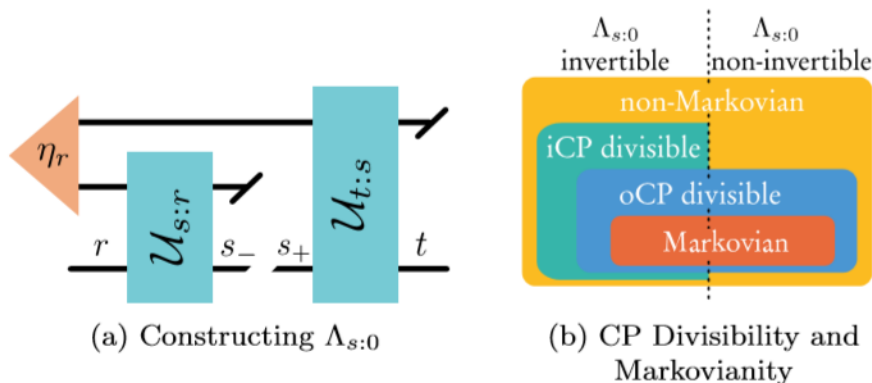
However, in Ref. [MKPM19] they have concluded that a process divisible by PCO can be seen as one that is Markovian on average: consider a multiple time process where an experimenter measures the system at all times, before independently preparing it in a new state; the divisibility of the PCP implies that if all previous measurement results are forgotten or averaged, future statistics only depend on the current preparation. This can be evidenced in the diagrams in Figs. 2-1 and 2-2



**Figure 2-1:** (a) Circuits for checking *iCP* and *oCP* divisibility. To construct the maps  $\hat{\epsilon}_{s,0}$  and  $\hat{\epsilon}_{t,0}$  we may set  $r = 0$  and measure the system at  $s$  or  $t$  respectively. (b) To construct  $\hat{\epsilon}_{t,s}$ , the system is discarded at  $s_-$  and a fresh state is fed in at  $s_+$ . The dotted line encapsulates the three – process tensor  $T_{t:s:r}$ . Source: Ref. [MKPM19].

In this case, they have provided an operationally motivated definition of *CP* divisibility that is stricter than the one frequently used, based on the invertibility of  $\hat{\epsilon}_{s,0}$ . Therefore, they have shown that the divisibility of the *oCP* is closely related to the conditions without signaling and implies the absence of information flow from

the environment to the system. Furthermore, they have shown that the divisibility of  $oCP$  can be interpreted as Markovianity on average, although the divisible processes of  $oCP$  can still show non-trivial memory effects, which have been fully characterized. Furthermore, they stress that short-term quantum technologies will require effective methods to detect and address non-Markovian noise [Pre18].



**Figure 2-2:** *Divisibility and Markovianity.* (a) The system interacts with one part of the correlated environment state leading to a non-Markovian  $oCP$ -divisible process. (b) The hierarchy of sets of process with varying degrees of temporal correlations: *machine learning, representation learning and deep learning*. Source: [MKPM19].

On the other hand, it follows that highlighting having shed light on divisibility from an operational point of view, which helps us to identify the kinds of temporal correlations that can evade non-Markovianity checks used regularly. However, there are trade-offs between discovering temporal correlations and the required number of experiments to be performed. In the past two years, some experiments have been carried out using generalizations of Born's rules and the fundamental principles of non-Markovian open quantum systems [dLSWS+20a].

This structure allows to detect memory effects even close to the validity of the Born-Markov approximation. An alternative operational based definition of environment-to-system backflow of information follows from this result. They provide experimental support to results by implementing the dynamics and measurements in a photonic experiment. They have calculated in an exact way the conditional past-future

correlation for the decay dynamics of a two– level system in a bosonic bath. Different measurement processes are considered.

In contrast to quantum memory measures based solely on system propagator properties, here memory effects are related to a convolution structure involving two system propagators and the environment correlation. Decoherence and dissipation are phenomena induced by the unavoidable coupling of an open quantum system with its environment. When describing this kind of system dynamics some important approximations are usually considered. A paradigmatic example is the Born Markov approximation (BMA), which considers that the reservoir is not altered significantly due to the presence of the system. The BMA has been used extensively, providing excellent agreement with many experiments such as for example in the context of quantum optics and magnetic resonance. The decay dynamics of a two level system induced by a bosonic bath is described by the Hamiltonian

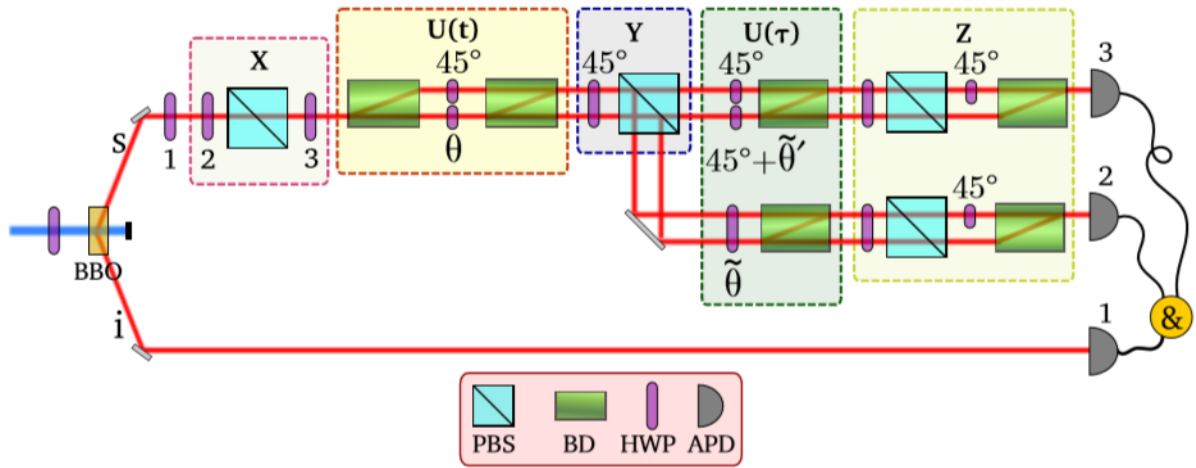
$$\hat{H}_{\text{tot}} = \frac{w_0}{2}\sigma_z + \sum_k w_k b_k^\dagger b_k + \sum_k (g_k \sigma_+ b_k + g_k^* \sigma_- b_k^\dagger). \quad (2.27)$$

Here,  $\sigma_z$  is  $z$ - Pauli matrix,  $\sigma_+ = |\uparrow\rangle\langle\downarrow|$  and  $\sigma_- = |\downarrow\rangle\langle\uparrow|$  are the raising and lowering operators of the qubit in the natural basis  $\{|\uparrow\rangle, |\downarrow\rangle\}$ . The bosonic operators satisfy the relations  $[b_k, b_k^\dagger] = 1$ . The "wave vector propagator"  $\vec{G}(t)$  obeys the convoluted evolution

$$\frac{d}{dt}\vec{G}(t) = - \int_0^t dt' \check{f}(t-t')\vec{G}(t'), \quad (2.28)$$

where the memory kernel is defined by the bath correlation  $\check{f}(t) \equiv \sum_k |g_k|^2 \exp[+i(w_0 - w_k)t]$ . To demonstrate the experimental feasibility of measuring memory effects close to the BMA, they develop a photonic platform that simulates the non-Markovian system dynamics. A continuous-wave (CW) laser, centered at 325 nm, is sent to a beta-barium-borate (BBO) crystal. Degenerated pairs of photons (wavelength centered at 650 nm), are produced in the modes signal "s" and idler "i" via spontaneous-parametricdown-conversion [KWW+99].

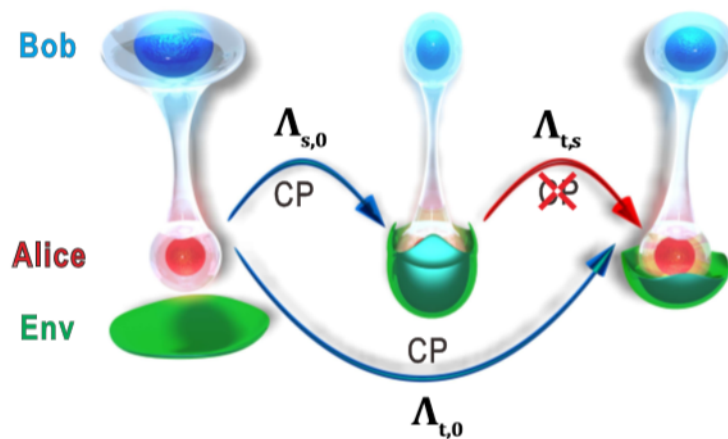
The respective experimental evidences indicate us, non-generalized measurements accessible experimentally in non-Markovian open quantum systems. Therefore, we are interested in defining a measure of the non-Markovian character in terms of a cross-correlation between the measured spectrum and Markovian simulated spectrum. Secondly, in the Ref. [dLSWS<sup>+</sup>20a] CPF correlation is measured through the sequence  $X \rightarrow U(t) \rightarrow Y \rightarrow U(\tau) \rightarrow Z$ , where  $X, Y$ , and  $Z$  are the measurement processes while  $U(t)$  and  $U(\tau)$  are the unitary transformation maps associated to the total Hamiltonian. Expanding on the respective formal analysis, note the 2-3



**Figure 2-3:** *Experimental setup.* Modules X, Y, and Z perform the projective measurements. Modules  $U(t)$  and  $U(\tau)$  implement the unitary system-environment maps. From coincidence counting, the avalanche photon detectors (APD) allow measuring the CPF correlation. Source: Ref. [dLSWS<sup>+</sup>20a].

Subsequently, it is shown in the Ref. [WHX<sup>+</sup>19b] the relationship between quantum Markovianity and coherence, providing an effective way to detect non-Markovianity based on the relative entropy of quantum incoherent coherence (QIREC). Theoretically, they have shown the relationship between completely positive divisibility (CP) and the monotonic behavior of the QIREC. Also, they have implemented all the optical experiments to demonstrate that the behavior of the QIREC coincides with the entanglement between the system and the anchor for both Markovian and non-Markovian evolution; while other coherence-based non-Markovian information carriers violate monotonicity, even in Markovian processes. Furthermore, they have experimentally

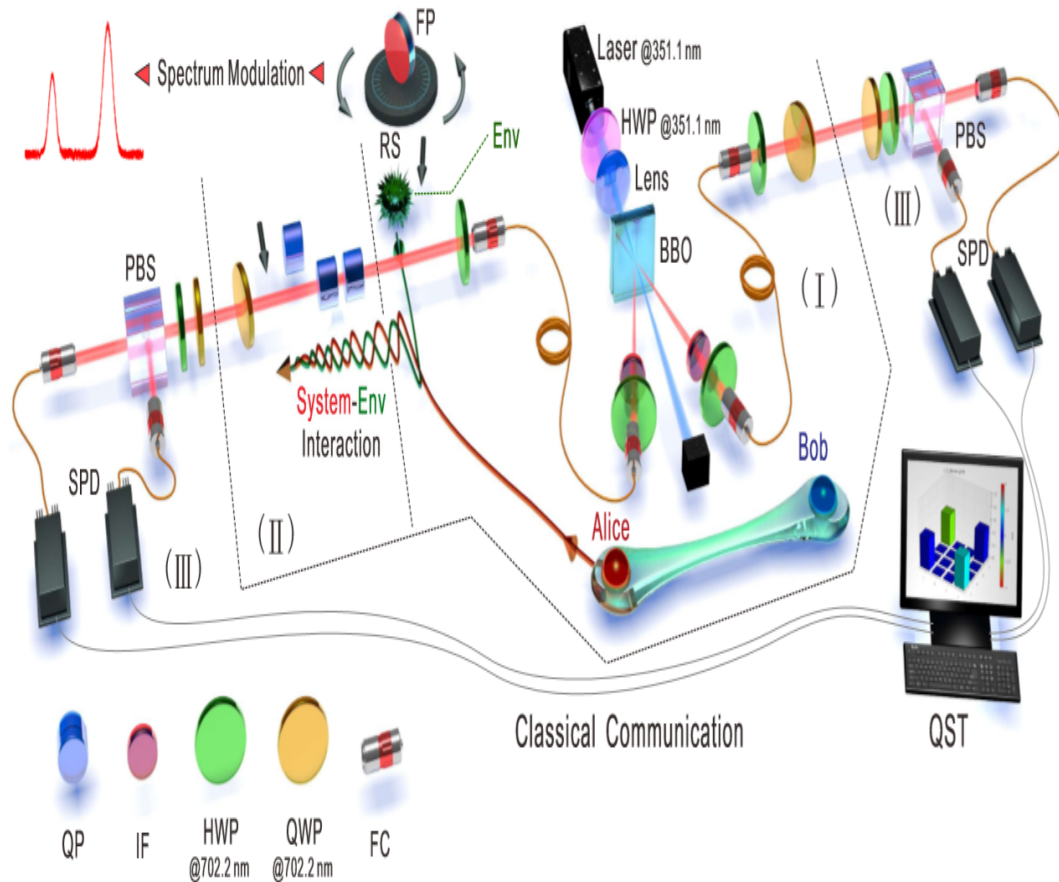
observed that non-Markovianity improves the ability to create coherence in an ancilla. This is the first experimental study of the relationship between the dynamic behavior of the QIREC and the phenomenon of information flow. Moreover, the authors have experimentally detected non-Markovianity via the non-monotonic behavior of both the QIREC and the SIC, which is coincident with previous results based on entanglement. Now, to motivate the development of the work a little, consider the following representation 2-4.



**Figure 2-4:** *Theoretical Framework.* Source: Ref. [WHX<sup>+</sup>19b].

In this case, in the figure 2-4 consider a bipartite system involving Alice (red, system) and Bob (blue, ancilla) with nonzero initial *QIREC*, which is shown by the bigger volume of Bob. The environment is shown as green and can interact with Alice's system, while Bob is immune to the environment. Then Alice undergoes a quantum evolution which can be characterized by a family of  $t$ -parameterized dynamical maps  $\{\Lambda_t\}$ . If the evolution is *CP* divisible, then *QIREC* decreases monotonically. The *CPTP* map on Alice's system also affects the ability of preparing coherent states on Bob's system, in both the asymptotic limit and single-shot regimes (this is shown by the behavior of the *SIC*, and theoretically proved in the Supplementary Materials), which is shown by the decrease of Bob's volume. However, any temporal increase of the *QIREC* or the *SIC* indicates the violation of *CPTP* of the intermediate map  $\Lambda_{t,s}$ , and non-Markovianity. The result demonstrates that the *QIREC* on Bob's side

provides a new method for characterizing the CP divisibility of a general quantum process on Alice's side. Also, the violation of monotonic behavior of either the  $QI$  REC or the SIC indicates non-Markovianity.



**Figure 2-5:** The experimental setup is constructed by three modules. (I) State preparation, (II) evolution, and (III) detection. Source:[WHX<sup>+</sup>19b].

In the figure 4-4, they showed the detailed experimental setup optical elements include: IF interference filter; HWP half-wave plate; QWP quarter-wave plate; QP quartz plate; FP Fabry-Perot cavity; BBO -bariumborate; SPD single photon detector; FC fiber coupler; PBS polarizing beam splitter; Env, environment QST, quantum state tomography. Although, notable contributions are evident in [WHX<sup>+</sup>19b], the question remains open, regarding the links between general quantum resources and non-Markovianity. Therefore, we will incorporate experimentally accessible measurements in open quantum systems. This with the aim of expanding these connections and,



therefore, concatenate the theoretical principles (composition law), with respect to the experimental possibilities.

Therefore, in this chapter we have exposed the different measures (theoretical-experimental) existing in the literature to describe non-Markovian dynamics. In addition, the conception of measurements in spaces (Hilbert,  $L^p$ , Sobolev) has been generalized, retracing the inherent elements of the Theory of measurement, functional spaces and the Linear Response Theory. This will prevail in the incorporation of the principle of divisibility in the two subsequent sections and also in the generation of an equivalent measure available for the experiment for open non-Markovian quantum systems.



# Chapter 3

## Quantum Brownian Motion: The Functional Integral Approach

In this section, a schematic of the quantum dynamics of a damped harmonic oscillator is made. This has been previously discussed in other works, taking into account anomalous behavior at low temperatures and the analysis of Ohmic dissipation [GSI88]. However, some inferences have recently been made about how the harmonic oscillator coupled to a linear thermal bath is special insofar as the linearity of the system implies that the sum of the pairs of paths satisfies the classical damped equation of motion. Also, they have shown that it is the non-local interaction that appears in a reduced description of the degree of freedom of the system that is responsible for the expansion of the Wigner delta type propagator in its Gaussian representation [PID10]. This constitutes a fundamental indicator to link the dynamics (Markovian and non-Markovian) to describe open quantum systems and the functional integral approach from the perspective of Brownian quantum movement. Therefore, we make a fundamental description of the existing theory of quantum damped harmonic oscillators.

### 3.1 General Theory

Similarly, as shown in Ref. [GSI88], we consider a Brownian particle of mass  $M$  that moves in a potential  $V(q, t)$  that can explicitly depend on time. The Brownian motion of the particle arises due to its interaction with the heat bath environment. Furthermore, as explained above, many authors have used a model in which the environment consists of a set of harmonic oscillators linearly coupled to the  $q$  coordinate of the Brownian particle. The system under study is governed by the Hamiltonian.

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_{SR}, \quad (3.1)$$

where

$$\hat{H}_S = \frac{p^2}{2M} + V(q, t) \quad (3.2)$$

is the Hamiltonian of the undamped particle,

$$\hat{H}_R = \sum_{n=1}^N \frac{1}{2} \left( \frac{p_n^2}{m_n} + m_n w_n^2 x_n^2 \right) \quad (3.3)$$

describes the reservoir consisting of  $N$  harmonic oscillators, and

$$\hat{H}_{SR} = -q \sum_{n=1}^N c_n x_n + q^2 \sum_{n=1}^N \frac{c_n^2}{2m_n w_n^2}, \quad (3.4)$$

introduce the coupling. The last term in the (3.4) compensates for the coupling-induced renormalization of the potential (see below) and it is introduced here as a matter of convenience.

## 3.2 Functional integral representation of the density matrix and elimination of the environment

We are interested in a reduced description of the system and focus on the time evolution of the Brownian particle only. Hence, we want to eliminate the environmental degrees of freedom. To that end it is convenient to employ the functional integral representation of quantum mechanics [FH63] introduced by Feynman. Since of our model integrals over environmental coordinates are Gaussian.

### 3.2.1 Euclidean functional integral

The coordinate representation of the equilibrium density matrix  $W_\beta$  of the entire system may be written as a so– called Euclidean functional integral [FH63]

$$W_\beta(\bar{q}, \bar{x}_n, \bar{q}', \bar{x}') = Z_\beta^{-1} \int \mathcal{D}\bar{q} \mathcal{D}\bar{x}_n \exp\left(-\frac{1}{\hbar} S^E[\bar{q}, \bar{x}_n]\right), \quad (3.5)$$

where the integral is over all paths  $\bar{q}(\tau)$ ,  $\bar{x}_n$ ,  $0 \leq \tau \leq \hbar\beta$  with  $\bar{q}(0) = \bar{q}'$ ,  $\bar{x}_n(0) = \bar{x}'_n$ , and  $\bar{q}(\hbar\beta) = \bar{q}$ ,  $\bar{x}_n(\hbar\beta) = \bar{x}_n$ . The path probability is weighted according to Euclidean action.

$$S^E[\bar{q}, \bar{x}_n] = S_0^E[\bar{q}] + S_R^E[\bar{x}_n] + S_{0R}^E[\bar{q}, \bar{x}_n], \quad (3.6)$$

where

$$S_0^E[\bar{q}] = \int_0^{\hbar\beta} d\tau \mathcal{L}_0^E(\bar{q}, \dot{\bar{q}}) = \int_0^{\hbar\beta} d\tau \left[ \frac{1}{2} M \dot{\bar{q}}^2 + V(\bar{q}) \right] \quad (3.7)$$

is the Euclidean action of the undamped particle moving in the time-independent potential  $V(\bar{q})$  effective during the preparation of the initial state,

$$S_R^E[\bar{x}_n] = \int_0^{\hbar\beta} d\tau \mathcal{L}_R^E(\bar{x}, \dot{\bar{x}}_n) = \sum_{n=1}^N \int_0^{\hbar\beta} d\tau \left[ \frac{1}{2} m_{nn} \dot{\bar{x}}_n^2 + \frac{1}{2} m_n \omega_n^2 \bar{x}_n^2 \right] \quad (3.8)$$

describes the reservoir, and

$$S_{0R}^E[\bar{q}, \bar{x}_n] = \int_0^{\hbar\beta} d\tau \mathcal{L}_{0R}^E(\bar{q}, \bar{x}_n) = \sum_{n=1}^N \int_0^{\hbar\beta} (-c_n \bar{q} \bar{x}_n + \bar{q}^2 \frac{c_n^2}{2m_n w_n^2}) \quad (3.9)$$

the interaction.

### 3.2.2 Real time functional integral

A pure state  $\Psi(q_i, x_{n_i}, 0)$  of the entire system evolves in time according to

$$\Psi(q_f, x_{n_f}, t) = dq_i dq_{n_i} K(q_f, x_{n_f}, t; q_i, x_{n_i}, 0) \Psi(q_i, x_{n_i}, 0) \quad (3.10)$$

where  $K(q_f, x_{n_f}, t; q_i, x_{n_i}, 0)$  is the coordinate representation of the time evolution operator  $\exp(-\frac{iHt}{\hbar})$  of the entire system which may again be represented as a functional integral [FH63]

$$K(q_f, x_{n_f}, t; q_i, x_{n_i}, 0) = \int \mathcal{D}q \mathcal{D}x_n \exp(\frac{i}{\hbar} S[q, x_n]), \quad (3.11)$$

where the integral is over all paths  $q(s)$ ,  $x_n(s)$ ,  $0 \leq s \leq t$  with  $q(0) = q_i, x_n(0) = x_{n_i}$ , and  $q(t) = q_f, x_n(t) = x_{n_f}$ . Here the path probability is weighted according to the usual action

$$S[q, x_n] = \int_0^t ds \mathcal{L}(q, \dot{q}, x_n, \dot{x}_n, s), \quad (3.12)$$

where  $\mathcal{L}$  is the Lagrangian associated with the Hamiltonian (3.1). Hence

$$\mathcal{L}_0(q, \dot{q}) = \frac{1}{2} M \dot{q}^2 - V(q, s), \quad (3.13)$$

$$\mathcal{L}_R(x_n, \dot{x}_n) = \sum_{n=1}^N [\frac{1}{2} m_n \dot{x}_n^2 - \frac{1}{2} m_n w_n^2 x_n^2] \quad (3.14)$$

$$\mathcal{L}_{0R}(q, \dot{x}_n) = \sum_{n=1}^N [c_n q x_n - q^2 \frac{c_n^2}{2m_n w_n^2}]. \quad (3.15)$$

Note that in the Euclidean action functional (3.6) kinetic and potential energies are added, while the potential energy is subtracted from the kinetic term in the familiar action (3.12).

### 3.3 Quantum damped harmonic oscillator

We consider a Brownian particle in a harmonic potential

$$V(\hat{q}) = \frac{m}{2}w_0^2\hat{q}^2 - qF(t), \quad (3.16)$$

where we allow for a time-dependent external force  $F(t)$  coupled linearly to the particle. As has been stated before,  $F(t)$  is assumed not to influence the initial state, i.e.

$$F(t) = 0, t \leq 0. \quad (3.17)$$

Inserting (3.16), the potential term in the effective action  $\Sigma[x, r, \bar{q}]$  (see B), becomes

$$-V(r + \frac{x}{2}, s) + V(r - \frac{x}{2}, s) = -Mw_0^2rx + xF(s). \quad (3.18)$$

Now, for a harmonic oscillator, the complex action is stationary for trajectories satisfying

$$\begin{aligned} m\ddot{q}_{\pm}(s) + mw_0^2q_{\pm}(s) \mp \frac{1}{2}\frac{d}{ds}\int_s^t du\eta(s-u)[q_+(u) - q_-(u)] \\ + \frac{1}{2}\frac{d}{ds}\int_s^t du\eta(s-u)[q_+(u) - q_-(u)] \\ = i\int_0^t duK'(s-u)[q_+(u) - q_-(u)]. \end{aligned} \quad (3.19)$$

As in the undamped case, the paths are subject to the boundary conditions  $q_{\pm}(0) = q'_{\pm}$  and  $q_{\pm}(t) = q''_{\pm}$ . To make the discussion transparent, we consider the special case of Ohmic damping in addition to the assumption of factorizing initial conditions and the restriction to the real part of the equations of motion. We thus set  $I(w) = m\gamma w$  and

$\gamma(t) = \eta(t)/m = 2\gamma\delta(t)$ , so that the equations of motion, the (3.19) reduce to

$$\ddot{q}_{\pm} + w_0^2 q_{\pm} + \gamma \dot{q}_{\mp} = 0, \quad (3.20)$$

where the damping term couples the trajectories  $q_+$  and  $q_-$ . It is interesting to note that  $\gamma \dot{q}_{\mp}$  acts actually as a driving instead of a damping in the sense that the separation between trajectories grows exponentially. This can be seen more clearly by decoupling the two equations of motion, using sum,  $q = (q_+ + q_-)/2$ , and difference coordinates,  $\tilde{q} = q_+ - q_-$ . The (3.20) then read

$$\begin{aligned} \ddot{q} + \gamma \dot{q} + w_0^2 q &= 0, \\ \ddot{\tilde{q}} - \gamma \dot{\tilde{q}} + w_0^2 \tilde{q} &= 0. \end{aligned} \quad (3.21)$$

The solutions of the equations of motion (3.21) read

$$q(s) = q' \frac{G_-(t-s)}{G_-(t)} + q'' \frac{G_+(s)}{G_+(t)} \quad (3.22)$$

$$\tilde{q}(s) = \tilde{q}' \frac{G_+(t-s)}{G_+(t)} + \tilde{q}'' \frac{G_-(s)}{G_-(t)}, \quad (3.23)$$

where

$$G_{\pm}(t) = \frac{1}{w_d} \exp\left[\mp \frac{1}{2} \gamma t\right] \sin(w_d t). \quad (3.24)$$

Here,  $w_d = \sqrt{w_0^2 - \frac{\gamma^2}{4}}$ . The undamped time evolution of the Wigner function can immediately be transferred to the dissipative case if we relate the Wigner propagating function to the propagating function by means of

$$G_w(\mathbf{r}'', \mathbf{r}', t) = \frac{1}{2\pi\hbar} \int d\tilde{q}' d\tilde{q}'' \exp\left[\frac{i}{\hbar}(p'\tilde{q}' - p''\tilde{q}'')\right] J(\tilde{q}'', q'', t; \tilde{q}', q'), \quad (3.25)$$



where we call that  $\mathbf{r} = (p, q)$  is the phase-space vector. Performing the transformation in the (3.25), we therefore arrive at the Wigner propagating function

$$G_w(\mathbf{r}'', \mathbf{r}', t) = \delta[\mathbf{r}'', \mathbf{r}^{cl}(\mathbf{r}', t)], \quad (3.26)$$

where the classical phase-space trajectory

$$p^{cl}(t) = \dot{G}_+(t)p' + m \left[ \frac{|\dot{G}_+(t)|^2}{G_+(t)} - \frac{1}{G_-(t)} \right] q', \quad (3.27)$$

$$q^{cl}(t) = \frac{G_+(t)}{m}p' + \dot{G}_+(t)q', \quad (3.28)$$

with  $G_{\pm}(t)$  defined by (3.24) is now damped. While, in the (3.27) and (3.28) satisfies  $q^{cl}(0) = q'$  as expected, the initial momentum is given by  $p^{cl}(0) = p' - m\gamma q'$ . This initial slip is typical for factorizing initial conditions [FH63, AES82]. Now, from (3.26), it follows that

$$G_w(\mathbf{r}'', \mathbf{r}', t) = \frac{m}{\pi\hbar\Lambda(t)^{\frac{1}{2}}} \left| \frac{\dot{G}_+(t)}{G_+(t)} \right| \exp\left[-\frac{1}{\pi\hbar\Lambda(t)} [\mathbf{r}'' - \mathbf{r}^{cl}(t)]^T \Sigma [\mathbf{r}'' - \mathbf{r}^{cl}(t)]\right], \quad (3.29)$$

whose center moves along the damped classical trajectory in (3.27) and (3.28). The matrix appearing in the exponent is given by its components.

$$\begin{aligned} \Sigma_{11} &= a(t), \\ \Sigma_{12} = \Sigma_{21} &= -m \frac{\dot{G}_+(t)}{G_+(t)} [a(t) + b(t)], \\ \Sigma_{22} &= m^2 \frac{[\dot{G}_+(t)]^2}{[G_+(t)]^2} [a(t) + 2b(t) + c(t)], \\ \Lambda(t) &= \frac{\det(\Sigma)}{m^2} = a(t)c(t) - b(t)^2. \end{aligned} \quad (3.30)$$

The functions

$$\begin{aligned}
a(t) &= [\dot{G}_+(t)]^2 \Psi(t, t), \\
b(t) &= \dot{G}_+(t) G_+(t) \frac{\partial \Psi(t, t')}{\partial t} \Big|_{t' \nearrow t}, \\
c(t) &= [G_+(t)]^2 \frac{\partial^2 \Psi(t, t')}{\partial t \partial t'} \Big|_{t' \nearrow t},
\end{aligned} \tag{3.31}$$

can all be expressed in terms of a single function

$$\Psi(t, t') = \int_0^t ds \int_0^{t'} du K'(s-u) \frac{G_+(t-s)}{G_+(t)} \frac{G_+(t'-u)}{G_+(t')}. \tag{3.32}$$

This function is completely determined by the thermal position autocorrelation function  $\langle q(t)q(0) \rangle$  and its time derivatives. We employ the law of composition (divisibility principle) in the Wigner propagation function for the study of non-Markovianity in open quantum systems. Specifically, in the (3.29), this is:

$$\begin{aligned}
G_w(p'', q'', t_f, t_0, p', q') &= \frac{m}{\pi \hbar \Lambda (t_f - t_0)^{\frac{1}{2}}} \left| \frac{\dot{G}_+(t_f - t_0)}{G_+(t_f - t_0)} \right| \\
&\times \exp\left[ \frac{1}{\pi \hbar \Lambda (t_f - t_0)} [\mathbf{r}'' - \mathbf{r}^{cl}(t_f - t_0)]^T \Sigma [\mathbf{r}'' - \mathbf{r}^{cl}(t_f - t_0)] \right].
\end{aligned} \tag{3.33}$$

Therefore, we are interested in verifying, under what conditions the composition law (divisibility principle) is verified, this is done taking into account in the 2.7 and 3.33. That is to say,

$$G_w(p'', q'', t_f, t_0, p', q') = G_w(p'', q'', t_f, t_i, p''', q''') G_w(p''', q''', t_i, t_0, p', q'). \tag{3.34}$$

In this case, it has been shown that the principle of divisibility incorporated in the (3.34) is only satisfied, for  $\gamma = 0$ . That is to say, the process is Markovian. On the other hand, for values of  $\gamma \neq 0$ , the composition implies that it has memory effects (non-Markovian dynamics). Also, the Normalization Factor (NF) of the respective

composition is given by

$$NF(t_f, t_i, t_0) = \frac{2\pi}{\sqrt{4f_2(t_f, t_i, t_0) - \frac{f_3^2(t_f, t_i, t_0)}{f_4(t_f, t_i, t_0)} \sqrt{f_4(t_f, t_i, t_0)}}} \frac{m^2}{4\pi^2 \hbar^2 \sqrt{\Lambda(t_f - t_i)} \sqrt{\Lambda(t_i - t_0)}} \left| \frac{\dot{G}_+(t_f - t_i)}{G_+(t_f - t_i)} \right| \left| \frac{\dot{G}_+(t_i - t_0)}{G_+(t_i - t_0)} \right| \quad (3.35)$$

Furthermore, it follows that

$$G_w(p'', q'', t_f, t_i, p''', q''') G_w(p''', q''', t_i, t_0, p', q') = \frac{2\pi}{\sqrt{4f_2(t_f, t_i, t_0) - \frac{f_3^2(t_f, t_i, t_0)}{f_4(t_f, t_i, t_0)} \sqrt{f_4(t_f, t_i, t_0)}}} \frac{m^2}{4\pi^2 \hbar^2 \sqrt{\Lambda(t_f - t_i)} \sqrt{\Lambda(t_i - t_0)}} \left| \frac{\dot{G}_+(t_f - t_i)}{G_+(t_f - t_i)} \right| \left| \frac{\dot{G}_+(t_i - t_0)}{G_+(t_i - t_0)} \right| \exp\left[\frac{\Upsilon_1(t_f, t_i, t_0)}{\Upsilon_2(t_f, t_i, t_0)} - \Upsilon_3(t_f, t_i, t_0)\right]. \quad (3.36)$$

Details of representations  $f_n(t_f, t_i, t_0)$ , for all  $n = 1, 2, 3, 4, 5$  and  $\Upsilon_m(t_f, t_i, t_0)$  with  $m = 1, 2, 3$  are given in (B). Therefore, we introduce trajectories in the phase space, taking into account a non-unit dynamics at the quantum level, similar to the (3.27) and (3.28). This is,

$$p_1(t_f, t_0, p', q') = \dot{G}_+(t_f - t_0)p' + m(\gamma\dot{G}(t_f - t_0) + \ddot{G}(t_f - t_0))q', \quad (3.37)$$

$$q_1(t_f, t_0, p', q') = \frac{G_+(t_f - t_0)}{m}p' + (\gamma G_+(t_f - t_0) + \dot{G}(t_f - t_0))q'. \quad (3.38)$$

Analogously, inserting the (3.37) and (3.38) in the (3.34) it follows that the composition is only valid for  $\gamma = 0$ . The application of the principle of divisibility in the Wigner propagation function in the phase space, considering: the damping, the dissipation and, therefore, the sudden coupling of the bath to the environment, does not admit an experimental accessibility, implying the use of tomography process quantum.



# Chapter 4

## Time-Divisibility in the Energy Domain

We have previously analyzed the different correlation functions in the time domain. Furthermore, we apply the divisibility criterion on the Gaussian Wigner propagation function. Therefore, we are interested in observing the respective correlations or characterizations in the energy domain.

In this chapter, we present the necessary and sufficient criteria in the energy domain to compose in the time domain. This was done by applying the principle of divisibility (composition), taking into account the Hilbert and Liouville spatial partition. Later, we will show the characterization of the Gaussian or Lorentzian profiles and, therefore, we will classify the dynamics as Markovian or non-Markovian. Finally, we will set the discussion with some examples, based on a two-level electronic system by the normal modes of the vibrational degree of freedoms and the spin boson model.

However, given a non-unit quantum mechanical process, the question of whether the loss of coherence followed by a physical system is non-Markovian (and to what extent), is of great relevance [dVA17] since it defines the predictions that can be do for physical observables. Furthermore, non-local correlations over time are the quintessential effect of non-Markovian dynamics. Since time and energy are (canonical conjugate variables) in quantum mechanics, it is natural to expect that correlations in time can be observed in the energy domain. Therefore, in this chapter, we incorporate an experimentally

accessible measure in the energy domain to quantify the non-Markovian character of open quantum system dynamics.

## 4.1 Projection Operators, Reduced Equations of Motion, and Effective Hamiltonians

Projection operators are defined as follows: we consider a basis set in our Hilbert space  $|\phi_i\rangle$ . We then partition the space into two parts,  $\hat{\mathbf{P}}$  and  $\hat{\mathbf{Q}}$ , and introduce the operators [EGP13, MK79]:

$$\hat{\mathbf{P}} = \sum_{i=1}^n |\phi_i\rangle\langle\phi_i|, \hat{\mathbf{Q}} = \sum_{i=n+1}^{\infty} |\phi_i\rangle\langle\phi_i| \quad (4.1)$$

where  $n$  is some chosen cutoff that defines the partitioning. From these definitions it immediately follows that

$$\hat{\mathbf{P}} + \hat{\mathbf{Q}} = 1, \quad (4.2)$$

$$\hat{\mathbf{P}}^2 = \hat{\mathbf{P}}, \hat{\mathbf{Q}}^2 = \hat{\mathbf{Q}}, \quad (4.3)$$

$$\hat{\mathbf{P}}\hat{\mathbf{Q}} = \hat{\mathbf{Q}}\hat{\mathbf{P}} = 0. \quad (4.4)$$

Operators that satisfy (4.2-4.4) are called *projection operator*. Equation 4.3 implies that projection operators are *idempotent*. We now return to the *Schrödinger* equation. Inserting the partitioning of the unit operator (4.2) between the  $\hat{H}$  and the  $\psi$ , and multiplying both sides from the left either  $\hat{\mathbf{P}}$  or  $\hat{\mathbf{Q}}$ ,

$$\dot{\psi} = -\frac{i}{\hbar}\hat{H}\psi \quad (4.5)$$

we obtain two coupled equations for  $\hat{\mathbf{P}}\psi$  and  $\hat{\mathbf{Q}}\psi$

$$\hat{\mathbf{P}}\dot{\psi} = -\frac{i}{\hbar}(\hat{\mathbf{P}}\hat{H}\hat{\mathbf{P}})(\hat{\mathbf{P}}\psi) - \frac{i}{\hbar}(\hat{\mathbf{P}}\hat{H}\hat{\mathbf{Q}})(\hat{\mathbf{Q}}\psi), \quad (4.6)$$

$$\hat{\mathbf{Q}}\dot{\psi} = -\frac{i}{\hbar}(\hat{\mathbf{Q}}\hat{H}\hat{\mathbf{P}})(\hat{\mathbf{P}}\psi) - \frac{i}{\hbar}(\hat{\mathbf{Q}}\hat{H}\hat{\mathbf{Q}})(\hat{\mathbf{Q}}\psi), \quad (4.7)$$

In matrix form these equations read

$$\begin{bmatrix} \hat{\mathbf{P}}\dot{\psi} \\ \hat{\mathbf{Q}}\dot{\psi} \end{bmatrix} = -\frac{i}{\hbar} \begin{bmatrix} \hat{\mathbf{P}}\hat{H}\hat{\mathbf{P}} & \hat{\mathbf{P}}\hat{H}\hat{\mathbf{Q}} \\ \hat{\mathbf{Q}}\hat{H}\hat{\mathbf{P}} & \hat{\mathbf{Q}}\hat{H}\hat{\mathbf{Q}} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{P}}\psi \\ \hat{\mathbf{Q}}\psi \end{bmatrix}$$

Solving for  $\hat{\mathbf{Q}}\psi$  we have

$$\hat{\mathbf{Q}}\psi(t) = \hat{\mathbf{Q}}\psi(0) - \frac{i}{\hbar} \int_0^t d\tau \exp[-\frac{i}{\hbar}\hat{\mathbf{Q}}\hat{H}\hat{\mathbf{Q}}(t-\tau)]\hat{\mathbf{Q}}\hat{H}\hat{\mathbf{P}}[\hat{\mathbf{P}}\psi(\tau)]. \quad (4.8)$$

Substituting into the equation for  $\hat{\mathbf{P}}\psi$ , and assuming that the system is initially in the  $\hat{\mathbf{P}}$  space so that  $\hat{\mathbf{Q}}\psi(0) = 0$  we finally obtain

$$\hat{\mathbf{P}}\dot{\psi} = -\frac{i}{\hbar}\hat{\mathbf{P}}\hat{H}\hat{\mathbf{P}}(\hat{\mathbf{P}}\psi) + (\frac{i}{\hbar})^2 \int_0^t d\tau \hat{\mathbf{P}}\hat{H}\hat{\mathbf{Q}} \exp[-\frac{i}{\hbar}\hat{\mathbf{Q}}\hat{H}\hat{\mathbf{Q}}(t-\tau)]\hat{\mathbf{Q}}\hat{H}\hat{\mathbf{P}}[\hat{\mathbf{P}}\psi(\tau)]. \quad (4.9)$$

We next introduce a similar partitioning of the Green function

$$\begin{bmatrix} \hat{\mathbf{P}}\psi \\ \hat{\mathbf{Q}}\psi \end{bmatrix} = -\frac{i}{\hbar} \begin{bmatrix} \hat{\mathbf{P}}G(t)\hat{\mathbf{P}} & \hat{\mathbf{P}}G(t)\hat{\mathbf{Q}} \\ \hat{\mathbf{Q}}G(t)\hat{\mathbf{P}} & \hat{\mathbf{Q}}G(t)\hat{\mathbf{Q}} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{P}}\psi(0) \\ \hat{\mathbf{Q}}\psi(0) \end{bmatrix}$$

where

$$\hat{\mathbf{P}}G(t)\hat{\mathbf{P}} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dE \exp[(\frac{i}{\hbar})Et]\hat{\mathbf{P}}G(E)\hat{\mathbf{P}}. \quad (4.10)$$

By performing a Fourier transform on (4.9) we have

$$\hat{\mathbf{P}}G(E)\hat{\mathbf{P}} = \frac{1}{E - \hat{\mathbf{P}}\hat{H}_{\text{eff}}(E)\hat{\mathbf{P}}}, \quad (4.11)$$

with the effective Hamiltonian

$$\hat{H}_{\text{eff}}(E) = \hat{H} + \hat{H}\hat{Q}\tilde{G}(E)\hat{Q}\hat{H}, \quad (4.12)$$

where

$$\tilde{G}(E) = \frac{1}{E - \hat{Q}\hat{H}\hat{Q}}. \quad (4.13)$$

We next partition the Hamiltonian, and assume that the zero-order Hamiltonian  $\hat{H}_0$  commutes with the  $\hat{\mathbf{P}}$  projection-operator so that

$$\hat{\mathbf{P}}\hat{H}_0\hat{\mathbf{Q}} = \hat{\mathbf{Q}}\hat{H}_0\hat{\mathbf{P}} = 0 \quad (4.14)$$

The effective Hamiltonian thus assumes the form

$$\hat{\mathbf{P}}\hat{H}_{\text{eff}}(E)\hat{\mathbf{P}} = \hat{\mathbf{P}}\hat{H}_0\hat{\mathbf{P}} + \hat{\mathbf{P}}R(E)\hat{\mathbf{P}}, \quad (4.15)$$

with the self energy operator

$$\hat{\mathbf{P}}R(E)\hat{\mathbf{P}} = \hat{\mathbf{P}}V\hat{\mathbf{P}} + \hat{\mathbf{P}}V\hat{Q}\tilde{G}(E)\hat{Q}V\hat{\mathbf{P}} \quad (4.16)$$

Equation (4.9) or (4.11) allows us to consider only partial information and solve for  $\hat{\mathbf{P}}\psi$ . The effect of  $\hat{\mathbf{Q}}\psi$  is rigorously incorporated in the effective Hamiltonian  $\hat{H}_{\text{eff}}$  through the self-energy operator  $R(E)$ . The other projections of the Green function can be obtained in a similar way. As an example of an application for the projected Green function, consider a model system of a single state  $|s\rangle$  coupled to a continuum  $|l\rangle$ .

$$H = |s\rangle E_s \langle s| + \sum_{l=1}^N |l\rangle E_l \langle l| + \sum_{l=1}^N (V_{sl}|s\rangle \langle l| + V_{ls}|l\rangle \langle s|), \quad (4.17)$$



This model is proposed by Wigner and Weisskopf [SB12], it is a prototype for irreversible decay. It can represent radiative-damping, autoionization in atoms, intramolecular relaxation, coupling to a photon bath, etc. We shall be interested in calculating the probability of the system to be found in the  $|s\rangle$  at time  $t$ , given that it was prepared in the same state as  $t = 0$ . To that end we need to calculate the matrix element  $G_{ss}$ . The straightforward (and most tedious) way to do that is by calculating the eigenstates and eigenvalues of this Hamiltonian, which requires the diagonalization of an  $(N + 1) \times (N + 1)$  matrix. We then have

$$\hat{H}|j\rangle = E_j|j\rangle, \quad (4.18)$$

and

$$G_{ss}(E) = \sum_j \frac{|\langle s|j\rangle|^2}{E - E_j + i\epsilon}, \quad (4.19)$$

where,

$$P_{ss} \equiv |G_{ss}(t)|^2 = \left| \sum_j |\langle s|j\rangle|^2 \exp\left(-\frac{i}{\hbar}E_j t\right) \right|^2. \quad (4.20)$$

The way in which the partition of the respective projectors is introduced is similar to Ref. [SB12], that is to say

$$\hat{\mathbf{P}} = |s\rangle\langle s|; \hat{\mathbf{Q}} = \sum_l |l\rangle\langle l|. \quad (4.21)$$

Therefore, we write

$$G_{ss}(t) = \theta(t) \exp\left[\frac{-i}{\hbar}(E_s + \Delta_s)(t) - \frac{\Gamma_s}{2}(t)\right], \quad (4.22)$$

with

$$R_{ss}(E) = \sum_l \frac{|V_{sl}|^2}{E - E_l + i\epsilon} \equiv \Delta_s(E) - \frac{i}{2}\hbar\Gamma_s(E). \quad (4.23)$$

Assuming that the  $|l\rangle$  variety is sufficiently dense, it follows that

$$R_{ss}(E) = \int dE_l \frac{|V_{sl}|^2 \rho(E_l)}{E - E_l + i\epsilon}. \quad (4.24)$$

Thus,

$$\Delta_s(E) = \text{PP} \int dE_l \frac{|V_{sl}|^2 \rho(E_l)}{E - E_l}, \quad (4.25)$$

$$\hbar\Gamma_s(E) = 2\pi \int |V_{sl}|^2 \delta(E - E_l) \rho(E_l) dE_l. \quad (4.26)$$

If the set is dense, then

$$\Delta_s(E) \cong \Delta_s(E_s); \quad \Gamma_s(E) \cong \Gamma_s(E_s), \quad (4.27)$$

$$\mathfrak{J}(t - t_0) = \frac{-1}{2\pi i} \int_{-\infty}^{\infty} dE \frac{\exp[(-\frac{i}{\hbar})E(t - t_0)]}{E - E_s - \Delta_s(E) + \frac{i}{2}\Gamma_s(E)}. \quad (4.28)$$

In this case, we are interested in studying the links of the environment – system, considering discrete or continuous states (varieties) and incorporating sufficient and necessary criteria in the domain of energy to compose  $G_{ss}(t)$  in the time domain, this is done taking into account in the (2.7) and (4.28). However, we are interested in composing  $\mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0)$ . In this case, we propose a theorem with the respective proof and, therefore, we show that is in the Markovian regime, applying the principle of divisibility (2.24). The different intermediate details of the test can be seen (A).

**Theorem 1.** . *Let  $\Gamma_s, \Delta_s$  parameters, then  $G_{ss}(t - t_0) = G_{ss}(t - t_p)G_{ss}(t_p - t_0) \forall t \in \mathbf{R}$ .*

Proof: Let  $\Gamma_s, \Delta_s : S \subset \mathbf{R} \rightarrow \mathbf{R}$  continuously differentiable functions. Therefore, from (4.22), it follows that

$$\begin{aligned} G_{ss}(t - t_0) &= \theta(t - t_0) \exp \left[ -\frac{i}{\hbar}(E_s + \Delta_s)(t - t_0) - \frac{\Gamma_s}{2}(t - t_0) \right] \\ &= \theta(t - t_p) \exp \left[ -\frac{i}{\hbar}(E_s + \Delta_s)(t - t_p) - \frac{\Gamma_s}{2}(t - t_p) \right] \times \theta(t_p - t_0) \exp \left[ -\frac{i}{\hbar}(E_s + \Delta_s)(t_p - t_0) - \frac{\Gamma_s}{2}(t_p - t_0) \right] \\ &= G_{ss}(t - t_p)G_{ss}(t_p - t_0) \end{aligned} \quad (4.29)$$

The previous theorem shows that the quantum system coupled to a structureless

continuum implies Markovian dynamics. That is, for all  $\Gamma_s$  and  $\Delta_s$  parameters, the measure is accessible experimentally.

**Theorem 2.** (*Pachón, Triviño*). *Let  $\Gamma_s(E), \Delta_s(E) : S \subset \mathbf{R} \rightarrow \mathbf{R}$  continuously differentiable functions, if  $\Gamma_s(E) + 2i\Delta_s(E) = k$  then  $\mathfrak{J}(t - t_0) = \mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0)$ , being  $k$  a real number and  $\forall t \in \mathfrak{R}$*

Proof: We are interested in observing under what conditions  $\mathfrak{J}(t - t_0) = \mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0)$  at different orders. Therefore, taking into account in the (4.28), follow immediately

$$\mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0) = \frac{-1}{2\pi i} \frac{1}{2\pi} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\tau \frac{\exp[-\frac{i}{\hbar}E(t-t_p)] \exp[\frac{i}{\hbar}\tau(\epsilon-E)]}{E - E_s - \Delta_s(\epsilon) + \frac{i}{2}\Gamma_s(\epsilon)} \quad (4.30)$$

Now expanding  $\frac{1}{E - E_s - \Delta_s(\epsilon) + \frac{i}{2}\Gamma_s(\epsilon)}$ , around  $\epsilon$  and performing the Fourier transformation, it follows that the second order composition is given by

$$\begin{aligned} \mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0) &= [2\hbar - (t - t_p)(\Gamma_s(E_s) + 2i\Delta_s(E_s))] \\ &\quad \times (2\hbar + (t_0 - t_p)(\Gamma_s(E_s) + 2i\Delta_s(E_s))) \times (\Gamma'_s(E_s) + 2i\Delta'_s(E_s))^2 \end{aligned} \quad (4.31)$$

That being the case, it is necessary that  $\Gamma_s(E) + 2i\Delta_s(E) = k$ . That is to say,  $\Gamma_s(E) = k_1$  and  $\Delta_s(E) = \frac{k_2}{2}$ ,  $\forall k_1, k_2 \in \mathfrak{R}$  or  $\Gamma'_s(E_s) + 2i\Delta'_s(E_s) = 0$ . Now, this is valid for all functions that satisfy  $\Gamma_s(E) = k - 2i\Delta_s(E)$ . On the other hand, if  $\Gamma_s(E), \Delta_s(E)$  are independent of  $E$ , it follows that  $\Gamma_s^n(E) + 2i\Delta_s^n(E) = 0$ , where  $n$ , represents the  $n$ -th derivate of order  $\mathcal{O}^{2n}$ . Also,  $\Gamma$  and  $\Delta$  have real coefficients in a ring  $A[E]$ .

Now, if the functions  $\Gamma_s(E)$  and  $\Delta_s$  depend on energy, it implies non-Markov dynamics. That is, the measure is not accessible experimentally, since the continuum acquires structure.

Despite, the fact that a wide family of functions are obtained that satisfy this condition  $\Gamma_s^n(E) = k - 2i\Delta_s^n(E)$ . This allows a new window to be opened in the study of open quantum systems (Markovian or non-Markovian). In fact, all function families (distributions) satisfy this condition. For example,  $\Gamma(E) = \int_0^{\infty} t^{E-1} \exp(-t) dt$ ,

$\Gamma(E) = (E - 1)!, \forall E > 0$ . On the other hand,  $\Delta_s(E) = E \pm k$ , for every real  $k$  number.

In this section, we incorporate sufficient and necessary criteria in the domain of energy to compose in the domain of time. All this was generated through the divisibility approach, study of the Nakjima-Zwanzing equations, partition of the space of Hilbert or Louville. And also, the topology was studied in  $\mathfrak{R}^n$  to formalize the theorems.

## 4.2 Experimental Observables and Non-Markovian

Although the formal in the (4.19) allows for an intuitive introduction of our proposal, our objectives is to identify the time correlation in an energy domain experimentally accessible observable. In doing so, we make a connection with the field of non-linear spectroscopy and discuss the influence of the non-Markovian dynamics in the fluorescence and absorption spectra. To illustrate our proposal, let us consider the Hamiltonian of two electronic states  $|g\rangle$  and  $|e\rangle$  in contact with their own normal vibrational modes, which are described by the Hamiltonian  $H_g$  and  $H_e$ , respectively,

$$\hat{H}_{g,e} = \langle g|H_g|g\rangle + \langle e|H_e|e\rangle, \quad (4.32)$$

with  $\hat{H}_g = \frac{1}{2} \sum_j \hbar w_j (\mathbf{p}_j + \mathbf{q}_j)$ ,  $\hat{H}_e = \hbar w_{eg}^0 + \frac{1}{2} \sum_j \hbar w_j [\mathbf{p}_j + (\mathbf{q}_j + \mathfrak{d}_j)^2]$ , where we have introduced the dimensionless coordinates  $\mathbf{p}_j = (\hbar w_j m_j)^{-\frac{1}{2}} p_j$ ,  $\mathbf{q}_j = (\hbar w_j m_j)^{\frac{1}{2}} q_j$  and  $\mathfrak{d}_j = (\hbar w_j m_j)^{\frac{1}{2}} d_j$ . The electronic energy gap is  $w_{eg} = w_{eg}^0 + \frac{1}{2} \sum_j \mathfrak{d}_j w_j$ .

For this model, the response function  $C(t)$  is given by  $C(t) = \sum_j w_j^2 S_j [(\bar{n}_j + 1) \exp(-it) + \bar{n}_j \exp(it)]$ , being  $\bar{n}_j = [\exp(\beta \hbar w_j) - 1]^{-1}$  the thermally averaged occupation number of the  $j$ -th mode. We have introduced the dimensionless Huang-Rhys factor  $S = \frac{1}{2} \mathfrak{d}_j^2$ , which is related to the coupling strength of the nuclear degree of freedoms to the electronic transition and can be obtained from the absorption and

fluorescence spectra (see Chap. 8 in Ref. [Muk99] for detail), which are defined as

$$A(w) = \frac{1}{\pi} \Re \int_0^\infty dt \exp[i(w - w_{\text{eg}})t - g(t)], \quad (4.33)$$

$$F(w) = \frac{1}{\pi} \Re \int_0^\infty dt \exp[i(w - w_{\text{eg}} - 2\lambda)t - g^*(t)], \quad (4.34)$$

respectively,

$$g(t) = \sum_j S_j \left[ \coth\left(\frac{\beta \hbar w_j}{2}\right) (1 - \cos w_j t) + i(\sin(w_j t) - w_j t) \right], \quad (4.35)$$

is the line-broadening function and  $\lambda = \sum_j S_j w_j$ .

By defining the spectral density as  $\tilde{C}(w) = 2\Re \int_0^\infty dt \exp(iwt)C(t)$ , and assuming for it the particular for  $\tilde{C}'' = 2\lambda \frac{w\Lambda}{w^2 + \Lambda^2}$ , we get (cf. Chap. 8 in Ref. [Muk99])  $g(t) = g' + ig''$ , whit  $g'' = -(\frac{\lambda}{\Lambda})[\exp(-\Lambda t) + \Lambda t - 1]$  and  $g' = -g'' \coth(\frac{\beta \hbar w_j}{2}) + \frac{4\lambda\Lambda}{\hbar\beta} \sum_{n=1}^\infty \frac{\exp(-\nu_n t) + \nu_n t - 1}{\nu_n(\nu_n^2 - \Lambda^2)}$ , being  $\nu_n \equiv \frac{2\pi}{\hbar\beta} n$  the Matsubara frequencies. For our subsequent discussion, let us define the dimensionless parameter  $\kappa = \frac{\Lambda}{\Delta} = (\frac{\hbar\Lambda^2}{2\lambda\kappa_B T})^2$ . However, if  $\kappa \ll 1$  the nuclear dynamics is slow (with time scales  $\Lambda^{-1}$ ), i.e., it is non Markovian. For this case we  $g = \frac{1}{\hbar} \lambda \kappa_B T t^2$  and therefore

$$A(w) \sim \exp\left(-\frac{(w - w_i)^2}{2\Delta^2}\right), \quad (4.36)$$

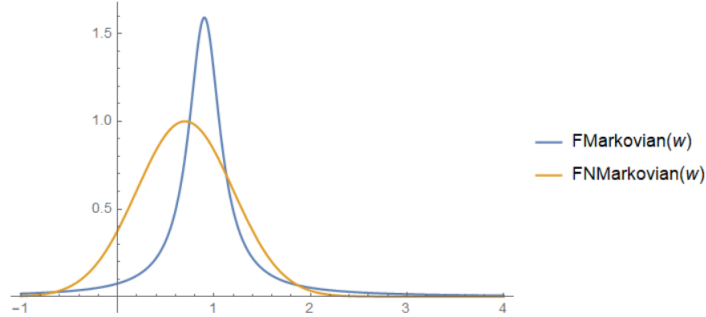
$$F(w) \sim \exp\left(-\frac{(w - w_i + 2\lambda)^2}{2\Delta^2}\right), \quad (4.37)$$

acquires a Gaussian profile. On the other hand, if  $\kappa \gg 1$ , the nuclear dynamics is fast compared to the coupling strength, i.e., it is Markovian. For this case, get  $g = \Gamma t - i\lambda t$ , whit  $\Gamma = \frac{\lambda\kappa_B T}{\hbar\Lambda}$ . Therefore

$$A(w) = F(w) = \frac{1}{\pi} \frac{\hat{\Gamma}}{(w - w_{\text{eg}}) + \hat{\Gamma}^2}. \quad (4.38)$$

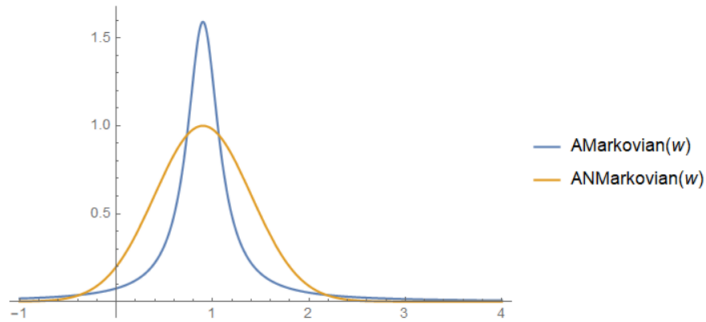
acquires a Lorentzian profile.

We show the behavior of the Markovian and Non-Markovian profiles which is related to the coupling strength of the nuclear degree of freedoms to the electronic transition and can be obtain from the fluorescence spectra



**Figure 4-1:** *Markovian and non-Markovian profile of fluorescence.* It is inferred, the Non-Markovian profile *Gaussian* and, therefore, the Markovianity, characterized by its *Lorentzian*. This, according to the equations 4-1, 4.38. In addition, we have taken into account:  $w_{eg} = 0.9$ ,  $\hbar = 1$ ,  $\lambda = 0.1$ ,  $\Lambda = 10$ ,  $w = [-1, 4]$

Analogously, we show the behavior of the Markovian and Non-Markovian profiles which is related to the coupling strength of the nuclear degree of freedoms to the electronic transition and can be obtain from the Absorption spectra



**Figure 4-2:** *Markovian and non-Markovian profile of absorption.* It is observed, the Non-Markovian profile *Gaussian* and, therefore, the Markovianity, characterized by its *Lorentzian*. This, according to the equations 4-2, 4.38. In addition, we have taken into account:  $w_{eg} = 0.9$ ,  $\hbar = 1$ ,  $\lambda = 0.1$ ,  $\Lambda = 10$ ,  $w = [-1, 4]$

The figures 4-1 and 4-2 corroborate the Markovian or non-Markovian profile of the fluorescence or absorption spectra. In fact, they are the foundation quantification of the non-Markovian dynamics, see 4-3.

### 4.3 Non-Markovian driven by stochastic processes

In previous case, we consider the dynamics induced in a two level electronic system by the normal modes of the vibrational degrees of freedom. Here we assume that the energy gap is stochastically modulated a random force  $\Omega(t)$ . Let us consider a two-level system described by the Hamiltonian

$$\hat{H}_S = \frac{1}{2}\hbar w_0 \sigma_z + \frac{1}{2}\hbar \Delta \sigma_z \Omega(t), \quad (4.39)$$

and coupled to a Gaussian stochastic function  $\Omega(t)$  determined by the quantum Liouville equation (cf. [Tan06] for detail) via the coupling term  $\frac{1}{2}\hbar \Delta \sigma_z \Omega(t)$ . This mimics the presence of a Gaussian bath with coupling term  $\frac{1}{2}\hbar \Delta \sum_{\alpha} g_{\alpha} (b_{\alpha}^{\dagger} + b_{\alpha})$ , with the correlation of the noise denoted by  $\gamma$ . If  $\gamma \gg \Delta$  for a fixed  $\gamma' = \frac{\Delta}{\gamma}$  (motional narrowing limit), the spectrum takes a Lorentzian form as

$$F(w) = \frac{2\gamma'}{\gamma'^2 + (w - w_0^2)}. \quad (4.40)$$

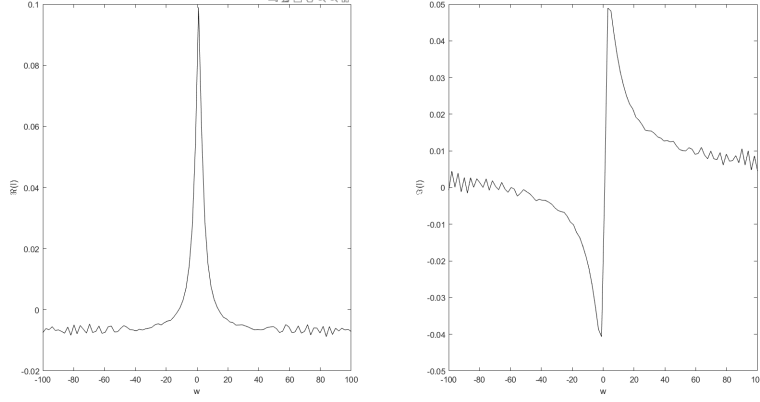
In the slow-modulation limit  $\gamma \ll (w - w_0^2) \ll \sqrt{2}\Delta$ , the spectrum takes a Gaussian distribution

$$F(w) = \frac{2\sqrt{2}}{2} \exp\left[-\frac{(w - w_0)^2}{2\Delta^2}\right]. \quad (4.41)$$

Here  $\gamma$  corresponds to the usual decay rate and in this formalism it is defined in terms of the two-point correlation function of the stochastic function  $\Omega(t)$  [Tan06].

### 4.4 Quantification of the non-Markovian dynamics

Above we have discussed two extreme cases, however, for a given physical process one non-Markovian contribution, i.e., we expect that the line profile is between a Lorentzian and a Gaussian.

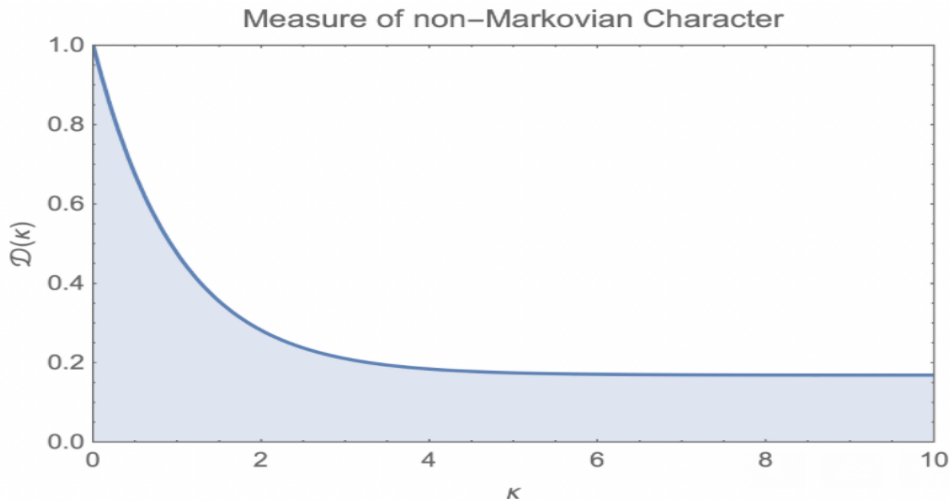


**Figure 4-3:** *Measured Spectrum.* We have calculated, the representation 4.34, using numerical integration. In addition, we consider  $w_{eg} = 0.9$ ,  $\hbar = 1$ ,  $\lambda = 0.1$ ,  $\Lambda = 10$ ,  $w = [-100, 100]$ .

Thus, our proposal is to quantify how different a given measured spectrum is from a simulated Lorentzian spectrum, i.e., we are interested in defining a measure of the non-Markovian character in terms of a cross-correlation between the measured spectrum and a Markovian simulated spectrum. In doing so, we define

$$\mathcal{D}(w_0) = \frac{\int dw \Lambda_m(w_0 + w) \Lambda_M(w)}{\int dw \Lambda_{nM}(w_0 + w) \Lambda_M(w)}, \quad (4.42)$$

where  $\Lambda$  denotes the either the absorption or fluorescence spectrum.  $\Lambda_m$  denotes the measured spectrum,  $\Lambda_M$  the simulated Markovian one ( $\kappa \geq 1$ ),  $\Lambda_{nM}$  stands for the simulated non-Markovian spectrum ( $\kappa \ll 1$ ).



**Figure 4-4:** *Measure of non-Markovian Character.*



In figure 4.4, we show the measure of the non-Markov character of a quantum system (electronic states) coupled to the bath (normal vibrational modes). Now, if  $\Lambda_m(w) = \Lambda_{nM}(w)$ ,  $\kappa \ll 1$ , it implies non-Markovian dynamics. Now, for  $\kappa \gg 1$ , Markovian dynamics follows. Therefore, we have found an experimentally accessible measure. That is, we can quantify the respective Markovian or non-Markov profiles, mediated by the absorption and fluorescence spectra.

## 4.5 Examples

Within an externally-driven spin-boson model description [ERT09], one could consider two equivalent models that arise, in principle, from two different physical situations: (a) consider a qubit coupled to its detector, which can be represented by a single harmonic oscillator mode of frequency  $\Omega_p$  and interaction strength  $g$ . Here, the harmonic oscillator mode interacts, in turn, with a set of harmonic oscillators, and we can write the model Hamiltonian as (qubit-oscillator plus oscillator-bath)  $\hat{H}_a(t) = \hat{H}_{qO}(t) + \hat{H}_{OB}$ , with

$$\begin{aligned} \hat{H}_{qO}(t) &= -\frac{\hbar\Delta}{2}\sigma_x - \frac{\hbar\varepsilon(t)}{2}\sigma_z + \hbar g\sigma_z X + \hbar\Omega_p B^\dagger B, \\ \hat{H}_{OB} &= X \sum_k \hbar\nu_k(b_k^\dagger + b_k) + \sum_k \hbar\omega_k b_k^\dagger b_k + X^2 \sum_k \hbar\frac{\nu_k^2}{\omega_k}, \end{aligned} \quad (4.43)$$

where  $B$  is the annihilation operator of the single harmonic mode,  $X = B^\dagger + B$ ,  $b_k$  and  $b_k^\dagger$  denote the bath mode operators,  $\sigma_i$  are the usual Pauli matrices,  $\hbar\Delta$  give the tunnel splitting, and the external driving  $\varepsilon(t) = \varepsilon_0 + A \cos(\Omega t)$  has the static bias  $\varepsilon_0$ . For  $A = 0$ , the level splitting of the isolated qubit is  $\hbar\nu = \hbar\sqrt{\varepsilon_0^2 + \Delta^2}$ . We recall that the spectral density for the continuous bath modes is Ohmic with dimensionless damping strength  $\gamma$ :

$$J_{\text{Ohm}}(\omega) = \sum_k \nu_k^2 \delta(\omega - \omega_k) = \gamma\omega \frac{\omega_D^2}{\omega^2 + \omega_D^2}, \quad (4.44)$$

with the usual high-frequency cut-off at  $\omega_D$ . In this model, the relevant physical system of interest is comprised by the qubit and the single mode.

Now the equivalent, second model corresponds to (b) the driven spin-boson Hamiltonian (the one you enter with a “different external driving”, and that we have recently used for modelling coupled chromophores):

$$H_{\text{SB}}(t) = -\frac{\hbar\Delta}{2}\sigma_x - \frac{\hbar\varepsilon(t)}{2}\sigma_z + \frac{1}{2}\sigma_z\hbar\sum_k\tilde{\lambda}_k(\tilde{b}_k^\dagger + \tilde{b}_k) + \sum_k\hbar\tilde{\omega}_k\tilde{b}_k^\dagger\tilde{b}_k, \quad (4.45)$$

where  $\tilde{b}_k$  is the annihilation operator of the  $k$ -th bath mode with frequency  $\tilde{\omega}_k$ . Let us assume a spectral density with a Lorentzian peak of width  $\Gamma = 2\pi\kappa\Omega_p$  at the characteristic detector frequency  $\Omega_p$ . This behaves Ohmically at low frequencies with the dimensionless coupling strength  $\alpha = \lim_{\omega\rightarrow 0} J_{\text{eff}}(\omega)/2\omega$ , that is:

$$J_{\text{eff}}(\omega) = \frac{2\alpha\omega\Omega_p^4}{(\Omega_p^2 - \omega^2)^2 + (\gamma\omega)^2}. \quad (4.46)$$

and  $g = \Omega_p\sqrt{\alpha/8\kappa}$ . Here, the detector acts as the qubit environment.

In conclusion, we have introduced the sufficient and necessary criteria in the domain of energy to compose in the domain of time. This composition has been made taking into account the algebraic structures and general topology. On the other hand, it is priorized in nonlinear spectroscopy to characterize Markovian dynamics in Gaussian or Lorentzian profiles. Similarly, a study of the fluorescence and absorption spectra has been carried out and, consequently, corresponding to the quantification of measurements accessible to the experiment.

# Chapter 5

## Conclusions and remarks

An exhaustive study of the literature was carried out to identify the main measures or approaches in the description of unitary or non-unit dynamics in open Markovian or non-Markovian quantum systems. In this case, we extend the measure 2.15 into the spaces  $L_p$  and Sobolev. Well, we don't just restrict ourselves to Hilbert spaces. In fact, we extrapolate metrics in terms of others. In addition, it was necessary to compare the existing theoretical results and, therefore, the latest experimental advances in the accessibility of Markovian quantification.

We apply the principle of divisibility (composition law) finding the sufficient and necessary criteria in the energy domain to compose in the time domain. For this, it was necessary to study the dynamics of open quantum systems, master equations, Hilbert or Liouville space partitioning, general topology, algebraic structures. In this case, we propose some theorems or corollaries that allowed us to formalize the theory and extend the result to different orders. The results are applicable to radioactive damping, atom ionization, intramolecular relaxation, photon bath coupling, based on the Weiskopf model.

The absorption and fluorescence spectra were studied, characterizing the Gaussian or Lorentzian representations in Markovian or non-Markovian profiles. Subsequently, we proposed a measure to describe the dynamics of non-Markovian open quantum systems in terms of the cross-correlation between the measured spectrum and a simulated Markovian spectrum. In fact, the Markovian (Lorentzian) or non-Markovian

(Gaussian) profile is immediately recognized in two electronic states in contact with their own normal vibrational modes. Therefore, we generate an experimentally accessible measure in non-Markovian open quantum systems.

We have demonstrated under what conditions the Wigner function along damped classical trajectories with unit dynamics or, on the contrary, inheriting quantum non-unit dynamics, satisfy the composition law (divisibility principle) or simply acquire memory effects (non-Markovian characterization).

On the other hand, there are still several aspects in which it is possible to deepen or feed back in the field of open quantum systems, from the non-Markovian perspective. Specifically, topological invariants, wound properties, topological groups or studies of complex systems immersed in algebraic or geometric varieties. In fact, we know that most of the tools of algebraic topology or Measurement Theory, imply the correct characterization of the spaces (Hilbert, Banach, Sobolev or  $L^p$ ). Therefore, future works allow the principle to be correlated with different complex systems (physicochemical), chaos, cryptography or biological systems.

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# Appendix A

## Sufficient and necessary criteria

We are interested in composing  $\mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0)$  at different orders.

$$\begin{aligned}\mathfrak{J}(t - t_p) &= \frac{-1}{2\pi i} \int_{-\infty}^{\infty} dE \frac{\exp[\frac{-i}{\hbar}E(t - t_p)]}{E - E_s - \Delta_s(E) + \frac{i}{2}\Gamma_s(E)} \\ &= \frac{-1}{2\pi i} \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dE d\tau \frac{\exp[\frac{-i}{\hbar}E(t - t_p)] \exp[\frac{i}{\hbar}\tau(\epsilon - E)]}{E - E_s - \Delta_s(\epsilon) + \frac{i}{2}\Gamma_s(\epsilon)}.\end{aligned}\quad (\text{A.1})$$

Now, expanding  $\frac{1}{E - E_s - \Delta_s(\epsilon) + \frac{i}{2}\Gamma_s(\epsilon)}$ , around  $\epsilon$  it follows that

$$\begin{aligned}\left[ \frac{1}{E - E_s - \Delta_s(\epsilon) + \frac{i}{2}\Gamma_s(\epsilon)}, \epsilon, E_s, 2 \right] &= \\ \frac{1}{E - E_s - \Delta_s(E_s) + \frac{i}{2}\Gamma_s(E_s)} &+ \frac{(-2i\Gamma'_s(E_s) + 4\Delta'_s(E_s)(\epsilon - E_s))}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^2} + O(\epsilon - E_s)^3 + \\ \frac{((-2(\Gamma'_s(E_s) + 2i\Delta'_s(E_s)))^2 + (\Gamma_s(E_s) - 2i(E - E_s - \Delta_s(E_s))))(\Gamma''_s(E_s) + 2i\Delta''_s(E_s)))(\epsilon - E_s)^2}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^3}.\end{aligned}\quad (\text{A.2})$$

Let,

$$\begin{aligned}H(E_s) &= \frac{1}{E - E_s - \Delta_s(E_s) + \frac{i}{2}\Gamma_s(E_s)} + \frac{(-2i\Gamma'_s(E_s) + 4\Delta'_s(E_s)(\epsilon - E_s))}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^2} + O(\epsilon - E_s)^3 \\ &+ \frac{((-2(\Gamma'_s(E_s) + 2i\Delta'_s(E_s)))^2 + (\Gamma_s(E_s) - 2i(E - E_s - \Delta_s(E_s))))(\Gamma''_s(E_s) + 2i\Delta''_s(E_s)))(\epsilon - E_s)^2}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^3}.\end{aligned}\quad (\text{A.3})$$

$$\begin{aligned}
\mathfrak{J}(t - t_p) &= \frac{-1}{2\pi i} \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dE d\tau \exp \left[ \frac{-i}{\hbar} E(t - t_p) \right] \exp \left[ \frac{i}{\hbar} \tau(\epsilon - E) \right] H(E_s), \\
&= \frac{-1}{2\pi i} \int_{-\infty}^{\infty} dE \exp \left[ \frac{-i}{\hbar} E(t - t_p) \right] H(E_s). \tag{A.4}
\end{aligned}$$

In an analogous way, the series process is carried out at different orders. Now, taking into account the following representation at order zero and introducing the Inverse Fourier Transform (IFT), it follows that  $(-\frac{1}{2\pi i})\sqrt{2\pi}(IFT[\frac{1}{E-E_s-\Delta_s(E_s)+\frac{i}{2}\Gamma_s(E_s)}, E, \frac{1}{\hbar}\tau])$  con  $Im(\Delta_s) == 0, Im(E_s) == 0$ , expanding and simplifying, it continues

$$\mathfrak{J}(\tau) = \exp \left[ -\frac{\tau(\Gamma_s(E_s) + 2i(E_s + \Delta_s(E_s)))}{2\hbar} \right] \Theta(\tau). \tag{A.5}$$

On the other hand, the first-order mathematical representation is given by

$$\begin{aligned}
\mathfrak{J}_1(\tau) &= e^{-\frac{\tau(\Gamma_s(E_s)+2i(E_s+\Delta_s(E_s)))}{2\hbar}} \Theta(\tau) \\
&\quad \left( -\frac{i}{2}\Gamma'_s(E_s) + \Delta'_s(E_s) \right) - e^{-\frac{\tau(\Gamma_s(E_s)+2i(E_s+\Delta_s(E_s)))}{2\hbar}} \\
&\quad \Theta(\tau)(-i\Gamma'_s(E_s) + 2\Delta'_s(E_s)) \frac{\tau(\Gamma_s(E_s) + 2i\Delta_s(E_s))}{4\hbar}. \tag{A.6}
\end{aligned}$$

Therefore, in second order, the respective composition

$$\mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0) = [\mathfrak{J}(t - t_p) + \mathfrak{J}_1(t - t_p)][\mathfrak{J}(t_p - t_0) + \mathfrak{J}_1(t_p - t_0)], \tag{A.7}$$

$$\begin{aligned}
&= [2\hbar - (t - t_p)(\Gamma_s(E_s) + 2i\Delta_s(E_s))] \times \\
&\quad [2\hbar + (t_0 - t_p)(\Gamma_s(E_s) + 2i\Delta_s(E_s))][\Gamma'_s(E_s) + 2i\Delta'_s(E_s)]^2. \tag{A.8}
\end{aligned}$$

Now for higher orders the procedure is similar. Without loss of generality in the third

order,

$$\begin{aligned}
\mathfrak{J}_3(\tau) = & \frac{1}{6(2E \cdot E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^4} e^{-\frac{iE_s\tau}{\hbar}} \delta^3(\tau) \\
& (12i\Gamma'_s(E_s)^3 - 72\Gamma'_s(E_s)^2\Delta'_s(E_s) + 96\Delta'_s(E_s)^3 \\
& \quad - 12i\Gamma'_s(E_s)(12\Delta'_s(E_s)^2 \\
& \quad + (\Gamma'_s(E_s) + 2i\Delta_s(E_s))(\Gamma''_s(E_s) + 2i\Delta''_s(E_s))) \\
& + 24(\Gamma_s(E_s) + 2i\Delta_s(E_s))\Delta'_s(E_s)(\Gamma''_s(E_s) + 2i\Delta''_s(E_s)) \\
& + i(\Gamma_s(E_s) + 2i\Delta_s(E_s))^2(\Gamma_{s^3}(E_s) + 2i\Delta_{s^3}(E_s)) \\
& \quad + \frac{H_1(E_s)}{(3(2E(E_s) + i)\Gamma_s(E_s - 2)\Delta_{s^3}(E_s))^4} \\
& \quad + \frac{2ie^{-\frac{iE_s\tau}{\hbar}}(\Gamma_s^3(E_s) + 2i\Delta_s^3(E_s))\delta\delta^5(\tau)}{3(2EE_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^4}
\end{aligned} \tag{A.9}$$

where,

$$\begin{aligned}
H_1(E_s) = & (2e^{-\frac{iE_s\tau}{\hbar}}(6(-i\Gamma'_s(E_s) + 2\Delta'_s(E_s)) \\
& (\Gamma''_s(E_s) + 2i\Delta''_s(E_s) + i(\Gamma_s(E_s) + 2i\Delta_s(E_s)) \\
& \quad (\Gamma_s^3(E_s) + 2i\Delta_s^3(E_s))))\delta^4(\tau)
\end{aligned} \tag{A.10}$$

Analogously, it continues

$$\begin{aligned}
& (\mathfrak{J}_0(t - t_p) + \mathfrak{J}_{11}(t - t_p))(\mathfrak{J}_0(t_p - t_0) + \mathfrak{J}_{11}(t_p - t_0)) \\
= & 4e^{\frac{iE_s(t+t_0)}{\hbar}} \hbar(2\hbar - (t - t_p)(\Gamma_s(E_s) + 2i\Delta_s(E_s)))(-i\Gamma'_s(E_s) + 2\Delta'_s(E_s)).
\end{aligned} \tag{A.11}$$

So,  $\mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0)$  is given by

$$\begin{aligned}
& (\mathfrak{J}(t - t_p)\mathfrak{J}(t_p - t_0) = \left(\frac{-1}{2\pi i} \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t - t_p)\right] \right. \\
& \left. \left(\frac{1}{E - E_s - \Delta_s(E_s) + \frac{i}{2}\Gamma_s(E_s)} + \frac{(-2i\Gamma'_s(E_s) + 4\Delta'_s(E_s))(E - E_s)}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^2} \right. \right. \\
& \left. \left. + \frac{H_2(E_s)}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^3} \right. \right. \\
& \left. \left. + O(E - E_s)^3\right)\right) dE \\
& \left(\frac{-1}{2\pi i} \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E_p(t_p - t_0)\right] \right. \\
& \left. \left(\frac{1}{E_p - E_s - \Delta_s(E_s) + \frac{i}{2}\Gamma_s(E_s)} + \frac{(-2i\Gamma'_s(E_s) + 4\Delta'_s(E_s))(E_p - E_s)}{(2E_p - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^2} \right. \right. \\
& \left. \left. + \frac{H_2(E_s)}{(2E_p - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^3} \right. \right. \\
& \left. \left. + O(E_p - E_s)^3\right)\right) dp \\
& = \frac{-1}{2\pi i} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t - t_p)\right] \\
& \left(\frac{1}{E - E_s - \Delta_s(E) + \frac{i}{2}\Gamma_s(E)}\right) dE \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t_p - t_0)\right] \\
& \frac{1}{E_p - E_s - \Delta_s(E_s) + \frac{i}{2}\Gamma_s(E_s)} dE_p \\
& \frac{-1}{2\pi i} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t - t_p)\right] \\
& \left(\frac{1}{E - E_s - \Delta_s(E) + \frac{i}{2}\Gamma_s(E)}\right) dE \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t_p - t_0)\right] \\
& + \frac{(-2i\Gamma'_s(E_s) + 4\Delta'_s(E_s))(E_p - E_s)}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^2} \\
& + \frac{H_2(E_s)}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^3} \\
& + O(E_p - E_s)^3) dE_p + \frac{-1}{2\pi i} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t_p - t_0)\right] \\
& \frac{1}{E_p - E_s - \Delta_s(E_s) + \frac{i}{2}\Gamma_s(E_s)} dE \int_{-\infty}^{\infty} \exp\left[\frac{-i}{\hbar} E(t - t_p)\right] \\
& \frac{(-2i\Gamma'_s(E_s) + 4\Delta'_s(E_s))(E - E_s)}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^2} \\
& + \frac{H_2(E_s)}{(2E - 2E_s + i\Gamma_s(E_s) - 2\Delta_s(E_s))^3} \\
& + O(E - E_s)^3) dE) \tag{A.12}
\end{aligned}$$

$$\begin{aligned}
H_2(E_s) = & ((-2(\Gamma'_s(E_s))^2 - 8i\Gamma'_s(E_s)\Delta'_s(E_s) + 8\Delta'_s(E_s)^2 + (\Gamma_s(E_s) - 2i(E - E_s - \Delta_s(E_s))) \\
& (\Gamma''_s(E_s) + 2i\Delta''_s(E_s)))(E - E_s)^2)
\end{aligned} \tag{A.13}$$

On the other hand, it continues

$$\begin{aligned}
& \left(-\frac{1}{2\pi i}\right)\sqrt{2\pi}e^{-\frac{i}{\hbar}E_s\tau}IFT\left[\frac{E_p}{4(E_p + \frac{i}{2}\Gamma_s(E_s) - \Delta_s(E_s))^2}, E_p, \tau\right] \\
= & -\frac{1}{8}e^{-\frac{\tau(\hbar\Gamma_s(E_s) + 2i(E_s + \hbar\Delta_s(E_s)))}{2\hbar}}\Theta(\tau)(-2 + \tau\Gamma_s(E_s) + 2i\tau\Delta_s(E_s)),
\end{aligned} \tag{A.14}$$

$$\begin{aligned}
& \left(-\frac{1}{2\pi i}\right)\sqrt{2\pi}e^{-\frac{i}{\hbar}E_s\tau}IFT\left[\frac{H_3}{(8(E_p + \frac{i}{2}\Gamma_s(E_s) - \Delta_s(E_s)))^3}, E_p, \tau\right] \\
& = \frac{1}{4}\delta(\tau)\Gamma''_s(E_s) - \frac{1}{32}e^{-\frac{1}{2}\tau(\Gamma_s(E_s) + \frac{2i(E_s + \hbar\Delta_s(E_s))}{\hbar})}\Theta(\tau) \\
& ((8 + \tau(\Gamma_s(E_s) + 2i\Delta_s(E_s)))(-8 + \tau\Gamma_s(E_s) + 2i\tau\Delta_s(E_s)))\Gamma'_s(E_s)^2 \\
& + 4i(8 + \tau(\Gamma_s(E_s) + 2i\Delta_s(E_s)))(-8 + \tau\Gamma_s(E_s) + 2i\tau\Delta_s(E_s))\Gamma'_s(E_s)\Delta'_s(E_s) \\
& + 2(-2(8 + \tau(\Gamma_s(E_s) + 2i\Delta_s(E_s)))(-8 + \tau\Gamma_s(E_s) + 2i\tau\Delta_s(E_s)))\Delta'_s(E_s)^2 \\
& - (\Gamma_s(E_s) + 2i\Delta_s(E_s))(-4 + \tau\Gamma_s(E_s) + 2i\tau\Delta_s(E_s)) \\
& (\Gamma''_s(E_s) + 2i\Delta''_s(E_s))) + \frac{1}{2}i\delta(\tau)\Delta''_s(E_s).
\end{aligned} \tag{A.15}$$

$$\begin{aligned}
H_3(E_s) = & (E_p^2(-2\Gamma'_s(E_s)^2 - 8i\Gamma'_s(E_s)\Delta'_s(E_s) + 8\Delta'_s(E_s)^2 + (\Gamma_s(E_s) - 2i(E_p - \Delta_s(E_s))) \\
& (\Gamma''_s(E_s) + 2i\Delta''_s(E_s))))
\end{aligned} \tag{A.16}$$

Thus, in order to compose in the domain of time, it is necessary

$$\frac{\partial^n}{\partial E} \Delta_s(E)|_{E=E_s} = 0, \tag{A.17}$$

$$\frac{\partial^n}{\partial E} \Gamma_s(E)|_{E=E_s} = 0 \tag{A.18}$$





# Appendix B

## Minimal action paths and damping kernel

We have considered a particle coupled to a finite number of reservoir oscillators [GSI88]. However, the environment can only be considered as a proper heat bath causing dissipation in the spectrum of environmental oscillator is quasi-continuous. Hence, we introduce a spectral density of the environment through

$$I(w) = \pi \sum_{n=1}^N \frac{c_n^2}{2m_n w_n} \delta(w - w_n). \quad (\text{B.1})$$

Using the general relation

$$\sum_{n=1}^N \frac{c_n^2}{2m_n w_n} f(w_n) = \int_0^\infty \frac{dw}{\pi} I(w) f(w), \quad (\text{B.2})$$

we find

$$K(\theta) = \int_0^\infty \frac{dw}{\pi} I(w) \frac{\cosh[w(\frac{1}{2}\hbar\beta - i\theta)]}{\sinh(\frac{1}{2}\hbar\beta)}, \quad (\text{B.3})$$

$$\mu = \int_0^\infty \frac{dw}{\pi} I(w) \frac{2}{w}. \quad (\text{B.4})$$

In the following we shall first transform the exponent (see, Ref. [GSI88], Eq. (3.28)) of the influence functional into a form particularly suitable for further evaluation. The

result of this calculations allows us to relate the influence kernel to the phenomenological damping kernel. The kernel  $K(\theta)$  defined for complex times  $\theta = s - i\tau$  still contains a purely reversible renormalization of the potential [CL83b, CL83a] which will be split off in the sequel. Let us first decompose  $K(\theta)$  into its real and imaginary part

$$K(s - i\tau) = K'(s - i\tau) + iK''(s - i\tau), \quad (\text{B.5})$$

where

$$K'(s - i\tau) = \int_0^\infty \frac{dw}{\pi} \frac{\cosh[w(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\hbar\beta)} \cos(ws), \quad (\text{B.6})$$

$$K''(s - i\tau) = - \int_0^\infty \frac{dw}{\pi} \frac{\sinh[w(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\hbar\beta)} \sin(ws). \quad (\text{B.7})$$

Since the imaginary part of the argument varies only within the interval  $0 \leq \tau \leq \hbar\beta$ , it is convenient to expand these kernels into a Fourier series with respect to  $\tau$ . Introducing the characteristic frequencies  $\nu_n$  of the interval  $\hbar\beta$  given by

$$\nu_n = \frac{2\pi n}{\hbar\beta}, \quad (\text{B.8})$$

however, for  $0 \leq \tau \leq \hbar\beta$ , it follows that,

$$\frac{\cosh[w(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\hbar\beta)} = \frac{2}{\hbar\beta} \sum_{n=-\infty}^{\infty} w \frac{\exp(i\nu_n\tau)}{w^2 + \nu_n^2}, \quad (\text{B.9})$$

$$\frac{dw}{\pi} \frac{\sinh[w(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\hbar\beta)} = -\frac{2}{\hbar\beta} \sum_{n=-\infty}^{\infty} i\nu_n \frac{\exp(i\nu_n\tau)}{w^2 + \nu_n^2} \quad (\text{B.10})$$

by virtue of which (B.6) and (B.7) take the form

$$K'(s - i\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} g_n(s) \exp(i\nu_n\tau), \quad (\text{B.11})$$

$$K''(s - i\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} i f_n(s) \exp(i\nu_n\tau) \quad (\text{B.12})$$

where,

$$g_n(s) = \frac{1}{M} \int_0^\infty \frac{dw}{\pi} I(w) \frac{2w}{w^2 + \nu_n^2} \cos(ws), \quad (\text{B.13})$$

$$f_n(t) = \frac{1}{M} \int_0^\infty \frac{dw}{\pi} I(w) \frac{2w}{w^2 + \nu_n^2} \sin(ws). \quad (\text{B.14})$$

Since the real part  $K'(s-i\tau)$  of the influence kernel has the symmetry  $K'(s-i\hbar\beta+i\tau) = K'(s-i\tau)$  its Fourier coefficients are real and satisfy  $g_{-n}(s) = g_n$ . On the other hand, the imaginary part  $K''$  has the symmetry  $K''(s-i\hbar\beta+i\tau) = K''(s-i\tau)$  which leads to imaginary Fourier coefficients  $if_n(s)$  with  $f_{-n}(s) = -f_n(s)$ . Now, the first term in the exponent (see, Ref. [GSI88], Eq. (3.28)) of the influence functional only involves  $K(\theta)$  for imaginary time  $\theta = -i\tau$ . Noting  $K''(s-i\tau)$  vanish for  $s = 0$ , so

$$K(-i\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} g_n(s) \exp(i\nu_n \tau), \quad (\text{B.15})$$

where  $g_n = g_n(s=0)$ . Using (B.4) it is readily seen that  $g_n$  may be written as

$$g_n = \frac{\mu}{M} - \xi_n, \quad (\text{B.16})$$

taking into account that

$$\xi_n = \frac{1}{M} \int_0^\infty \frac{dw}{\pi} \frac{I(w)}{w} \frac{2\nu_n^2}{w^2 + \nu_n^2}. \quad (\text{B.17})$$

Since

$$\frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \exp(i\tau) =: \delta(\tau) = \sum_{n=-\infty}^{\infty} \delta(\tau - n\hbar\beta) \quad (\text{B.18})$$

is a  $\delta$ - function periodically repeated at  $\tau = \pm n\hbar\beta$ , the decomposition (B.16) of  $g_n$  splits the imaginary time kernel (B.15) into a local and a nonlocal part. According, the first term of the exponent  $\tilde{\Phi}[q, q', \bar{q}]$  may be written as

$$\begin{aligned}
& - \int_0^{\hbar\beta} d\tau \int_0^\tau \sigma K(-i\tau + i\sigma) \bar{q}(\tau) \bar{q}(\sigma) = \\
& - \int_0^{\hbar\beta} d\tau \frac{1}{2} \mu \bar{q}^2(\tau) + \frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k(\tau - \sigma) \bar{q}(\tau) \bar{q}(\sigma), \tag{B.19}
\end{aligned}$$

where

$$k(\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} \xi_n \exp(i\nu_n \tau). \tag{B.20}$$

Subsequently, in Ref. [GSI88] It follows that,

$$\begin{aligned}
& \frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k(\tau - \sigma) \bar{q}(\tau) \bar{q}(\sigma) \\
& = -\frac{1}{4} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k(\tau - \sigma) \bar{q}(\tau) - \bar{q}(\sigma)^2, \tag{B.21}
\end{aligned}$$

clearly displaying its nonlocal character. In the (B.21) is readily verified by performing the square and noting that

$$\int_0^{\hbar\beta} d\tau k(\tau) = M\xi_0 = 0 \tag{B.22}$$

For real time the real and imaginary parts of the kernel (B.3)

$$K'(s) = \int_0^\infty \frac{dw}{\pi} I(w) \coth\left(\frac{1}{2}w\hbar\beta\right) \cos(ws), \tag{B.23}$$

$$K'' = - \int_0^\infty \frac{dw}{\pi} I(w) \sin(ws). \tag{B.24}$$

Now, the fourth term of the exponent of the influence functional splits into

$$\begin{aligned}
& \int_0^t ds \int_0^s du \{q(s) - q'(s)\} \{K(s-u)q(u) - K^*(s-u)q'(u)\} \\
&= \int_0^t ds \int_0^s du K'(s-u) \{q(s) - q'(s)\} \{q(u) - q'(u)\} \\
&+ i \int_0^t ds \int_0^s du K''(s-u) \{q(s) - q'(s)\} \{q(u) - q'(u)\}. \tag{B.25}
\end{aligned}$$

The imaginary part  $K''(s)$  of the kernel again contains a reversible renormalization of the potential and may be written

$$K''(S) = \frac{1}{2} \frac{d\eta(s)}{ds}, \tag{B.26}$$

where

$$\eta(s) = w \int_0^\infty \frac{ds}{\pi} \frac{I(w)}{w} \cos(w). \tag{B.27}$$

By virtue of (B.26) the second terms of (B.25) may be integrated by part with respect to  $u$  to yield

$$\begin{aligned}
i \int_0^t ds \int_0^s du K''(s-u) \{q(s) - q'(s)\} \{q(u) - q'(u)\} = \\
- \frac{i}{2} \int_0^t ds \eta(0) \{q^2(s) - q'^2(s)\} + \frac{i}{2} \{q(0) + q'(0)\} \int_0^t ds \eta(s) \{q(s) + q'(s)\} \\
+ \frac{i}{2} \int_0^t ds \int_0^s du \eta(s-u) \{q(s) + q'(s)\} \{\dot{q}(u) + \dot{q}'(u)\}. \tag{B.28}
\end{aligned}$$

Because of  $\eta(0) = \mu$  the first term in (B.28) just cancels the last term (see, Ref. [GSI88], Eq. (3.28)). Hence, the potential renormalization implicit in  $K(s)$  is again eliminated by the counterterm. The last term in (B.28) contains no further potential renormalization since it does not have the structure of a potential energy contribution due to its dependence on the particle velocity. Collecting the results in the (B.19),

(B.25) and (B.28), the exponent of the influence functional now takes the form

$$\begin{aligned}
\tilde{\Phi}[q, q', \bar{q}] &= \frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k(\tau - \sigma) \bar{q}(\tau) \bar{q}(\sigma) - i \int_0^{\hbar\beta} d\tau \int_0^t ds \bar{q}(\tau) \{q(s) + q'(s)\} \\
&+ \int_0^t ds \int_0^t du K'(s - u) \{q(s) - q'\} \{q(u) - q'\} \\
&+ \frac{i}{2} \int_0^t ds \int_0^t du \eta(s - u) \{q(s) + q'(s)\} \{\dot{q}(u) + \dot{q}'(u)\} \\
&+ \frac{i}{2} \{q(0) + q'(0)\} \int_0^t ds \eta(s) \{q(s) + q'(s)\}. \tag{B.29}
\end{aligned}$$

The first two terms describes the effects of initial correlations between the environment and the Brownian particle on the subsequent time evolution of the particle. The remaining three terms just constitute the exponent of the influence functional of the conventional Feynman – Vernon theory which neglects correlation between the particle and the environment in the initial state. We remark that Caldeira and Leggett [CL83a] omitted the last term in (B.29) in their treatment of the conventional theory. The result in (B.29) suggests the introduction of sum and difference coordinates of the Brownian particle, i.e.

$$x = q - q', r = \frac{q + q'}{2}, \tag{B.30}$$

which initial and final values defined according. The functional integral representations (see, Ref. [GSI88], Eq. (3.4)) of the density matrix is then recast into

$$\rho(x_f, r_f, t) = \int dx_i dr_i d\bar{q} d\bar{q}' J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') \lambda(x_i, r_i, \bar{q}, \bar{q}'), \tag{B.31}$$

$$\begin{aligned}
J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') &= Z^{-1} \int \mathcal{D}x \mathcal{D}r \mathcal{D}\bar{q} \exp\left\{ (S_0[r + \frac{x}{2}] - S_0[r - \frac{x}{2}]) - \frac{1}{\hbar} S_0^E[\bar{q}] \right\} \tilde{F}[x, r, \bar{q}] \\
&\tag{B.32}
\end{aligned}$$

is a functional over all paths  $x(s), r(s), 0 \leq s \leq t$  in real time with

$$x(0) = x_i, r(0) = r_i, x(t) = x_f, r(t) = r_f \quad (\text{B.33})$$

and over all paths  $\bar{q}(\tau), 0 \leq \tau \leq \hbar\beta$  in imaginary time with  $\bar{q}(0) = \bar{q}', \bar{q}(\hbar\beta) = \bar{q}$ . The influence functional now becomes

$$\tilde{F}[x, r, \bar{q}] = \exp\left(-\frac{1}{\hbar}\tilde{\Phi}[x, r, \bar{q}]\right), \quad (\text{B.34})$$

where the exponents is given by (B.29) expressed in terms of the new variables in the (B.30). The functional integral (B.32) can thus be written

$$J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') = Z^{-1} \int \mathcal{D}x \mathcal{D}r \mathcal{D}\bar{q} \exp\left(\frac{i}{\hbar}\Sigma[x, r, \bar{q}]\right). \quad (\text{B.35})$$

where  $\Sigma[x, r, \bar{q}]$  is an effective action given by

$$\begin{aligned} \Sigma[x, r, \bar{q}] = & i \int_0^{\hbar} d\tau \left[ \frac{M}{2} \dot{\bar{q}}^2 + V(\bar{q}) + \frac{1}{2} \int_0^{\hbar} d\sigma k(\tau - \sigma) \bar{q}(\tau) \bar{q}(\sigma) \right] \\ & + \int_0^{\hbar} d\tau \int_0^t ds K^*(s - i\tau) \bar{q}(\tau) x(s) \\ & + \int_0^t ds \left[ M \dot{x} \ddot{r} - V\left(r + \frac{x}{2}, s\right) + V\left(r - \frac{x}{2}, s\right) - r_i \eta(s) x(s) \right] \\ & - \int_0^t ds \left[ \int_0^s du \eta(s - u) x(s) \dot{r}(u) + \frac{i}{2} \int_0^t du K'(s - u) x(s) x(u) \right]. \quad (\text{B.36}) \end{aligned}$$

The kernel occurring in (B.35) has been defined in (B.3), (B.20), (B.23), and (B.27). Note that the potential may depend explicitly on time only for  $t > 0$ .





# Appendix C

## Auto-correlation function

The Gaussian nature of a harmonic oscillator coupled linearly to a bath of harmonic oscillators implies that its reduced dynamics can be expressed completely in terms of the thermal position autocorrelation function [GWT84, Ris85]

$$\begin{aligned} C(t) &= \langle q(t)q(0) \rangle = S(t) + iA(t) \\ &= \frac{\hbar}{\pi m} \int_{-\infty}^{\infty} dw \frac{w \hat{\gamma}(-iw)}{(w^2 - w_0^2)^2 + w^2 \hat{\gamma}(-iw)^2} \frac{\exp(-iwt)}{1 - \exp(\beta \hbar w)} \end{aligned} \tag{C.1}$$

$S(t)$  and  $A(t)$  denote the symmetrized and antisymmetrized correlation functions and correspond to the real and imaginary part of  $C(t)$ , respectively.  $\hat{\gamma}(z)$  is the Laplace transform of the friction kernel (See Ref.[PID10], Eq. (25)) divided by the oscillator mass  $m$ . The antisymmetric correlation function is related to the function  $G_+(t)$  introduced for the special Ohmic damping case in (3.24) by

$$G_+(t) = -\frac{2m}{\hbar} A(t) \Theta(t), \tag{C.2}$$

where  $\Theta(t)$  is the unit step function. The second moments of position and momentum appearing in (See Ref.[PID10], Eq. (49)) are related to the symmetrized correlation function by  $\langle q^2 \rangle = S(0)$  and  $\langle p^2 \rangle = -m\ddot{S}(0)$ , respectively. For the latter to be finite, the Laplace transform  $\hat{\gamma}(z)$  requires a high-frequency cutoff. The functions, in the

(3.31) are found to read [GSI88]

$$a(t) = \frac{m^2 [\dot{G}_+(t)]^2}{\hbar [G_+(t)]^2} \{ \langle q^2 \rangle [1 - \frac{[S(t)]^2}{\langle q^2 \rangle^2}] + \frac{\langle p^2 \rangle}{m^2} [G_+(t)]^2 + 2\dot{S}(t)G_+(t) \}, \quad (\text{C.3})$$

$$b(t) = -\frac{m^2 [\dot{G}_+(t)]}{\hbar [G_+(t)]} \{ \langle q^2 \rangle [1 - \frac{[S(t)]^2}{\langle q^2 \rangle^2}] \frac{[\dot{G}_+(t)]}{[G_+(t)]} + \dot{G}_+(t)\dot{S}(t) - G_+(\ddot{S}(t)) + \frac{S(t)\dot{S}(t)}{\langle q^2 \rangle} \}, \quad (\text{C.4})$$

$$c(t) = \frac{m^2}{\hbar} \{ \langle q^2 \rangle \frac{[\dot{G}_+(t)]^2}{[G_+(t)]^2} + \frac{\langle p^2 \rangle}{m^2} - \frac{1}{\langle q^2 \rangle} [\dot{S}(t) - \frac{[\dot{G}_+(t)]}{[G_+(t)]} S(t)]^2 \}. \quad (\text{C.5})$$

If one takes into account that  $G_+(t), S(t)$ , and their derivatives decay to zero for long times but not the ratio  $\frac{\dot{G}_+(t)}{G_+(t)}$ , one immediately finds the asymptotic expression (See Ref.[PID10], Eq. (48)).

# Appendix D

## Functions

In this section, we show the auxiliary functions  $f_n(t_f, t_i, t_0)$  and  $\Upsilon_m(t_f, t_i, t_0)$  that have emerged after integrations. That is, intermediate processes to obtain the composition, of (3.36).

$$\begin{aligned}
& (G_w(p'', q'', t_f, t_i, p''', q'''))(G_w(p''', q''', t_i, t_0, p', q')) \\
&= \frac{2\pi}{\sqrt{4f_2(t_f, t_i, t_0) - \frac{f_3^2(t_f, t_i, t_0)}{f_4(t_f, t_i, t_0)}}} \sqrt{f_4(t_f, t_i, t_0)} \\
& \frac{m^2}{4\pi^2 \hbar^2 \sqrt{\Lambda(t_f - t_i)} \sqrt{\Lambda(t_i - t_0)}} \left| \frac{\dot{G}_+(t_f - t_i)}{G_+(t_f - t_i)} \right| \left| \frac{\dot{G}_+(t_i - t_0)}{G_+(t_i - t_0)} \right| \\
& \exp\left[ \frac{\Upsilon_1(t_f, t_i, t_0)}{\Upsilon_2(t_f, t_i, t_0)} - \Upsilon_3(t_f, t_i, t_0) \right].
\end{aligned} \tag{D.1}$$

In this case,

$$\begin{aligned}
\Upsilon_1(t_f, t_i, t_0) &= f_1(t_f, t_i, t_0) f_3(t_f, t_i, t_0) f_5(t_f, t_i, t_0) \\
&- f_2(t_f, t_i, t_0) f_5^2(t_f, t_i, t_0) - f_1^2(t_f, t_i, t_0) f_4(t_f, t_i, t_0),
\end{aligned} \tag{D.2}$$

$$\Upsilon_2(t_f, t_i, t_0) = f_3^2(t_f, t_i, t_0) - 4f_2(t_f, t_i, t_0)f_4(t_f, t_i, t_0), \quad (\text{D.3})$$

$$\begin{aligned} \Upsilon_3(t_f, t_i, t_0) = & -\frac{p''\Sigma_{22}(t_f - t_i)}{2\hbar\Lambda(t_f - t_i)} \\ & -\frac{p''q''(\Sigma_{12}(t_f - t_i) + \Sigma_{21}(t_f - t_i))}{2\hbar\Lambda(t_f - t_i)} \\ & -\frac{q''^2\Sigma_{22}(t_f - t_i)}{2\hbar\Lambda(t_f - t_i)} - \frac{1}{2\hbar\Lambda(t_f - t_i)\Lambda(t_i - t_0)} \\ & (p^{cl2}(t_i, t_0, p', q')\Lambda(t_f - t_i)\Sigma_{11}(t_i - t_0) + p^{cl}(t_i, t_0, p', q') \\ & q^{cl}(t_i, t_0, p', q')\Lambda(t_f - t_i)(\Sigma_{12}(t_i - t_0) + \Sigma_{12}(t_i - t_0)) \\ & p^{cl2}(t_i, t_0, p', q')\Lambda(t_f - t_i)\Sigma_{22}(t_i - t_0)). \end{aligned} \quad (\text{D.4})$$

However,

$$\begin{aligned} f_1(t_f, t_i, t_0) = & \frac{1}{2\pi} \left( \frac{2p''\dot{G}_+(t_f - t_i)\Sigma_{11}(t_f - t_i)}{\Lambda(t_f - t_i)} \right. \\ & + \frac{p''G_+(t_f - t_i)(\Sigma_{12}(t_f - t_i) + \Sigma_{21}(t_f - t_i))}{m\Lambda(t_f - t_i)} \\ & + \frac{q''\dot{G}_+(t_f - t_i)(\Sigma_{12}(t_f - t_i) + \Sigma_{21}(t_f - t_i))}{\Lambda(t_f - t_i)} \\ & + \frac{1}{\Lambda(t_f - t_i)} + (2((p' + m\gamma q')\dot{G}_+(t_f - t_i) + mq'\ddot{G}(t_i - t_0)) \\ & \Sigma_{11}(t_i - t_0) + p^{cl}(t_i, t_0, p', q')(\Sigma_{12}(t_i - t_0) + \Sigma_{21}(t_i - t_0))) \\ & \left. + \frac{2q''G_+(t_f - t_i)\Sigma_{22}(t_f - t_i)}{m\Lambda(t_f - t_i)} \right), \end{aligned} \quad (\text{D.5})$$

$$\begin{aligned}
f_2(t_f, t_i, t_0) &= (m^2 \dot{G}_+^2(t_f - t_i) \Lambda(t_i - t_0) \\
&\Sigma_{11}(t_f - t_i) + m^2 \Lambda(t_f - t_i) \Sigma_{11}(t_i - t_0) \\
&+ m G_+(t_f - t_i) \dot{G}_+(t_f - t_i) \Lambda(t_i - t_0) \\
&\quad (\Sigma_{12}(t_f - t_i) + \Sigma_{21}(t_f - t_i)) \\
&\quad + \dot{G}_+^2(t_f - t_i) \Lambda(t_i - t_0) \Sigma_{22}(t_f - t_i)) \\
&\quad \left( \frac{1}{2m^2} \hbar \Lambda(t_f - t_i) \Lambda(t_i - t_0) \Lambda(t_i - t_0) \right),
\end{aligned}$$

(D.6)

$$\begin{aligned}
f_3(t_f, t_i, t_0) &= \frac{1}{2m \hbar \Lambda(t_f - t_i) \Lambda(t_i - t_0)} \\
&(m \dot{G}_+(t_f - t_i) \ddot{G}_+(t_f - t_i) \Lambda(t_i - t_0) (\Sigma_{12}(t_f - t_i) \\
&\quad + \Sigma_{21}(t_f - t_i)) + m \dot{G}_+^2(t_f - t_i) \Lambda(t_i - t_0) \\
&\quad (2m\gamma \Sigma_{11}(t_f - t_i) + \Sigma_{12}(t_f - t_i) + \Sigma_{21}(t_f - t_i)) \\
&\quad + m \Lambda(t_f - t_i) (\Sigma_{12}(t_i - t_0)) + \Sigma_{21}(t_i - t_0) \\
&\quad + 2\gamma \dot{G}_+^2(t_f - t_i) \Lambda(t_i - t_0) \Sigma_{22}(t_f - t_i) \\
&+ 2\dot{G}_+(t_f - t_i) \Lambda(t_i - t_0) (m^2 \ddot{G}_+(t_f - t_i) \Sigma_{11}(t_i - t_0) \\
&\quad \dot{G}_+(t_f - t_i) (m\gamma \Sigma_{12}(t_f - t_i) \\
&\quad + m\gamma \Sigma_{21}(t_f - t_i) + \Sigma_{22}(t_f - t_i))))
\end{aligned}$$

(D.7)

$$\begin{aligned}
f_4(t_f, t_i, t_0) &= \frac{1}{2\pi} \left( \frac{1}{\Lambda(t_f - t_i)} m^2 \right. \\
&\quad + (\gamma \dot{G}_+(t_f - t_i) + \ddot{G}_+(t_f - t_i))^2 \Sigma_{11}(t_f - t_i) \\
&\quad + \frac{1}{\Lambda(t_f - t_i)} m (\gamma G_+(t_f - t_i) + \dot{G}_+(t_f - t_i)) \\
&\quad (\gamma \dot{G}_+(t_f - t_i) + \ddot{G}_+(t_f - t_i)) (\Sigma_{12}(t_f - t_i) \Sigma_{21}(t_f - t_i)) \\
&\quad \left. + \frac{1}{\Lambda(t_i - t_0)} (\gamma G_+(t_f - t_i) + \dot{G}_+(t_f - t_i))^2 \right. \\
&\quad \left. \Sigma_{22}(t_f - t_i) \frac{\Sigma_{22}(t_f - t_i)}{\Lambda(t_i - t_0)} \right),
\end{aligned} \tag{D.8}$$

$$\begin{aligned}
f_5(t_f, t_i, t_0) &= \frac{1}{2\pi} \left( \frac{1}{\Lambda(t_f - t_i)} m p'' \right. \\
&\quad (\gamma \dot{G}_+(t_f - t_i) + \ddot{G}_+(t_f - t_i)) \Sigma_{11}(t_f - t_i) \\
&\quad + \frac{1}{\Lambda(t_f - t_i)} p'' (\gamma G_+(t_f - t_i) + \dot{G}_+(t_f - t_i)) \\
&\quad (\Sigma_{12}(t_f - t_i) \Sigma_{21}(t_f - t_i)) + \frac{1}{\Lambda(t_f - t_i)} m q'' \\
&\quad (\gamma \dot{G}_+(t_f - t_i) + \ddot{G}_+(t_f - t_i)) (\Sigma_{12}(t_f - t_i) \Sigma_{21}(t_f - t_i)) \\
&\quad \left. + \frac{1}{\Lambda(t_f - t_i)} 2q'' (\gamma G_+(t_f - t_i) + \dot{G}_+(t_f - t_i)) \Sigma_{22}(t_f - t_i) \right. \\
&\quad \left. + \frac{p^{cl}(t_i, t_0, p', q') (\Sigma_{12}(t_i - t_0) + \Sigma_{21}(t_i - t_0))}{\Lambda(t_i - t_0)} \right. \\
&\quad \left. + \frac{2q^{cl}(t_i, t_0, p', q') \Sigma_{22}(t_i - t_0)}{\Lambda(t_i - t_0)} \right).
\end{aligned} \tag{D.9}$$

# Appendix E

## Fundamental notions of algebraic topology and measurement theory

Algebraic topology has contributed significantly to the proof of strong theorems or conjectures. Therefore, we present in this section different notions of algebraic structures (groups, semigroups, rings, fields, algebras), principles of topology and generalities in measurable spaces, which have already been exhaustively studied in the literature [Fra87, Kos92, Nav92, Apo96]. We have used, topological-algebraic tools prevail in the construction of the definitions and representation of theorems to explain the principle of divisibility (law of composition) in open non-Markovian quantum systems (memory effects).

### E.1 Algebraic structures

In mathematics, a group is a set equipped with a binary operation that combines any two elements to form a third element in such a way that four conditions called group axioms are satisfied, namely closure, associative, identity and invertibility. Example,  $(\mathbf{Z}, +)$ ;  $(\mathbf{R}, +)$ ;  $\mathbf{R}^* = \mathbf{R} - 0$  ;  $(\mathbf{R}^*, \times)$ ;  $(\mathbf{C}, +)$ ;  $(\mathbf{M}_{n \times n}, +)$ .

In algebra, given a group  $G$  with a binary operation  $(\diamond)$ , a non-empty subset  $H$  of  $G$  is said to be a subgroup of  $G$  if  $H$  also forms a group under the operation  $(\diamond)$ . Or else,  $H$  is a subgroup of  $G$  if the constraint from  $(\diamond)$  to  $H$  satisfies the group axioms,

example:  $G \rightarrow \{G, \{1\}\}$ ,  $\mathbf{Z} \rightarrow \{\mathbf{Z}_n = k \cdot n : k, n \in \mathbf{Z}, n \geq 0\}$ .

It is noteworthy that we can denote the binary operation in a set with any symbol, for example,  $+$ ,  $*$ ,  $\star$ ,  $\circ$ ,  $\bullet$ ,  $\diamond$ . Also, the order of a group  $(G, *)$  is the number of elements of  $G$  and we will denote it with  $o(G)$  or with  $|G|$  indistinctly. On the other hand, if  $G$  is finite (infinite) we will say that  $G$  is finite or (Infinite). For example,  $\mathbb{Z}$  is an infinite group, under the usual sum.

**Definition 4.** Let  $(G, \star)$  and  $(G', \diamond)$  two groups. A group homeomorphism is a function  $f : G \rightarrow G'$  such that  $f(x \star y) = f(x) \diamond f(y)$ .

**Definition 5.** Let  $\Omega$  and  $A$  be two sets. An action of  $\Omega$  in  $A$  is a function  $\Omega \times A$  in set  $A$ .

**Definition 6.** A ring is a triplet  $(A, +, \cdot)$  where  $A$  is a set,  $+$  and  $\cdot$  are binary operations such that.

- *i)*  $(A, +)G$  is a commutative group.
- *ii)*  $(A, \cdot)$  is a semi-group
- *iii)*  $x(y + z) = xy + xz$ , and  $(x + y)z = xz + yz$ .

Some examples of rings are:  $(\mathbf{Z}, +, \cdot)$ ,  $(\mathbf{Z}_n, +, \cdot)$ ,  $(\mathbf{Q}, +, \cdot)$ ,  $(\mathbf{R}, +, \cdot)$ ,  $(\mathbf{C}, +, \cdot)$ . Also, if  $A$  is a commutative subgroup, then  $(A, +, \cdot)$  will be called a commutative ring. On the other hand, remember that if the product of two nonzero elements of a ring  $A$  is zero element of the ring, then those two elements are said to be divisors of zero. If the ring  $(A, +, \cdot)$  with  $1 \neq 0$  does not have divisors of zero, it will be called an *integer domain*. If an integer domain has a multiplicative universe for each nonzero element, it is said to be a *division ring*. Finally, a *field* is a commutative ring with division. The rings are related by functions that preserve the ring structures. If  $(A, \diamond, \square)$  and  $(A', +, \diamond)$  are rings, a ring homeomorphism is a function that is a homomorphism of the commutative group of  $A$  in the commutative group  $A'$  and that is also a homomorphism of semigroup  $A$  in semigroup  $A'$ , that is,

$$f(x \diamond y) = f(x) + f(y) \quad \text{and} \quad f(x \square y) = f(x) \cdot f(y). \quad (\text{E.1})$$



If in the definition of vector space we consider a commutative ring  $(A, +, \cdot)$  with 1 instead of a field  $K$ , we will obtain an algebraic structure called  $A$ - *Left module*. So, as a particular case of the  $A$ -modules are the  $K$  - *modules*, that is, the vector spaces on a  $K$  field.

**Definition 7.** *An algebra over  $A$  ( $A$  a commutative ring with one) is a set  $A$  that simultaneously is a ring and an  $A$  - modulo. That is, an algebra  $(A, +, \mu, \cdot)$  is an  $A$  - modulo with another binary operation, called multiplication with an extra condition that makes binary operations and scalar multiplication compatible, which is the following:*

$$i) (\lambda x + \lambda' y)z = \lambda(xz) + \lambda'(yz)$$

$$ii) z(\lambda x + \lambda' y) = \lambda(zx) + \lambda'(zy), \text{ for, } \lambda, \lambda' \in A; x, y, z \in A.$$

Now, if the multiplicative conditions of an algebra are imposed, we obtain *commutative algebras, associative algebras, algebras with one*. An associative algebra with one such that every nonzero element is invertible is called a *division algebra*. For example,  $(\mathbf{M}_n K, +, \cdot, \mu)$ , where  $\mathbf{M}_n K$  denotes all square matrices of  $n \times n$  with coefficients in a field  $K$  ( $\mu$  denotes scalar multiplication) is an algebra just like  $(K, +, \cdot, \mu)$  and  $(K[x], +, \cdot, \mu)$ . We define a *graduated algebra* as a sequence  $A = (A_0, A_1, A_2, \dots)$  of algebras  $A_i$ , one for each index  $i \in \mathbf{N}$ .

Example: Let  $T^k(V) = \bigotimes_k V = V \otimes_k \dots \otimes_k V$  the tensor product of a vector space  $V$  on a field  $K$ ,  $k$  times. We will call  $T^k(V)$  *tensor space of degree  $k$  of  $V$* . If we define a multiplication  $\cdot : T^k(V) \times T^l(V) \rightarrow T^{k+l}(V)$ , through  $(x_1 \otimes x_2 \dots \otimes x_k) \cdot (y_1 \otimes y_2 \dots \otimes y_l) = x_1 \otimes x_2 \dots \otimes x_k \otimes y_1 \otimes y_2 \dots \otimes y_l$  we have a graduated algebra (where we define  $T^0V = K$  and  $T^1V = V, TV = K, V, T^2V, T^3V, T^4V, \dots$ ) called a *tensor algebra of  $V$* .

## E.2 General topology

The General Topology has its own objectives, but it also nourishes the foundations of many mathematical areas such as Analysis, Geometry and other fields of topology

(Algebraic Topology, Topology). Geometric (or Differential Topology). Taking the metric spaces as models, a topology  $\tau \subseteq P(X)$  has been defined on a set  $X$  and the pair  $(X, \tau)$  is said topological space (e.t.) The relevant applications between two e.t. they are continuous applications and the concept of equivalence in topology is called homeomorphism. One of the objectives of any mathematical area is to classify and count. In particular, to classify it is necessary to know how to discern when two objects are or are not equivalent (in our case, when two e.t. are or are not homeomorphic). In general, this is a very difficult problem and is far from being solved. We have introduced some elements of the topology in sets of points, specifically, let  $\mathbf{a}$  a point of  $\mathbf{R}^n$  and  $r$  a given positive number. The set of all points  $\mathbf{x}$  de  $\mathbf{R}^n$  such that  $\|\mathbf{x} - \mathbf{a}\| < r$ , It is called open  $n - ball$  of radius  $r$  and center  $\mathbf{a}$ . We designate this set  $B(\mathbf{a})$  or by  $B(\mathbf{a}; r)$ .

**Definition 8.** Let  $S$  be a subset of  $\mathbf{R}^n$ , and suppose that  $\mathbf{a} \in S$ . Then,  $\mathbf{a}$  is called the interior point of  $S$  if there is an open  $n - ball$  with center in  $\mathbf{a}$ , contained in  $S$ .

**Definition 9.** A set  $S$  of  $\mathbf{R}^n$  is open if all its points are interior. In other words,  $S$  is open if, and only if,  $S = \text{int}(S)$ .

**Definition 10.** Let  $X$  be a set and  $\tau \subseteq P(X)$ .  $(X, \tau)$  is said to be a topological space, if and only if, the following properties are met:

- i)  $\phi, X \in \tau$
- ii) If  $U, V \in \tau$ , then,  $U \cap V \in \tau$
- iii) If  $\{U_i\}_{i \in I}$  is a family of elements of  $\tau$ , then  $\bigcup_{i \in I} U_i \in \tau$

If  $(X, \tau)$  is a topological space, we will say that  $\tau$  is a topology of  $X$ .

**Definition 11.** Let  $X$  be a set and  $\mathcal{B} \subseteq P(X)$ .  $\mathcal{B}$  is said to be a basis of a topology of  $X$ , if and only if the following properties are met:

- i) For all  $x \in X$ , there exists  $B \in \mathcal{B}$  such that  $x \in B$ .
- ii) For all  $B_1, B_2 \in \mathcal{B}$  and all  $x \in B_1 \cap B_2$ , there exists  $B \in \mathcal{B}$  such that  $x \in B \subseteq B_1 \cap B_2$ .

## E.3 Measurable space

In mathematics, a  $\sigma$ -algebra (read sigma-algebra) on a set  $X$  is a non-empty family  $\Sigma$  of subsets of  $X$ , closed under accounting complements, unions and intersections. The  $\sigma$ -algebras (also known as "tribes") are mainly used to define measures in  $X$ . The concept is very important in mathematical analysis and in probability theory.

Formally, a family of sets of  $X$  (or, equivalently, a subset of the set of parts of  $X$ ), which we will call  $\Sigma$  is a  $\sigma$ -algebra over  $X$  if and only if the following properties are met:

- i) The empty set is in  $\Sigma$
- ii) If  $E$  is in  $\Sigma$ , there is also its complementary set  $E^c$
- iii) If  $E_1, E_2, E_3, \dots$  is a sequence (accounting) in  $\Sigma$ , then its union (accounting) is also in  $\Sigma$ . Understand accounting as finite or countable.

An ordered pair  $(X, \Sigma)$ , where  $X$  is a set and  $\Sigma$  a  $\sigma$ -algebra on it, is called Measurable Space.

In the Euclidean space  $\mathbf{R}^n$ , another  $\sigma$ -algebra stands out: that formed by the Lebesgue-measurable sets. This contains more sets than Borel algebra in  $\mathbf{R}^n$ , and is the one preferred in integration theory.

## E.4 Measurement theory

A measurement space is a set for which a  $\sigma$ -algebra of measurable sets has been defined and a specific measured function that assigns a real or measured value to each element of the  $\sigma$ -algebra

The triplet  $(\mathbb{R}, \mathcal{B}, \lambda)$  where,  $\mathbb{R}$  is the set of real numbers,  $\mathcal{B}$  la  $\sigma$ -boreal algebra and  $\lambda$  Lebesgue's measure based on the length of the intervals, constitute a measurement space. A probabilistic space is a particular case of measurement space, where every measurable set has a finite measure or "size", given by its probability.

We have introduced algebraic and topological principles in the study of open Markovian or non-Markovian quantum systems. Specifically, we had applied mathematical structures (groups, rings, algebras, topological or measurable spaces) to incorporate sufficient and necessary criteria in the energy domain to compose in the time domain, mediated by the principle of divisibility (composition law) and the study of the Wigner function in damped systems. This was developed in the Chapters (3 and 4).

# Appendix F

## System-Environment (Reservoir)

Generally, the dynamics of open quantum systems is described through a master equations and perturbation theory. It is then necessary to specify that the theory of perturbations acquires relevance in obtaining approximations of the eigenvalues and proper functions of a system coupled to a reservoir (classical-quantum). In this case, we are interested in carrying out different extrapolations and analysis of the behavior of a reservoir-system [SB12]. In addition, it must be guaranteed that the reference system must have some similarity (analogy) with the case under study. This method of approximation is widely used in various branches (applied mathematics, chemistry, and physics) to find approximate solutions to many types of equations, including algebraic, differential, or integral equations. Therefore, we will show a general sketch of the differential-integral equations associated with this case. Specifically, let  $H(t)$  Hamiltonian be represented as follows

$$H = H_0 + \hat{V}, \quad (\text{F.1})$$

where,

$$H_0 = H_S + \sum_a \Phi_{aa}(z)|a\rangle\langle a| + H_R, \quad (\text{F.2})$$

$$\equiv \sum_a (E_a + H_R + \Phi_{aa}(z))|a\rangle\langle a|. \quad (\text{F.3})$$

Generally,  $\Phi_{ab}(z) = \langle a|H_{S-B}|b\rangle$ , the (F.3) suggests that the Hamiltonian can be introduced

$$H_a = E_a + H_R + \Phi_{aa}(z), \quad (\text{F.4})$$

which describes the behavior of the reservoir when the system is in the eigenstate  $|a\rangle$ . The perturbation  $\hat{V}$  represents the diagonal elements of  $\Phi_{aa}(z)$ , thus

$$\hat{V} = \sum_{a,b} (1 - \delta_{ab}) \Phi_{aa}(z) |a\rangle\langle b|. \quad (\text{F.5})$$

Once the diagonal matrix element is found  $\Phi_{aa}(z)$  a non-disturbing description of the system coupling – reservoir is achieved. To establish a description of the non-disturbing part of the reservoir system, an appropriate definition is introduced for the projection operators. Since a simultaneous description of several states  $|a\rangle$  is required, it is necessary to generalize the projection operator  $\mathcal{P}$ . If the latter acts on an arbitrary operator  $\hat{O}$ , it is represented

$$\mathcal{P}\hat{O} = \hat{R}_{\text{eq}} \text{tr}_R \hat{O} \equiv \hat{R}_{\text{eq}} \sum_{a,b} \text{tr}_R \{ \langle a|\hat{O}|b\rangle \} |a\rangle\langle b|. \quad (\text{F.6})$$

This projector is constructed in such a way that it introduces a common equilibrium state in the reservoir modes represented by  $\hat{R}_{\text{eq}}$ . In contrast, the new projection operator takes the form

$$\tilde{\mathcal{P}}\hat{O} = \sum_a \hat{R}_{\text{eq}} \{ \langle a|\hat{O}|a\rangle \} |a\rangle\langle a| \quad (\text{F.7})$$

Instead of including the space of all the states related to the Hamiltonian system, as is the case for the projection operator  $\mathcal{P}$ . The new amount  $\tilde{\mathcal{P}}$  projects on the diagonal of the elements of the system states and each state of the system is characterized by a separate reservoir equilibrium operator [SB12]

$$\hat{R}_a = \frac{\exp(\frac{-H_a}{k_B T})}{\text{tr}_R \exp(\frac{-H_a}{k_B T})} \quad (\text{F.8})$$

The introduction of the Hamiltonian corresponding to the vibrational part, in (F.4), allows to obtain a representation for the statistical equilibrium operators. For additional use, the  $\hat{\pi}_a = |a\rangle\langle a|$  projector and the combined static-reservoir system balance operator are introduced

$$\hat{W}_a = \hat{R}_a \hat{\pi}_a. \quad (\text{F.9})$$

If  $\tilde{\mathcal{P}}$  acts on the complete statistical operator, it is obtained

$$\tilde{\mathcal{P}}\hat{W}_a(t) = \sum_a P_a(t)\hat{W}_a. \quad (\text{F.10})$$

This expression indicates a specification of the various equilibrium states of the reservoir (with the statistical operator  $\hat{R}_a$ ) controlled by the actual population of the states of the respective system. The population of the state is extracted, if the matrix element of the respective state of the diagonal system is taken and traced with respect to the space of the state of the reservoir

$$P_a(t) = \text{tr}_R\{\langle a|\tilde{\mathcal{P}}\hat{W}(t)|a\rangle\}. \quad (\text{F.11})$$

Given the equation of Liouville-von Neumann

$$\frac{\partial}{\partial t}\hat{W}(t) = -i\mathcal{L}\hat{W}(t), \quad (\text{F.12})$$

where  $\mathcal{L}\dots = \frac{[H,\dots]}{\hbar}$ . Introducing the orthogonal complement,  $\tilde{\mathcal{Q}} = 1 - \tilde{\mathcal{P}}$ , also, making a separation in two parts orthogonal, it follows that

$$\frac{\partial}{\partial t}\tilde{\mathcal{P}}\hat{W}(t) = -i\tilde{\mathcal{P}}\mathcal{L}(\tilde{\mathcal{P}}\hat{W}(t) + \tilde{\mathcal{Q}}\hat{W}(t)), \quad (\text{F.13})$$

$$\frac{\partial}{\partial t}\tilde{\mathcal{Q}}\hat{W}(t) = -i\tilde{\mathcal{Q}}\mathcal{L}(\tilde{\mathcal{P}}\hat{W}(t) + \tilde{\mathcal{Q}}\hat{W}(t)). \quad (\text{F.14})$$

The solution to the equation for  $\tilde{\mathcal{Q}}\hat{W}$  includes the fact that  $\tilde{\mathcal{Q}}\hat{W}(t_0) = 0$  and can be written as follows way:

$$\hat{\mathcal{Q}}\hat{W}(t) = -i \int_{t_0}^t d\bar{t} \mathcal{U}_{\tilde{\mathcal{Q}}}(t - \bar{t}) \tilde{\mathcal{Q}}\mathcal{L}\tilde{\mathcal{P}}\hat{W}(\bar{t}), \quad (\text{F.15})$$

where, the super time-propagation-operator

$$\mathcal{U}_{\tilde{\mathcal{Q}}}(t) = \exp\{-i\tilde{\mathcal{Q}}\mathcal{L}t\}, \quad (\text{F.16})$$

must be introduced. The result for the equation  $\tilde{\mathcal{P}}\hat{W}$  (Nakjima- Zwanzing equation) is a closed equation with respect to  $\tilde{\mathcal{P}}\hat{W}$  and be write as follows

$$\frac{\partial}{\partial t} \tilde{\mathcal{P}}\hat{W}(t) = -i\tilde{\mathcal{P}}\mathcal{L}\tilde{\mathcal{P}}\hat{W}(t) - i \int_{t_0}^t d\bar{t} \tilde{\mathcal{P}}\mathcal{L}\mathcal{U}_{\tilde{\mathcal{Q}}}(t - \bar{t}) \tilde{\mathcal{Q}}\mathcal{L}\tilde{\mathcal{P}}\hat{W}(\bar{t}). \quad (\text{F.17})$$

Using the (F.11) it is possible to derive the corresponding movement equations for the populations of the state. For this the general expressions are considered

$$\text{tr}_R\{\langle a|\tilde{\mathcal{P}}\mathcal{L}\hat{O}|a\rangle\} \equiv \text{tr}_R\{\langle\langle a|\mathcal{L}\hat{O}|a\rangle\rangle\}, \quad (\text{F.18})$$

$$\hat{O}_1 = \tilde{\mathcal{P}}\hat{W}(t), \quad (\text{F.19})$$

as much as

$$\hat{O}_2 = \mathcal{U}_{\tilde{\mathcal{Q}}}(t - \bar{t}) \tilde{\mathcal{Q}}\mathcal{L}\tilde{\mathcal{P}}\hat{W}. \quad (\text{F.20})$$

By inserting  $\hat{O}_1$  in (F.18), it is easily verified that the resulting expression is canceled. The term with  $\hat{O}_2$  suggests the definition of the so-called memory kernels  $K_{ab}$  of the *generalized master equation* (GME). First we have to

$$\text{tr}_R\{\langle a|\mathcal{L}\hat{O}_2|a\rangle\} = \sum_b \text{tr}_R\{\langle a|(\mathcal{L}\mathcal{U}_{\tilde{\mathcal{Q}}}(t - \bar{t}) \tilde{\mathcal{Q}}\mathcal{L}\hat{W}_b)|a\rangle\} P_b(\bar{t}). \quad (\text{F.21})$$



To get to the memory core, the trace expression is multiplied by  $-1$  and the unit step function  $\theta(t - \bar{t})$ . Thus,

$$K_{ab}(t - \bar{t}) = -\theta(t - \bar{t}) \text{tr}_R \{ \langle a | (\mathcal{L} \mathcal{U}_{\tilde{\mathcal{Q}}}(t - \bar{t}) \tilde{\mathcal{Q}} \mathcal{L} \hat{W}_b) | a \rangle \}. \quad (\text{F.22})$$

To configure the (GME) we change  $\tau = t - \bar{t}$  and from the (F.17), the following compact relationship reads:

$$\frac{\partial}{\partial t} P_a(t) = \sum_b \int_{-\infty}^{t-t_0} d\tau K_{ab}(\tau) P_b(t - \tau). \quad (\text{F.23})$$

The time  $t_0$  can be moved to  $-\infty$  if the initial time is directly counted in the population definition ( $P_a \sim \theta(t - \bar{t})$ ). A more detailed inspection of the memory cores leads to further simplification. First it is noted that the introduction of the projector  $\hat{\pi}_a$  it allows replacing the trace with respect to the states of the reservoir with a complete trace.

In addition, the Green super-operator  $\mathcal{G}_{\tilde{\mathcal{Q}}}(\tau)$  is introduced as

$$\mathcal{G}_{\tilde{\mathcal{Q}}}(\tau) = -i\theta(\tau) \mathcal{U}_{\tilde{\mathcal{Q}}}(\tau), \quad (\text{F.24})$$

so that

$$K_{ab}(\tau) = -i \text{tr} \{ \hat{\pi}_a \mathcal{L} \mathcal{G}_{\tilde{\mathcal{Q}}}(\tau) \tilde{\mathcal{Q}} \mathcal{L} \hat{W}_b \}. \quad (\text{F.25})$$

For further simplification,  $\mathcal{L}$  is separated over  $\mathcal{L}_0 \dots = \frac{[H_0, \dots]}{\hbar}$  as well as in the coupling  $\mathcal{L}_V \dots = \frac{[\hat{V}]}{\hbar}$  and reach

$$\tilde{\mathcal{P}} \mathcal{L}_0 = \mathcal{L}_0 \tilde{\mathcal{P}} = 0 \quad (\text{F.26})$$

These relationships are easily verified when applied to an arbitrary operator  $\hat{O}$ .

In the same way, it follows

$$\tilde{\mathcal{P}}\mathcal{L}_V\tilde{\mathcal{P}} = 0. \quad (\text{F.27})$$

Using these identities and replacing  $\hat{\pi}_a\mathcal{L}$  in (F.25) again for  $\hat{\pi}_a\tilde{\mathcal{P}}\mathcal{L}$  we have  $\tilde{\mathcal{P}}\mathcal{L}\mathcal{G}_{\tilde{\mathcal{Q}}}(t) = \tilde{\mathcal{P}}\mathcal{L}_V\mathcal{G}_{\tilde{\mathcal{Q}}}(t)$ . In addition, it is observed that  $\tilde{\mathcal{Q}}\mathcal{L}\hat{W}_b = \tilde{\mathcal{Q}}\mathcal{L}\tilde{\mathcal{P}}\hat{W}_b = \mathcal{L}_V\hat{W}_b$ , result in the following notation of memory cores:

$$K_{ab}(\tau) = -i\text{tr}\hat{\pi}_a\mathcal{L}_V\mathcal{G}_{\tilde{\mathcal{Q}}}(\tau)\mathcal{L}_V\hat{W}_b \equiv \text{tr}\hat{\pi}\mathcal{T}(\tau)\hat{W}_b. \quad (\text{F.28})$$

In the last expression the super transfer operator is presented

$$\mathcal{T}(\tau) = -i\mathcal{L}_V\mathcal{G}_{\tilde{\mathcal{Q}}}(\tau)\mathcal{L}_V, \quad (\text{F.29})$$

provides an adequate interpretation of the memory kernel as the description of the probability transfer from state  $b$  to state  $a$  through the temporal evolution of the operator statistic,  $\hat{W} = \hat{R}_b\hat{\pi}_b$ . However,

$$K_{ab}(\omega) = L_{ab}(\omega) - \frac{i}{\omega + i\epsilon}\Sigma_c L_{ac}(\omega)K_{cb}(\omega), \quad (\text{F.30})$$

where,

$$L_{ab}(\omega) = -i\text{tr}\hat{\pi}\mathcal{L}_V\mathcal{G}(\omega)L_V\hat{W}_b. \quad (\text{F.31})$$

Once all the  $L_{ab}$  have been determined, the  $K_{ab}$  rates that enter the rate equations can be calculated according to this equation.

# Appendix G

## LRT

From another point of view, the study of non-Markovianity has also been supported by the Linear Response Theory (LRT), which is based on the theory of first-order disturbances for a system in thermal equilibrium, which is one of the most useful methods of connecting physical quantities to the underlying theoretical description of a system. Recently, a LRT was developed for open quantum systems, taking the non-Markovian effect [SLY17]. There, a description was made of a system coupled to a determined environment in an external field and the susceptibility was derived in the non-Markovian regime. The results obtained were applied to the theory of topological quantum materials, specifically to Hall's conductance [SLY17]. The general development of the LRT for the Markovian case is presented below. For this case, consider Hamiltonian  $\hat{H}$ , which is represented as follows

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_I + \varrho \hat{H}_{ext}(t), \quad (\text{G.1})$$

where  $\hat{H}_S$  is the Hamiltonian of the quantum system,  $\hat{H}_R$  is the Hamiltonian of the environment,  $\hat{H}_I$  stand for the coupling between the system and the environment,  $\varrho$  stands for the perturbation parameter and  $\hat{H}_{ext}(t)$  describes the coupling of the quantum system to an classical external field. The density operator  $\hat{\rho}(t)$  of the total

system satisfies,

$$\dot{\hat{\rho}}(t) = -\frac{i}{\hbar}[\hat{H}(t), \hat{\rho}(t)] \equiv -\frac{i}{\hbar}\hat{\mathcal{L}}(t)\hat{\rho}(t) \quad (\text{G.2})$$

Subsequently, the total density matrix is divided into two parts, as follows,

$$\hat{\rho}(t) = \hat{\rho}_0(t) + \delta\hat{\rho}_{exp}(t), \quad (\text{G.3})$$

where  $\hat{\rho}_0(t)$  is the total density matrix and initial condition  $\hat{\rho}(0) = \hat{\rho}_0(0)$ .  $\delta\hat{\rho}_{exp}(t)$  denotes the change of  $\hat{\rho}(t)$  due to the external field. By analogy, the Liouville operator can be divided into

$$\hat{\mathcal{L}}(t) = \hat{\mathcal{L}}_0(t) + \hat{\mathcal{L}}_{ex}(t). \quad (\text{G.4})$$

Collecting all these together, they obtain the susceptibility function

$$\chi_{\mu\nu}(\omega) = \int_0^\infty dt \exp(i\omega t) \text{Tr}_S[\hat{B}_\mu \zeta_\nu(t)], \quad (\text{G.5})$$

$$\zeta_\nu(\omega) = \int_0^\infty dt \exp(i\omega t) \zeta_\nu(t). \quad (\text{G.6})$$

Making a modified Laplace transformation to (G.5):  $\chi_{\mu\nu}(\omega) = \int_0^\infty dt \exp(i\omega t) \chi_{\mu\nu}(t)$ , therefore

$$\chi_{\mu\nu}(\omega) = \text{Tr}_S[\hat{B}_\mu \zeta_\nu(\omega)]. \quad (\text{G.7})$$

where  $\hat{B}_\mu$  an observable of the system. This result suggests that in order to calculate the susceptibility, they have to calculate  $\zeta_\nu(\omega)$ , i.e., the Laplace transform of  $\zeta_\nu(t)$

Before continuing, it is necessary to encourage the use of a fundamental tool for these calculations. Specifically, the Born series that comes out of using the Lipman-Schwinger equation, making approximations to first, second, third and higher orders and interactions. Now, it is necessary to specify that the Born approximation allows obtaining expressions for all observable dispersion. In fact, this is concatenated with

open quantum systems and, it is always possible to inspect the successive orders and see if the necessary condition for convergence is fulfilled [dLSWS<sup>+</sup>20b]. In this case, the axioms of completeness, square-integrable functions and separable Hilbert spaces must be respected. In particular, it follows  $\zeta_\nu(t) = \text{Tr}_B \tilde{\zeta}_\nu(t) \equiv \text{Tr}_B \{ \frac{i}{\hbar} \exp(-\frac{i}{\hbar} \hat{L}_0(t)) [\hat{A}_\nu, \rho_{\text{eq}}] \}$  up to the second order of coupling between the reservoir–system. It must be assumed that the system is in equilibrium at a temperature T. In addition,  $\tilde{\zeta}_\nu(0) = \zeta_\nu(0) \otimes \rho_R + O(\hat{H}_I)$ , with  $\zeta_\nu(0) \approx \frac{i}{\hbar} [\hat{A}_\nu, \rho_S]$ , where  $\hat{A}_\nu$  denotes hermitian system operators,  $\rho_x = \frac{e^{-\beta \hat{H}_x}}{\text{Tr}_x e^{-\beta \hat{H}_x}}$ ,  $x = S$  and  $R$ . Without loss of generality, choose  $H_S$ , couplings and define the interaction. Now, the second order calculations will be made taking into account the approximation of Born for the respective operator. That is to say,

$$\dot{\xi}_{I\nu} = -\frac{1}{\hbar^2} \text{tr}_B \int_0^t dt' [\hat{H}_I(t), [\hat{H}_I(t'), \xi_{I\nu}(t') \otimes \rho_R]], \quad (\text{G.8})$$

where,  $\xi_{I\nu}(t) = \hat{U}^\dagger \xi_\nu(t) \hat{U}(t)$ ,  $\xi_\nu(t)$  in the interaction picture. The functions of the environment at zero temperature  $f(t)$  and finite temperature  $\bar{f}(t)$  take

$$f(t) = \sum_j \|g_j\|^2 e^{-i\omega_j t} \equiv \int_0^\infty J(\omega) e^{-i\omega_j t} d\omega, \quad (\text{G.9})$$

$$\bar{f}(t) = \sum_j \|g_j\|^2 N(\omega_j) e^{-i\omega_j t} \equiv \int_0^\infty J(\omega) N(\omega_j) e^{-i\omega_j t} d\omega, \quad (\text{G.10})$$

where  $J(\omega)$  denotes the spectral density of the environment,  $N(\omega) = \frac{1}{e^{\frac{\hbar\omega}{\kappa_B T}} - 1}$  is the average photon number of the environment, and  $\kappa_B$  the Boltzmann constant. Furthermore, the function  $\zeta_\nu(t)$  plays an important role in the intermediate process of the study of the detection of the degree of Markovianity or non-Markovianity in the interaction (system-reservoir) in the presence of an external field. Consider now an observable  $\hat{B}_\mu$  of the system and guarantee that the operators are hermitian  $\hat{A}_\nu$ . On the other hand, the degree of non-Markovianity (memory effects), comes from the information associated with the second order terms of the integrable equations. Furthermore, theoretically or experimentally the degrees of Markovianity could be calibrated according to the variation of the parameters of the environment or the

incidence of the external field. Likewise, without loss of generality, the advances of the LRT combined with the Born approach, can be extended to different orders without any problem.