Leonardo da Silva Souza

Dynamical Maps for Reduced States of Indistinguishable Particles

Belo Horizonte

2019

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Tese apresentada ao Programa de Pós-Graduação em Física do Instituto de Ciências Exatas da Universidade Federal de Minas Gerais como requisito parcial para obtenção do título de Doutor em Física.

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Belo Horizonte

2019

Dados Internacionais de Catalogação na Publicação (CIP)

S729d Souza, Leonardo da Silva.
Dynamical maps for reduced states of indistinguishable particles / Leonardo da Silva Souza. – 2019.
70f., enc. : il.

Orientador: Reinaldo Oliveira Vianna.
Coorientador: Tiago Debarba.
Tese (doutorado) – Universidade Federal de Minas Gerais, Departamento de Física.
Bibliografia: f. 59-62.

1. Sistemas quânticos. 2. Mapas quânticos. 3. Partículas.
I. Título. II. Vianna, Reinaldo Oliveira. III. Universidade Federal de Minas Gerais, Departamento de Física.

CDU – 530.145 (043)

Ficha catalográfica elaborada por Romário Martins Ribeiro – CRB6 3595
Biblioteca Professor Manoel Lopes de Siqueira – Departamento de Física - UFMG

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ATA DA SESSÃO DE ARGUIÇÃO DA 361ª TESE DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA, DEFENDIDA POR Leonardo da Silva Souza orientado pelo professor Reinaldo Oliveira Vianna e coorientado pelo professor Tiago Debarba, para obtenção do grau de **DOUTOR EM CIÊNCIAS, área de concentração Física**. Às 09:00 horas de vinte e seis de novembro de dois mil e dezenove, na sala 4123A do Departamento de Física da UFMG, reuniu-se a Comissão Examinadora, composta pelos professores **Reinaldo Oliveira Vianna** (Orientador - Departamento de Física/UFMG), **Pablo Lima Saldanha** (Departamento de Física/UFMG), **Raphael Campos Drumond** (Departamento de Matamática/UFMG), **José Geraldo Peixoto de Faria** (Departamento de Matemática/ CEFET-MG) e **Nadja Kolb Bernardes** (Departamento de Física /UFPE) para dar cumprimento ao Artigo 37 do Regimento Geral da UFMG, submetendo o Mestre **Leonardo da Silva Souza** à arguição de seu trabalho de Tese de Doutorado, que recebeu o título de **"Dynamical Maps for Reduced States of Indistinguishable Particles"**. Às 14:00 horas do mesmo dia, o candidato fez uma exposição oral de seu trabalho durante aproximadamente 50 minutos. Após esta, os membros da comissão prosseguiram com a sua arguição, e apresentaram seus pareceres individuais sobre o trabalho, concluindo pela aprovação do candidato.

Belo Horizonte, 26 de Novembro de 2019.

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Acknowledgements

Primeiramente, pelo extraordinário apoio, gostaria de agradecer à minha família: aos meus pais Francisco e Almerinda, ao meu irmão Jadson e minha cunhada Cristiene, às minhas sobrinhas Vitória e Anna Laura.

Gostaria de expressar minha gratidão ao meu orientador, professor Reinaldo Oliveira Vianna, pela sua paciência, apoio e ensinamentos. A porta do gabinete do professor Reinaldo sempre esteve aberta quando precisei conversar. Obrigado por me guiar pelo estudo que resultou nesta tese.

Agradeço aos professores Fernando Iemini, Raphael Drumond e Tiago Debarba que sempre estiveram disponíveis para discussões desde a primeira conversa, grande parte do que aprendi sobre informação quântica e sistemas abertos foi ensinado por eles.

Agradeço ao pessoal do grupo Infoquant (André, Diego, Felipe, Fernando, João Vitor, Lucas, Ludmila, Marcelo, Reinaldo, Tiago, Thiago), foi ótimo compartilhar o "cafofo" com vocês durante os últimos quatro anos. Ao Diego Ferreira e Thiago Maciel, muito obrigado pelas discussões sobre informação quântica e algoritmos.

Aos amigos Amanda, Cintia, Diego, Halaine, Natália, Rosemberg, Oziel e Tarcísio pela agradável convivência.

Agradeço as agências CAPES e CNPq, pelo suporte financeiro.

Resumo

Na presente tese, examinamos dois tópicos da teoria de sistemas quânticos abertos. O primeiro tópico trata da descrição da dinâmica de sistemas inicialmente correlacionados com o ambiente. Na teoria de sistemas quânticos abertos, mapas que caracterizam a dinâmica do sistema quântico em contato com o ambiente são usualmente considerados completamente positivos. No entanto, isso não é necessariamente verdadeiro se o sistema e seu ambiente forem inicialmente correlacionados, a menos que se restrinja o domínio no qual o mapa atua, ou seja, apenas um subconjunto do conjunto de estados do sistema é mapeado para outros estados pelo mapa dinâmico. Nós introduzimos um quadro para a construção de mapas dinâmicos reduzidos para subsistemas de partículas fermiônicas indistinguíveis. Nesse cenário, um mapa reduzido na representação de Kraus é possível para alguns conjuntos de estados onde a única correlação não clássica presente é a de troca. O segundo tema estudado está relacionado à caracterização de dinâmicas não-markovianas com os critérios de divisibilidade e emaranhamento. Obtemos uma expressão analítica para a decomposição de Kraus do mapa quântico de um ambiente modelado por um hamiltoniano fermiônico quadrático arbitrário atuando em um ou dois qubits, derivamos funções simples para verificar a não positividade do mapa intermediário. No caso particular de um ambiente representado pelo Hamiltoniano de Ising, discutimos as duas fontes de não-Markovianidade no modelo, uma devido ao tamanho finito da rede, e outra devido ao tipo de interação.

Palavras-chave: sistema quântico aberto, mapa quântico, partículas indistinguíveis, não-Makovianidade, sistemas de muitos corpos.

Abstract

In the present thesis, we examine two subjects in the theory of open quantum systems. The first subject deals with the description of the dynamics of open systems initially correlated with the environment. In the theory of open quantum systems, maps characterizing the dynamics of a quantum system in contact with the environment are usually thought to be completely positive. However, this is not necessarily true if the system and its environment are initially correlated, unless we restrict the domain on which the map acts, in other words, only a subset of the set of states of the system gets mapped to other states by the dynamical map. We present a framework for the construction of reduced dynamical maps for subsystems of indistinguishable fermionic particles. We show that in this scenario, a reduced map in the Kraus representation is possible for some sets of states where the only non-classical correlation present is exchange. The second subject studied is related to the characterization of non-Markovian dynamics with the divisibility and entanglement criteria. We obtain the analytical expression for the Kraus decomposition of the quantum map of an environment modeled by an arbitrary quadratic fermionic Hamiltonian acting on one or two qubits, we derive simple functions to examine the non positivity of the intermediate map. In the particular case of an environment represented by the Ising Hamiltonian, we discuss the two sources of non-Markovianity in the model, one due to the finite size of the lattice, and another due to the kind of interactions.

Keywords: open quantum system, quantum map, indistinguishable particles, non-Markovianity, many-body system.

List of Publications

Thesis' publications:

1. *Dynamical matrix for arbitrary quadratic fermionic bath Hamiltonians and non-Markovian dynamics of one and two qubits in an Ising model environment*
   Fernando Iemini, **Leonardo da Silva Souza**, Tiago Debarba, Andre T. Cesário, Thiago O. Maciel, Reinaldo O. Vianna
   Eur. Phys. J. D 71, 119 (2017).

2. *Completely Positive Maps for Reduced States of Indistinguishable Particles*
   Leonardo da Silva Souza, Tiago Debarba, Diego L. Braga Ferreira, Fernando Iemini, Reinaldo O. Vianna
   Phys. Rev. A 98, 052135 (2018).

Publications as co-author:

3. *Decoherence of odd compass states in the phase-sensitive amplifying/dissipating environment*
   V. V. Dodonov, C. Valverde, **L. S. Souza** and B. Baseia
   Ann. Phys. 371, 296-312 (2016).

Contents

1 Introduction

The characterization of the dynamics of a system that may be correlated with other systems has been subject of investigation in several areas, varying from quantum information processing to cosmology [1, 2]. A closed system, an idealization of a system perfectly isolated from its environment, evolves unitarily according to the Schrödinger equation. On the other hand, the dynamics of a system whose interaction with its surroundings cannot be negligible is not necessarily unitary. The interaction with the environment affects properties of the system. For example, leads to the disappearance of quantum superpositions, a phenomenon known as decoherence. The theory of open quantum systems provides the mathematical framework to treat such systems. In this context, we speak of system and environment, and say that the system, which is just a part of the whole, is open. The standard characterization of an open quantum system dynamics is based on the supposition that system and environment start in an uncorrelated global state (factorable), since this is the case where the reduced dynamics is guaranteed to be completely positive (CP). The interaction with the environment naturally generates correlations, therefore the assumption of a special instant of time where there is no correlation between system and environment, from which one starts to monitor the evolution of the open system, is not always possible. For example, we will study a case where such time does not exist, dealing with indistinguishable particles.

One may also be interested in how an initial correlation with the environment can affect the system dynamics. The extension of the formalism to characterize reduced dynamics of system-environment initially correlated is much more problematic, subject that still generates discussion and has not yet been closed. A map characterizing the dynamics of a system, in a context that the system is initially correlated with the environment, is in general not completely positive, which can be seen as only a subset of the set of states is mapped to states by the map. The problems emerging in the description of reduced dynamics in presence of initial correlation were first explored by Pechukas and Alicki [3–5]. Pechukas introduced the idea of 'assignment map' ($\mathcal{A}$), which characterizes initial system-environment states ($\mathcal{A}[\rho_S] = \rho_{SE}$) for open quantum systems, and showed that imposing three 'natural' conditions, namely: (linearity) $\mathcal{A}$ preserves mixtures; (consistency) it is consistent, in the sense that $\rho_S = Tr_E(\mathcal{A}[\rho_S])$; and (positivity) $\mathcal{A}[\rho_S]$ is positive for all positive ρ_S; this implies the initial state of the system and environment is factorable ($\mathcal{A}[\rho_S] = \rho_S \otimes \rho_E$). In order to handle the problem, it was proposed to relax the condition of positivity by Pechukas [3, 5] or consistency by Aliciki [4]. The two suggestions can be reduced to a evolution with restricted domain of the assignment map. Stelmachovic et al. [6] demonstrated the need to characterize the correlation between system and environment in order to describe the evolution of the system. In their work it was presented an interesting example of two qubits (one for the system, one for the environment), with the dynamics given by a C-NOT gate. Assuming two initial states for the composed system (system-environment), a maximally entangled state and a maximally mixed global state, the reduced state of the system has the same one qubit maximally mixed states, but the dynamics leads to radically distinct states. Due to the important role of the initial correlation, a large portion of the literature on the subject has been dedicated to study set of correlated states that are taken to states by dynamical maps. Many authors worked out sets of classicaly [7, 8] or quantum [9, 10] correlated initial global states. In this work, we are interested in exploring set of states presenting exchange correlations, correlations due to indistinguishability of particles, that guarantee the definition of complete positivity dynamics for the domain compatible with the correlation. The subject has recently regained impetus, with many interesting discussions [10–17].

Another subject that has been of great interest in the field of open quantum systems concerns the Markovian or non-Markovian nature of quantum dynamics [18–20]. Many witnesses and quantifiers have been proposed in order to characterize the non-Markovianity of a quantum processes [21]. For example, the information flow between system and environment, quantified by the distinguishability of any two quantum states [22–24], or by the Fisher information [25], or mutual information [26]. Another interesting quantifier is the entanglement based measure of non-Markovianity [27], it is related to the classical information flow between system and environment [28].The behavior of the quantifiers depend on the kind of interactions and size of the system, as is discussed in [29]. In this work, we will focus on the divisibility criterion [30,31] which consist in checking the non-positivity of intermediate time quantum maps, and the entanglement [27], based on non-monotonic decreasing of the entanglement under local completely positive maps. We explored the system of an environment represented by the quantum one-dimensional Ising model acting on one central qubit, which in the case of finite size lattices can be solved analytically by means of the well known Jordan-Wigner and Bogoliubov transformations [56, 57]. The availability of an analytical solution for this representative critical model is the reason why this system is recurrently investigated in many instances. The study we perform here is complementary to previous investigations and, besides its pedagogical purpose, reveals functional dependencies among different indicators of non-Markovianity, and also stresses that there are two sources of non-divisibility in the dynamics, one intrinsic to the kind of interactions, and another due to the finite size of the lattice.

The thesis is organized as follows. In Chapter 2, we introduce some main notions in quantum information theory and open quantum systems theory, we define the mathematical framework to characterize quantum systems and their transformations, and we briefly revise the standard description of open quantum systems. Chapter 3 deals with the problem of describing the dynamics of open systems that are initially correlated with the environment. We present the pioneering work of Pechukas and Alicki [3–5] on the subject, we discuss the role of initial correlation with the environment in the dynamics of the open system. In Chapter 4, we present the construction of the reduced dynamical map for a system composed by N indistinguishable particles, in particular fermions. We briefly discuss indistinguishable particles formalism, we identify a class of initial global states that give rise to completely positive reduced dynamics for the compatible domain. Finally, we illustrate the formalism with an example of two fermions under a quadratic Hamiltonian. In Chapther 5, we introduce the concept of Markovianity in classical theory of stochastic processes, we briefly present differences and analogies with the quantum case. We define the divisibility criterion for measures of non-Markovianity for both, classical and quantum cases. In Chapter 6, we deduce the quantum map and the dynamical matrix for the intermediate map to a system of one and two qubits under the influences of a quadratic fermionic environment. In the case of the environment mapped in the Ising model with a transverse field, we characterize the dynamics of the open system (one or two qubits) using the divisibility criterion [30, 31], we investigate the non-Markovianity using the most negative eigenvalue of the intermediate map as a quantifier. We also use the increase of entanglement under local CP maps as a witness of non-Markovianity [27].

2 Preliminaries

In this chapter, we will present some fundamental concepts in quantum information theory and the basic notation used throughout the text. It is not intend to be a text to introduce the formalism of quantum information theory, but rather a brief presentation of the mathematical tools to characterize systems and their transformations. The concepts discussed in this chapter can be found in textbooks on quantum mechanics and quantum information [2, 32, 33].

2.1 Space of interest

Physical systems in quantum mechanics are associated with the Hilbert space $\mathcal{H}$, a complex Euclidean vector space, normed and with well defined inner product. In particular, the systems treated throughout this thesis are finite, which allows us to maintain the discussion for Hilbert spaces with finite dimension, i.e. $\mathcal{H}_N \cong \mathbb{C}^N$. It is typical to represent a vector $|\psi\rangle \in \mathcal{H}_N$ as a column vector of the form

$$|\psi\rangle = \sum_{j=0}^{N-1} \psi_j |j\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{pmatrix}, \tag{2.1}$$

where $\psi_j \in \mathbb{C}$ and $\{|j\rangle\}$ is the computational base. The inner product of two vectors $|\phi\rangle$, $|\psi\rangle \in \mathcal{H}$ is given by

$$\langle\phi|\psi\rangle = \sum_{j=0}^{N-1} \phi_j^* \psi_j, \tag{2.2}$$

where $\langle\psi|$ is an element of the dual space $\mathcal{H}_N^* \cong \mathbb{C}^N$ of $\mathcal{H}_N$, which is the space of linear maps from $\mathcal{H}_N$ to the complex numbers. The vector $\langle\psi| \in \mathcal{H}_N^*$ can be represented as a row vector defined by transposing its corresponding column vector in $\mathcal{H}_N$, Eq.(2.1), and taking the complex conjugate of its entries. Given a vector $|\psi\rangle \in \mathcal{H}_N$, the norm is defined by the relation

$$\||\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle} = \sqrt{\sum_{j=0}^{N-1} |\psi_j|^2}. \tag{2.3}$$

The set of linear operators mapping between two Hilbert spaces $A : \mathcal{H}_M \to \mathcal{H}_N$ also form their own Hilbert space $\mathcal{L}(\mathcal{H}_M, \mathcal{H}_N)$ named Hilbert-Schmidt space, therefore it is equipped with inner product and norm. Given the spaces $\mathcal{H}_M$ and $\mathcal{H}_N$, we can associate with each operator $A \in \mathcal{L}(\mathcal{H}_M, \mathcal{H}_N)$ a matrix with entries

$$A(j,k) = \langle j|A|k'\rangle, \tag{2.4}$$

where $|j\rangle \in \mathcal{H}_N$ and $|k'\rangle \in \mathcal{H}_M$. For any choice of operator pairs $A, B \in \mathcal{L}(\mathcal{H}_M, \mathcal{H}_N)$, one can define an inner product as

$$\langle A, B\rangle = Tr\left(A^\dagger B\right), \tag{2.5}$$

where $A^\dagger \in L(\mathcal{H}_N, \mathcal{H}_M)$ will be called adjoint of the operator A, defined by the relation $\langle k'|A^\dagger|j\rangle = \langle j|A|k'\rangle^*$, for all $|j\rangle \in \mathcal{H}_N$ and $|k'\rangle \in \mathcal{H}_M$. Thus, it is the operator whose matrix representation is obtained by transposing the matrix representation of A and taking the complex conjugate of its entries. The norm for an operator $A \in L(\mathcal{H}_M, \mathcal{H}_N)$ can be defined as

$$|M| = \sqrt{\langle A, A\rangle}, \tag{2.6}$$

which is known as Hilbert-Schmidt norm. Several others useful norms on operators can be defined. In sec. (4.2) we shall discuss in more detail the so called trace norm which is commonly used in the construction of distance measures between operators.

Some of the important classes of operators which will be mentioned in the text are:

1. *Normal.* An operator $A \in \mathcal{L}(\mathcal{H}_N)$ is normal if it commutes with its adjoint $[A, A^\dagger] = 0$, where $\mathcal{L}(\mathcal{H}_N)$ is a shorthand for $\mathcal{L}(\mathcal{H}_N, \mathcal{H}_N)$ and $[A, A^\dagger] = AA^\dagger - A^\dagger A$. Most of the operators that will be discussed are included in this class that have as main characteristic to be the operators for which the spectral theorem holds. Let $A \in \mathcal{L}(\mathcal{H}_N)$ be a normal operator and assume that the eigenvalues of A are $a_1, \ldots a_r$. There exists an orthonormal basis $\{|a_1\rangle, \ldots, |a_r\rangle\}$ in $\mathcal{H}_N$ such that,

$$A = \sum_{j=1}^{r} a_j |a_j\rangle\langle a_j|. \tag{2.7}$$

2. *Hermitian.* An operator $A \in \mathcal{L}(\mathcal{H}_N)$ is Hermitian if it is equal to its adjoint, i.e. $A = A^\dagger$. This class of operators is obviously a subset of normal operators with real eigenvalues. The set of Hermitian operators acting on a given Hilbert space $\mathcal{H}_N$ will be denoted $\mathrm{Herm}(\mathcal{H}_N)$. In the theory of quantum mechanics, observables are represented by Hermitian operators.

3. *Positive semidefinite and positive definite.* An operator $A \in \mathcal{L}(\mathcal{H}_N)$ is said to be positive semidefinite if it can be defined as $A = B^\dagger B$ for an operator $B \in \mathcal{L}(\mathcal{H}_N)$, or equivalently if satisfies $\langle\psi|A|\psi\rangle \geq 0$ for all $|\psi\rangle \in \mathcal{H}_N$. The notation $A \geq 0$ will be used to mean that P is positive semidefinite. Positive semidefinite operators that are invertible are called positive definite, or equivalently if satisfies $\langle\psi|A|\psi\rangle > 0$ for all $|\psi\rangle \in \mathcal{H}_N$.

4. *Orthogonal projections.* A positive semidefinite operator $P \in \mathcal{L}(\mathcal{H}_N)$ that satisfy the relation $P^2 = P$ is an orthogonal projection, hence, a Hermitian operator whose only eigenvalues are 0 and 1. Orthogonal projectors can expand any normal operator, in

other words, let $A \in \mathcal{L}(\mathcal{H}_N)$ be a normal operator and assume that the eigenvalues of A are $a_1, \ldots a_r$. There exists a set of orthogonal projection operators $\{P_1, \ldots P_r\}$, with $P_1 + \cdots + P_r = \mathbb{I}_N$ and $P_j P_k = 0$, for $j \neq k$, such that

$$A = \sum_{j=1}^{r} a_j P_k. \tag{2.8}$$

Note that this statement is equivalent to the spectral theorem.

5. *Density.* Positive semidefinite operators that have trace 1 are named density operators. The vector space whose elements are density operators acting on a given Hilbert space $\mathcal{H}_M$ will hereafter be denoted $\mathcal{D}(\mathcal{H}_N)$. In quantum mechanics, density operators $\rho \in \mathcal{D}(\mathcal{H}_N)$ represent quantum states of the physical system associated with the Hilbert space $\mathcal{H}_N$. The space $\mathcal{D}(\mathcal{H}_N)$ is a convex set whose extremal points are named pure states and can be written as

$$\rho = |\psi\rangle\langle\psi|, \tag{2.9}$$

where $|\psi\rangle \in \mathcal{H}_N$ with $\||\psi\rangle\| = 1$. In opposition, a state which is not pure is called mixed state and can be expressed as a convex combination of pure orthogonal states,

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|, \tag{2.10}$$

with $p_j \geq 0$, $\forall j$ and $\sum_j p_j = 1$.

6. *Linear isometries and unitary operators.* An operator $V \in \mathcal{L}(\mathcal{H}_M, \mathcal{H}_N)$ is a linear isometry if it preserves the norm, i.e., $\|V|\psi\rangle\| = \||\psi\rangle\|$, for all $|\psi\rangle \in \mathcal{H}_M$, or equivalently $V^\dagger V = \mathbb{I}_M$. Linear isometries mapping elements of $\mathcal{H}_N$ to itself are called unitary operators $U : \mathcal{H}_N \to \mathcal{H}_N$, where $U^\dagger U = UU^\dagger = \mathbb{I}_N$. The space of isometries $V : \mathcal{H}_M \to \mathcal{H}_N$ will be denoted $\mathcal{U}(\mathcal{H}_M, \mathcal{H}_N)$. Unitary operators characterize the dynamics of closed quantum systems, an idealization of a quantum systems perfectly isolated from its environment.

2.1.1 Composed systems

The characterization of open quantum systems is the key idea in this work and at its foundation lies the concept of composite quantum system, of which we will present some basic notions. Consider a system consisting of N subsystems $S_1, \ldots, S_N$, with their associated Hilbert spaces $\mathcal{H}_{S_1}, \ldots \mathcal{H}_{S_N}$. The Hilbert space of the composite system will be given by the tensor product of the Hilbert spaces of each subsystem, $\mathcal{H}_{S_1,\ldots,S_N} = \mathcal{H}_{S_1} \otimes \mathcal{H}_{S_2} \otimes \cdots \otimes \mathcal{H}_{S_N}$. Defining an orthonormal base $\{|j_i\rangle\}$ in each space $\mathcal{H}_{S_i}$, the composed system space admit the orthonormal base $\{|j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_N\rangle\}$, therefore a generic element in $\mathcal{H}_{S_1,\ldots,S_N}$ can be written as

$$|\psi\rangle = \sum_{j_1,j_2,\ldots,j_N} \alpha_{j_1,j_2,\ldots,j_N} |j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_N\rangle, \tag{2.11}$$

where $\alpha_{j_1,j_2,\ldots,j_N} \in \mathbb{C}$. In a similar way, given N linear operators $O_{S_1} \in \mathcal{L}(\mathcal{H}_{S_1})$, $\ldots$, $O_{S_N} \in \mathcal{L}(\mathcal{H}_{S_N})$, we can define a linear operator acting on $\mathcal{H}_{S_1} \otimes \cdots \otimes \mathcal{H}_{S_N}$ by taking the tensor product $O_{S_1} \otimes \cdots \otimes O_{S_N}$ and a generic element of $\mathcal{L}(\mathcal{H}_{S_1} \otimes \cdots \otimes \mathcal{H}_{S_N})$ can be defined as

$$O_{S_1,\ldots S_N} = \sum_k O^k_{S_1} \otimes O^k_{S_2} \otimes \cdots \otimes O^k_{S_N}. \tag{2.12}$$

As mentioned in the previous section, a density operator represents the state of the quantum system. Let us continue the discussion about composite systems for elements of the set $\mathcal{D}(\mathcal{H}_{S_1} \otimes \cdots \otimes \mathcal{H}_{S_N})$. A density operator $\rho \in \mathcal{D}(\mathcal{H}_{S_1} \otimes \cdots \otimes \mathcal{H}_{S_N})$ can be written in its spectral decomposition as

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|, \tag{2.13}$$

with $p_j \geq 0$, $\forall j$, $\sum_j p_j = 1$ and $|\psi_j\rangle$ has the form of Eq.(2.11) with $\| |\psi_j\rangle \| = 1$ for all j. From the density operator of the composed system we can obtain an operator characterizing the state of a subsystem by taking the trace over all subsystems except on the subsystem we are interested. Suppose we want to describe S_1 in the composed system $S_1, \ldots, S_N$, we should obtain the named reduced density operator of S_1, defined by the partial trace

$$\rho_{S_1} = \mathrm{Tr}_{S_2,\ldots,S_N}(\rho), \tag{2.14}$$

where $\rho_{S_1} \in \mathcal{H}_{S_1}$ and $\mathrm{Tr}_{S_2,\ldots,S_N}$ stand for the trace over the subspaces $S_2, \ldots, S_N$. Given an orthonormal base $\{|j_2\rangle \otimes \cdots \otimes |j_N\rangle\}$ in $\mathcal{H}_{S_2} \otimes \cdots \otimes \mathcal{H}_{S_N}$, the partial trace in Eq.(2.14) can be defined as

$$\rho_{S_1} = \sum_{j_2,\ldots,j_N} (\langle j_2| \otimes \cdots \otimes \langle j_N|)\, \rho\, (|j_2\rangle \otimes \cdots \otimes |j_N\rangle). \tag{2.15}$$

The simplest example of composite system states describes uncorrelated subsystems and has the form:

$$\rho = \rho_{S_1} \otimes \rho_{S_2} \otimes \cdots \otimes \rho_{S_N}, \tag{2.16}$$

where $\rho_{S_j} \in \mathcal{H}_{S_j}$ for all j. If a composed system can be written as Eq.(2.16) it is named a product state. The convex combination of states will also be a quantum state, thus we can generalize the notion of product states by taking the convex combination. The resulting state is the so-called separable state,

$$\rho = \sum_k p_k \rho^k_{S_1} \otimes \rho^k_{S_2} \otimes \cdots \otimes \rho^k_{S_N}, \tag{2.17}$$

where $p_j \geq 0$, $\forall j$ and $\sum_j p_j = 1$ and $\rho^k_{S_j} \in \mathcal{H}_{S_j}$ for all j, k. States of a composed system that cannot be written as Eq.(2.17) are called entangled states.

2.2 Linear maps on state space

In contrast to closed quantum systems that has the evolution given by unitary operators, to describe the evolution of open quantum systems we will use a more general transformation on the space of positive semidefinite operators having unit trace. In this section, we are going to describe the mapping between states without any mention of a temporal evolution, the link with the dynamics of the open quantum system will be discussed in the next section. A map $\Phi : \mathcal{D}(\mathcal{H}_M) \to \mathcal{D}(\mathcal{H}_N)$ must satisfy some conditions determined by the mathematical properties of the density operators:

1. *Linearity.* For any choice of density operator pairs $\rho, \sigma \in \mathcal{D}(\mathcal{H}_M)$, and any real number $p \in [0, 1]$, the map $\Phi \in T(\mathcal{H}_M, \mathcal{H}_N)$ is linear if $\Phi\left[(1-p)\rho + p\sigma\right] = (1-p)\Phi\left[\rho\right] + p\Phi\left[\sigma\right]$, where $T(\mathcal{H}_M, \mathcal{H}_N)$ is the space form by the set of maps $\Phi : \mathcal{D}(\mathcal{H}_M) \to \mathcal{D}(\mathcal{H}_N)$. The convex combination of quantum states is also a quantum state, the map must not depend on the way we choose the convex combination.

2. *Positivity and complete positivity.* A map $\Phi \in T(\mathcal{H}_M, \mathcal{H}_N)$ is positive if it preserves the positivity of an operator, $\Phi\left[A\right] \geq 0$ for all $A \geq 0$. As the density operator is a positive operator, the map must maintain its positivity. Moreover, considering the composition of systems in quantum mechanics, if the map only acts on a fraction of the composite system it is desirable that the resulted operator must remain a quantum state, which leads to the definition of a completely positive map. Given a bipartite system characterized by the state $\rho \in \mathcal{D}(\mathcal{H}_M \otimes \mathcal{H}_Z)$, the map Φ is completely positive if $\Phi \otimes \mathbb{I}_Z\left[\rho\right] \geq 0$, for any choice of ρ, where $\mathbb{I}_Z$ is the identity map on a space of density operators $\mathcal{D}(\mathcal{H}_Z)$. Completely positive maps are also positive, however the converse is not necessarily true, for example, the transpose map is positive but not completely positive.

3. *Trace preservation.* A map Φ is trace preserving if the following relation is satisfied $Tr\left(\Phi\left[\rho\right]\right) = Tr\left(\rho\right) = 1$. The trace preservation together with complete positivity ensures the mapping to a valid density operator, an operator whose eigenvalues characterizes a probability distribution.

2.2.1 Representations

There are many ways to represent quantum maps. Throughout this work, we use three represention s. We shall briefly introduce them below.

2.2.1.1 Kraus representation

Given a complety positive map $\Phi \in T(\mathcal{H}_M, \mathcal{H}_N)$, there exists a set of operators $\{E_j\} \in \mathcal{L}(\mathcal{H}_M, \mathcal{H}_N)$, such that we can represent the action of the map Φ in a quantum state $\rho \in \mathcal{D}(\mathcal{H}_M)$ as

$$\Phi\left[\rho\right] = \sum_j E_j \rho E_j^\dagger. \tag{2.18}$$

The operators E_j are known as Kraus operators. One may deduce that a map which can be written in the form (2.18) is completely positive by considering the map acting locally on a generic positive operator $A \in \mathcal{L}(\mathcal{H}_M \otimes \mathcal{H}_Z)$. The spectral decomposition of A can be written as $A = \sum_j a_j |a_j\rangle\langle a_j|$, with $a_j \geq 0$, then we have

$$\left(E_j \otimes \mathbb{I}_Z\right) A \left(E_j \otimes \mathbb{I}_Z\right)^\dagger = \sum_k a_k \left(E_j \otimes \mathbb{I}_Z\right) |a_k\rangle\langle a_k| \left(E_j \otimes \mathbb{I}_Z\right)^\dagger, \tag{2.19}$$

defining $|b_{j,k}\rangle = \left(E_j \otimes \mathbb{I}_Z\right)|a_k\rangle$, where $|b_{j,k}\rangle \in \mathcal{H}_N \otimes \mathcal{H}_Z$, we can see that the operator in Eq.(2.19) is positive. Therefore, the mapping of the form $\Phi_j : \rho \rightarrow E_j \rho E_j^\dagger$ is completely positive, which is also true for the linear combination in Eq.(2.18). Finaly, the map Φ is trace preserving for all $\rho \in \mathcal{D}(\mathcal{H}_M)$ if the Kraus operators satisfy the relation $\sum_j E_j^\dagger E_j = \mathbb{I}_{\mathcal{H}_M}$, as can be seen by the computation

$$\begin{aligned} Tr\left(\Phi[\rho]\right) &= Tr\left(\sum_i E_j \rho E_j^\dagger\right) \\ &= Tr\left(\sum_j E_j^\dagger E_j \rho\right) \\ &= Tr\left(\mathbb{I}_M \rho\right) = 1. \end{aligned} \tag{2.20}$$

All maps $\Lambda \in T(\mathcal{H}_M, \mathcal{H}_N)$, not necessarily completely positive, can be written as $\Lambda\left[\rho\right] = \sum_j E_j \rho F_j^\dagger$, where $E_j, F_j \in \mathcal{L}(\mathcal{H}_M, \mathcal{H}_N)$. Some authors assign the term Kraus representation for this general form, however in this work we will use just for the case $F_j = E_j$ for each j, Eq.(2.18).

2.2.1.2 The natural representation

Now, let us define the natural representation also known as superoperator representation. We use the idea of vectorization, a mapping between the spaces $\mathcal{L}(\mathcal{H}_M)$ and $\mathcal{H}_M \otimes \mathcal{H}_M$. Such mapping will be given by the *vec* operation that can be defined as

$$vec\left[|i\rangle\langle j|\right] = |i\rangle \otimes |j\rangle, \quad \forall\, i, j. \tag{2.21}$$

Consider the map $\Phi \in T(\mathcal{H}_M, \mathcal{H}_N)$, there exists an operator $K\left(\Phi\right) \in \mathcal{L}(\mathcal{H}_M \otimes \mathcal{H}_M, \mathcal{H}_N \otimes \mathcal{H}_N)$ such that

$$vec\left(\Phi\left[\rho\right]\right) = K\left(\Phi\right) vec\left[\rho\right], \tag{2.22}$$

where $\rho \in \mathcal{D}(\mathcal{H}_M)$. The operator $K\left(\Phi\right)$ is the natural representation of the map Φ. The natural representation of the map Φ can be defined as

$$K\left(\Phi\right) = \sum_{i,j,k,l} \langle |k\rangle\langle l|, \Phi\left[|i\rangle\langle j|\right]\rangle\, |i\rangle\langle j| \otimes |k\rangle\langle l|. \tag{2.23}$$

We can verify Eq.(2.23) by applying the map on some generic element of a base in $\mathcal{H}_A \otimes \mathcal{H}_B$,

$$\begin{aligned} K(\Phi)|m\rangle \otimes |n\rangle &= \sum_{k,l} \langle |k\rangle\langle l|, \Phi[|m\rangle\langle n|]\rangle |k\rangle \otimes |l\rangle \\ &= vec\left(\sum_{k,l} \langle |k\rangle\langle l|, \Phi[|m\rangle\langle n|]\rangle |k\rangle\langle l|\right) \\ &= vec(\Phi[|m\rangle\langle n|]), \end{aligned} \tag{2.24}$$

and using linearity, which leads to relation Eq.(2.22), for all ρ. There is no direct criterion in natural representation that shows if Φ is a CP-map. Using the following identity for product of three matrices (ABC):

$$vec[ABC] = \left(A \otimes C^T\right) vec[B], \tag{2.25}$$

we can rewrite the Kraus representation (Eq.2.18) as the natural representation, then with the superoperator $\sum_j E_j \otimes E_j^*$ acting on the vector $vec[\rho]$.:

$$|\Phi[\rho]\rangle = K(\Phi)|\rho\rangle, \quad K(\Phi) = \sum_j E_j \otimes E_j^*. \tag{2.26}$$

where $|\rho\rangle \equiv vec(\rho)$. In order to verify the complete positivity, its relation with the Choi-Jamiolkowski's representation is usually used.

2.2.1.3 Choi-Jamiolkowski representation

As the natural representation, Choi-Jamiolkowski is a representation of the map as a linear operator in an extended space. Consider the map $\Phi \in T(\mathcal{H}_M, \mathcal{H}_N)$, the Choi-Jamiolkowski representation of the map is given by

$$J(\Phi) = \sum_{i,j} \Phi[|i\rangle\langle j|] \otimes |i\rangle\langle j|, \tag{2.27}$$

where $\{|i\rangle\}$ is an orthonormal basis of $\mathcal{H}_M$. The operator $J(\Phi)$ is known as Choi matrix, or dynamical matrix. Given $J(\Phi)$, the action of the map Φ at a generic state $\rho \in \mathcal{D}(\mathcal{H}_M)$ is given by

$$\Phi[\rho] = Tr_N\left[J(\Phi)\left(\mathbb{I}_N \otimes \rho^T\right)\right]. \tag{2.28}$$

The Choi-Jamiolkowski representation can be thought of as the map acting locally on an unnormalized maximally entangled state $|\Phi^+\rangle = \sum_j |j\rangle \otimes |j\rangle$, that is

$$J(\Phi) = \Phi \otimes \mathbb{I}_M\left[|\Phi^+\rangle\langle\Phi^+|\right], \tag{2.29}$$

note that the operator $|\Phi^+\rangle\langle\Phi^+| \in \mathcal{D}(\mathcal{H}_M)$ is positive, thus the Choi-Jamiolkowski operator $J(\Phi)$ of a given completely positive map is also positive. As for the condition of trace preservation, if Φ is tracing preserving, then $Tr(\Phi(|i\rangle\langle j|)) = \delta_{i,j}$ which leads to

$$\begin{aligned} Tr_B(J(\Phi)) &= \sum_{i,j} Tr(\Phi[|i\rangle\langle j|])|i\rangle\langle j| \\ &= \sum_{i,j} \delta_{i,j}|i\rangle\langle j| = \mathbb{I}_M. \end{aligned} \tag{2.30}$$

For maps that can be written in the Kraus representation, that is complete positive, we can define the Choi-matrix in terms of Kraus operators $\{E_j\}$ as follows:

$$
\begin{aligned}
J(\Phi) \quad &= \Phi \otimes \mathbb{I}_M \left[\sum_{i,j} (|i\rangle \otimes |i\rangle) (\langle j| \otimes \langle j|) \right], \\
&= \sum_k E_k \otimes \mathbb{I}_M \left(vec[\mathbb{I}_M] \, vec[\mathbb{I}_M]^\dagger \right) E_k^\dagger \otimes \mathbb{I}_M \\
&= \sum_k vec[E_k] \, vec[E_k]^\dagger , \qquad (2.31)
\end{aligned}
$$

in the last line we use the identity Eq.(2.25). In section 5.2, we will show the relation between natural and Choi-Jamiolkowski representations.

2.3 Completely positive maps characterizing reduced dynamics of open quantum systems

The standard approach to the dynamics of open quantum systems considers an open system S with an associated Hilbert space $\mathcal{H}_S$ interacting with its environment E with associated Hilbert space $\mathcal{H}_E$ in such way that the composed system $S+E$ is closed and therefore its dynamics is governed by a Hamiltonian $H_{SE} \in \mathrm{Herm}(\mathcal{H}_S \otimes \mathcal{H}_E)$, which can be written as

$$H_{SE}(t) = H_S(t) \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E(t) + H_{int}(t), \qquad (2.32)$$

where $H_S \in \mathrm{Herm}(\mathcal{H}_S)$ and $H_E \in \mathrm{Herm}(\mathcal{H}_E)$ are Hamiltonians of system and environment, respectively, and $H_{int} \in \mathrm{Herm}(\mathcal{H}_S \otimes \mathcal{H}_E)$ is an interaction Hamiltonian. Thus, the state of the composite system is described by the unitary evolution

$$\rho_{SE}(t) = U_{SE}(t,t_0)\rho_{SE}(t_0)U_{SE}(t,t_0)^\dagger, \quad U_{SE}(t,t_0) = \mathcal{T}\exp\left(-i\int_{t_0}^{t} dt' H_{SE}(t')\right), \qquad (2.33)$$

where t_0 is the initial time, $\mathcal{T}$ is the time ordering operator and $\hbar$ is assumed to be one. The state of the open system S at time t is obtained by tracing over the environmental degrees of freedom, according to the following quantum dynamical process

$$\rho_S(t) = Tr_E\left(\rho_{SE}(t)\right) = Tr_E\left(U_{SE}(t,t_0)\rho_{SE}(t_0)U_{SE}(t,t_0)^\dagger\right). \qquad (2.34)$$

The process described above is a mapping for $\rho_{SE}(t_0)$ to $\rho_S(t)$. Moreover is a linear, trace preserving and completely positive mapping of $\mathcal{D}(\mathcal{H}_S \otimes \mathcal{H}_E)$ to $\mathcal{D}(\mathcal{H}_S)$, since the unitary and partial trace can be seen as maps that also satisfy the properties 1, 2 and 3 described in Sec.(2.2) . However, we are interested in a context where we only have access to the system S, therefore it is crucial to obtain a map on the set of the open system states $\Phi \in T(\mathcal{H}_S, \mathcal{H}_S)$, leading states at the initial time instant t_0 to a generic time t,

$\Phi(t,t_0)\rho_S(0) \to \rho_S(t)$. If the initial state of the system and its environment is a product state,

$$\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0), \tag{2.35}$$

then it is possible to define a linear, trace preserving and completely positive map Φ from the state space of the open system $\mathcal{D}(\mathcal{H}_S)$ into itself, as follows

$$\rho_S(t) = Tr_E\left(U_{SE}(t,t_0)\rho_S(t_0) \otimes \rho_E(t_0)U^\dagger_{SE}(t,t_0)\right). \tag{2.36}$$

Assuming the spectral decomposition of the environmental initial state as $\rho_E(t_0) = \sum_k p_k|\psi_k\rangle\langle\psi_k|$, we can write

$$\begin{aligned}
\rho_S(t) &= \sum_j \langle\phi_j|U_{SE}(t,t_0)\rho_S(t_0) \otimes \left(\sum_k p_k|\psi_k\rangle\langle\psi_k|\right) U^\dagger_{SE}(t,t_0)|\phi_j\rangle \\
&= \sum_{j,k} \left(\sqrt{p_k}\langle\phi_j|U_{SE}(t,t_0)|\psi_k\rangle\right)\rho_S(t_0)\left(\sqrt{p_k}\langle\psi_k|U^\dagger_{SE}(t,t_0)|\phi_j\rangle\right) \\
&= \sum_{j,k} K_{j,k}(t,t_0)\rho_S(t_0)K^\dagger_{j,k}(t,t_0),
\end{aligned} \tag{2.37}$$

where $\{|\phi_j\rangle\}$, $\{|\psi_k\rangle\}$ are orthonormal bases in $\mathcal{H}_E$ and $K_{j,k}(t,t_0) = \sqrt{p_k}\langle\phi_j|U_{SE}(t,t_0)|\psi_k\rangle$, this expression corresponds to the Kraus representation of the map, hence complete positivity is guaranteed and the trace-preserving is an immediate consequence of the operator U_{SE} being unitary. The formalism to describe systems that are initially correlated with the environment is much more problematic. In the next chapter, we will present some of the important results in this line of work.

3 Initial Correlation in Open Quantum Systems

In the previous chapter, we saw that if system and environment start in an uncorrelated global state, factorable, then it is possible to construct a map acting on the state space of the system, satisfying all the desirable properties, characterizing the dynamics of the system. However, if the system is initially correlated with the environment, the map associated with the dynamics of the system may not be completely positive or, as we will see, is valid only for a subset of the density state space. In the last two decades, more attention has been given to the construction of reduced dynamical maps of systems initially correlated [6–10, 34, 35], mainly motivated by discussions between Pechukas and Alicki [3–5].

3.1 Pechukas' theorem

Pechukas introduced the idea of 'assignment map' $\mathcal{A}:\mathcal{H}_S\rightarrow\mathcal{H}_{SE}$, which characterizes initial system-environment states for open quantum systems, i.e. $\mathcal{A}\left[\rho_S(t_0)\right]=\rho_{SE}(t_0)$. In his work, the dynamic map could be understood as the composition of three maps

$$\Phi(t,t_0)\left[\rho_S(t_0)\right]=Tr_E\left(U_{SE}(t,t_0)\mathcal{A}\left[\rho_S(t_0)\right]U_{SE}^{\dagger}(t,t_0)\right), \tag{3.1}$$

the partial trace $Tr_E:\mathcal{H}_{SE}\rightarrow\mathcal{H}_S$, an unitary $U_{SE}:\mathcal{H}_{SE}\rightarrow\mathcal{H}_{SE}$, both satisfying properties 1, 2 and 3 (2.2), and the assignment map $\mathcal{A}$. The trace preservation, linearity and the complete positivity of the dynamical map relies on the features of the assignment map. Imposing desirable requirements for the assignment map, compiled by Alicki in three conditions:

(i) *Linearity.* The assignment map $\mathcal{A}$ preserves mixtures, $\mathcal{A}\left[\sum_j p_j\rho_j\right]=\sum_j p_j\mathcal{A}\left[\rho_j\right]$.

(ii) *Consistency.* The assignment map $\mathcal{A}$ is consistent, in the sense that $\rho_S=Tr_E(\mathcal{A}\left[\rho_S\right])$.

(iii) *Positivity.* The assignment map is positive if $\mathcal{A}\left[\rho_S\right]\geq 0$ for all positive ρ_S.

Pechukas demonstrated that, when these three conditions are satisfied simultaneously, then the initial state of the system and environment is factorable, i.e. $\mathcal{A}\left[\rho_S\right]=\rho_S\otimes\rho_E$. In Pechukas' original work these ideas were presented to a single-qubit open quantum system, later Rodríguez-Rosario et al. [35], generalized its arguments to high dimension open systems. Assuming a set of linearly independent projectors $\{P_j\}$ that span the space of the open system $\mathcal{S}$, we can define a general assignment map $\mathcal{A}$ by its action on the projectors P_i, as follows

$$\mathcal{A}\left(P_j\right) = P_j \otimes \tau_j, \tag{3.2}$$

where $\tau_j \in \mathcal{L}(\mathcal{H}_E)$ is Hermitian $\tau_j = \tau_j^\dagger$ and have unit trace $Tr\left(\tau_j\right) = 1$ for all j, which are requirements to ensure that $\mathcal{A}$ is a trace and Hermitian preserving map. Any element of $\mathcal{D}(\mathcal{S})$ can be expanded by the projectors as $\rho_S = \sum_j a_j P_j$, with real coefficients a_j, not necessarily positive and satisfy $\sum_j a_j = 1$. The assignment map (3.2) satisfies the linearity, $\mathcal{A}\left[\sum_j a_j P_j\right] = \sum_j a_j \mathcal{A}\left(P_j\right)$, and consistency condition since τ_j has unit trace. The Pechucas' theorem tells us that the assignment (3.2) is positive for all ρ_S if and only if τ_j are the same, $\tau_j = \rho_E$, for all j. First we start with the "only if" part, suppose $\tau_j = \rho_E$ for all j, it is easy to see that $\mathcal{A}\left(\rho_S\right) \geq 0$,

$$\mathcal{A}\left[\rho_S\right] = \mathcal{A}\left[\sum_j a_j P_j\right] = \sum_j a_j P_j \otimes \rho_E = \rho_S \otimes \rho_E \geq 0, \tag{3.3}$$

note that $\rho_S \geq 0$, $\rho_E \geq 0$ and the composition of positive operators produces a positive operator. Now, let us show the "if" part, consider the positivity of the assignment map, $\mathcal{A}\left[\rho_S\right] \geq 0$, for all states $\rho_S \in \mathcal{D}(\mathcal{H}_S)$ and knowing that $\tau_j = \rho_E$, $\forall\, j$, is a possible solution, we just need to demonstrate that for at least one state in $\mathcal{D}(\mathcal{H}_S)$ this is the only valid solution. Defining a generic pure state σ_S, the assignment map $\mathcal{A}$ acting on σ_S provides a factorable state $\mathcal{A}\left[\sigma_S\right] = \sigma_S \otimes \rho_E$, since the reduced state of a correlated state is mixed. The set of projectors $\{P_j\}$ can expand any operator on the space of the open quantum system $\mathcal{H}_S$, therefore we can write $\sigma_S = \sum_j c_j P_j$ and consequently,

$$\mathcal{A}\left[\sigma_S\right] = \sum_j c_j P_j \otimes \rho_E. \tag{3.4}$$

But by acting the assignment map after the expansion $\sigma_S = \sum_j c_j P_j$ and using the definition Eq.(3.2), we can also define

$$\mathcal{A}\left[\sigma_S\right] = \sum_j c_j P_j \otimes \tau_j. \tag{3.5}$$

The Eqs.(3.4) and (3.5) imply in the relations $\mathcal{A}\left(P_j\right) = P_j \otimes \rho_E$ and $\mathcal{A}\left(P_j\right) = P_j \otimes \tau_j$, respectively, comparing these two relations and taking the trace with respect to the system gives that $\rho_E = \tau_j$, $\forall j$, finishing the proof.

To deal with the problem of characterizing reduced dynamics of initial correlated systems, Pechukas [3, 5] suggested to giving up positivity. On the other hand, Aliciki [4] argued to giving up consistency. In the end, it can be concluded that, one way or another, the domain of validity of the assignment map must be restricted to the set of states that lead to positivity for the first case and consistency for the second.

3.2 The role of initial correlation in the dynamics of open quantum systems

Shortly after the exchanges between Pechukas and Aliciki, Stelmachovic et al. [6] studied the influence of initial correlations between system and environment in the dynamics of the system, making clear that taking into account such correlations is paramount to the correct description of the evolution. They showed an instructive example with two qubits (one for the system S, one for the environment E), evolving under a C-NOT gate: both a maximally entangled state and a maximally mixed global state have the same one-qubit local maximally mixed states, but the evolution is radically different. Assume two qubits S and E, with their associated Hilbert spaces $\mathcal{H}_S \cong \mathcal{H}_2$ and $\mathcal{H}_E \cong \mathcal{H}_2$. The dynamics of the joint systems SE is given by the unitary $U_{SE} = \exp\left(-iH_{SE}t\right)$ governed by the Hamiltonian

$$H_{SE} = \frac{1}{2}\left(\mathbb{I}_2 - \sigma_z\right) \otimes \sigma_x + \frac{1}{2}\left(\mathbb{I}_2 + \sigma_z\right) \otimes \mathbb{I}_2, \tag{3.6}$$

where $\{\sigma_i\}_i = \{x, y, z\}$ are the well known Pauli operators, which together with the identity operator $\mathbb{I}_2$ form a base that can expand any operator on space $\mathcal{L}(\mathcal{H}_2)$. The unitary U_{SE} at time $t = \pi/2$ implements the controlled C-NOT, with qubit S being the control, while qubit E is the target. Consider two initial conditions $\rho_{SE}^{(1)}(0)$ and $\rho_{SE}^{(2)}(0)$ for the two-qubit state,

$$\begin{aligned}\rho_{SE}^{(1)}(0) &= \left(\alpha|00\rangle + \beta|11\rangle\right)\left(\alpha^*\langle 00| + \beta^*\langle 11|\right), \\ \rho_{SE}^{(2)}(0) &= |\alpha|^2|00\rangle\langle 00| + |\beta|^2|11\rangle\langle 11|,\end{aligned} \tag{3.7}$$

where $|jj\rangle$ is a shorthand to $|j\rangle \otimes |j\rangle$. Applying the partial trace it is easy to see that the reduced state for the two initial conditions are the same, i.e.,

$$\begin{aligned}\rho_S^{(1,2)}(0) &= Tr_E\left(\rho_{SE}^{(1,2)}(0)\right) = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|, \\ \rho_E^{(1,2)}(0) &= Tr_S\left(\rho_{SE}^{(1,2)}(0)\right) = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|.\end{aligned} \tag{3.8}$$

Even though the reduced states of the system S and the environment E at the initial time are the same for both cases, the reduced state S in each case will evolve to different states due to the difference in the initial correlation. One can also rapidly show that the density operators of the composed system SE for both conditions (3.7) at time $t = \pi/2$ are given by

$$\begin{aligned}\rho_{SE}^{(1)}(\pi/2) &= U_{SA}(\pi/2)\rho_{SE}^{(2)}(0)U_{SA}^\dagger(\pi/2) = \left(\alpha|00\rangle + \beta|10\rangle\right)\left(\alpha^*\langle 00| + \beta^*\langle 10|\right), \\ \rho_{SE}^{(2)}(\pi/2) &= U_{SA}(\pi/2)\rho_{SE}^{(1)}(0)U_{SA}^\dagger(\pi/2) = |\alpha|^2|00\rangle\langle 00| + |\beta|^2|10\rangle\langle 10|,\end{aligned} \tag{3.9}$$

and the reduced density matrix of qubit $\mathcal{S}$ in each case is:

$$\begin{aligned}\rho_S^{(1)}(\pi/2) &= Tr_E\left(\rho_{SE}^{(1)}(\pi/2)\right) = \left(\alpha|0\rangle + \beta|1\rangle\right)\left(\alpha^*\langle 0| + \beta^*\langle 1|\right), \\ \rho_S^{(2)}(\pi/2) &= Tr_E\left(\rho_{SE}^{(2)}(\pi/2)\right) = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|.\end{aligned} \tag{3.10}$$

Moreover, in ref. [6] was presented the definition of a map acting on the space of a N-dimensional open system in the presence of initial correlation, showing that the characterization of the initial correlation is necessary in obtaining the map. Let us assume as the Hilbert spaces associated with the open system $\mathcal{H}_S \cong \mathcal{H}_N$ and the environment $\mathcal{H}_E \cong \mathcal{H}_M$. Any operator for the composite system SE can be written in terms of the operator set $\{\mathbb{I}_S \otimes \mathbb{I}_E, \sigma_i \otimes \mathbb{I}_E, \mathbb{I}_S \otimes \tau_j, \sigma_i \otimes \tau_j\}$, with $i = 1, \ldots, N^2 - 1$; $j = 1, \ldots, M^2 - 1$ and where $\sigma_i \in \mathcal{L}(\mathcal{H}_S)$ and $\tau_j \in \mathcal{L}(\mathcal{H}_E)$ are the orthogonal generators of SU(N) and SU(M) that satisfy the relations

$$\begin{aligned} \sigma_i = \sigma_i^\dagger, \quad Tr_S\left(\sigma_i\right) = 0, \quad Tr_S\left(\sigma_i \sigma_{i'}\right) = 2\delta_{i,i'}, \\ \tau_j = \tau_j^\dagger, \quad Tr_E\left(\tau_j\right) = 0, \quad Tr_E\left(\tau_j \tau_{j'}\right) = 2\delta_{j,j'}. \end{aligned} \tag{3.11}$$

The Pauli operators are an example of such operators for the two-dimensional case. We can define a generic state of the composite system $\rho_{SE} \in \mathcal{H}_{SE}$ as

$$\rho_{SE} = \frac{1}{NM}\left[\mathbb{I}_S \otimes \mathbb{I}_E + \sum_i \alpha_i \sigma_i \otimes \mathbb{I}_E + \sum_j \beta_i \mathbb{I}_S \otimes \tau_j + \sum_{i,j} \gamma_{ij} \sigma_i \otimes \tau_j\right], \tag{3.12}$$

where α_i, β_i and γ_{ij} are real coefficients, conditioned that the operator ρ_{SE} characterizes a quantum system state of SE, i.e., it is a density operator. Tracing over the degrees of freedom of the environment, we obtain the density operator of the open system ρ_S,

$$\rho_S = Tr_E\left(\rho_{SE}\right) = \frac{1}{N}\left(\mathbb{I}_S + \sum_i \alpha_i \sigma_i\right), \tag{3.13}$$

and similarly one can get the state of the environment ρ_E by tracing over the open system

$$\rho_E = Tr_S\left(\rho_{SE}\right) = \frac{1}{M}\left(\mathbb{I}_E + \sum_i \beta_i \tau_i\right). \tag{3.14}$$

Now, from the respectives open system and environment states defined in Eqs.(3.13) and (3.14), we can write the composed system state Eq.(3.12) as

$$\rho_{SE} = \rho_S \otimes \rho_E + \sum_{i,j} \gamma'_{ij} \sigma_i \otimes \tau_j, \quad \gamma'_{ij} = \frac{\gamma_{ij} - \alpha_i \beta_j}{NM}. \tag{3.15}$$

The parameters γ'_{ij} characterize the initial system-environment correlations, $\gamma'_{ij} = \langle \sigma_i \otimes \tau_j \rangle - \langle \sigma_i \rangle \langle \tau_j \rangle$ where $\langle \cdot \rangle = Tr(\cdot \rho)$ is the mean value. Adopt (3.15) as the state of the composed system SE at initial time $t_0 = 0$ and its dynamics given by action of a unitary operator $U_{SE}(t)$, we can describe the process that leads to the reduced state of S for any time t as

$$\begin{aligned} \rho_S(t) &= Tr_E\left(U_{SE}(t)\left[\rho_S(0) \otimes \rho_E(0) + \sum_{i,j} \gamma'_{ij} \sigma_i \otimes \tau_j\right] U_{SE}^\dagger\right) \\ &= Tr_E\left(U_{SE}(t) \rho_S(0) \otimes \rho_E(0) U_{SE}^\dagger\right) + Tr_E\left(U_{SE}(t) \sum_{i,j} \gamma'_{ij} \sigma_i \otimes \tau_j U_{SE}^\dagger\right). \end{aligned} \tag{3.16}$$

The first term on the right side of equality was discussed in Eq.(2.36), corresponding to the Kraus representation generated in the scenario where initially there is no correlation between the system S and the environment. Consider the spectral decomposition of the environmental initial state as $\rho_E(t_0) = \sum_m p_m |\psi_m\rangle\langle\psi_m|$, we obtain

$$\rho_S(t) = \sum_{n,m} K_{nm}(t)\rho_S(0)K^{\dagger}_{nm}(t) + \sum_{n,i,j} \gamma'_{ij}\langle\phi_n|U_{SE}(t)\sigma_i \otimes \tau_j U^{\dagger}_{SE}(t)|\phi_n\rangle, \tag{3.17}$$

where $\{|\phi_n\rangle\}$ is a base in the environment space $\mathcal{H}_E$ and $K_{n,m}(t) = \sqrt{p_k}\langle\phi_n|U_{SE}(t)|\psi_m\rangle$. For fixed parameters β_j and γ'_{ij} characterizing the state of the environment and the initial correlation, respectively, Eq.(3.17) defines a map describing the evolution of S, $\Phi : \rho_S(0) \to \rho_S(t)$. However for non-null initial correlation, $\gamma'_{ij} \neq 0$ for any i, j, the map Φ is in general not positive and only a set of the states $\rho_S \in \mathcal{D}(\mathcal{H}_S)$ will be taken to quantum states. To illustrate this statement, imagine the case where the fixed parameter γ'_{ij} represents system and environment sharing a maximally entangled state, e.g. the first condition in Eq.(3.7), in this scenario the reduced initial state of S is always the normalized identity operator, $\rho_S = \frac{1}{N}\mathbb{I}_S$, applying the map to any other state could generate an operator outside the density operator set, because it would be equivalent to choosing a set $\{\alpha_i, \beta_j, \gamma'_{ij}\}$ that does not represent the density operator of SE in the dynamic process described in Eq (3.16). A remark is that depending on the form of the unitary operator U_{SA} we may have $\langle\phi_n|U_{SE}(t)\sigma_i \otimes \tau_j U^{\dagger}_{SE}(t)|\phi_n\rangle = 0$, making the contribution of γ'_{ij} negligible in the dynamics, for exemple, in a comment to [6], Salgado et al. [36] showed for two qubits that, whatever the initial correlations, the system dynamics has the Kraus representation form for all states, and is consequently completely positive, whenever the global dynamics is locally unitary, $U_{SE} = U_S \otimes U_E$, this was then proved for bipartite global systems of arbitrary dimension by Hayashi et al. [34]. As said in the Introduction (1), a great attention has been devoted to study general class of correlated initial states that lead to completely positive map for its compatible domain, the set of states of the open quantum system that are compatible with its initial correlation with the environment and are mapped to other states, many authors worked out sets of classicaly [7, 8] or quantum [9, 10] initial global states. In our work, we studied the reduced dynamics of initial states presenting exchange correlation in a framework to be presented in the next chapter.

4 Completely Positive Maps for Reduced States of Indistinguishable Fermions

The subtle notion of quantum correlations of indistinguishable particles has been investigated by many authors, with introduction of seminal ideas, as entanglement of modes [37], or entanglement of particles [38–46]. Our own group has scrutinized the concepts like entanglement of particles [41,42] and 'quantumness of correlations' of indistinguishable particles [47, 48], performing interesting applications where general properties of many particle systems were obtained from the reduced state of one particle [49]. Despite that, the role of initial exchange correlations in the reduced dynamics was still unexplored. In this chapter, we present our results on the topic [Phys. Rev. A 98, 052135 (2018)]. We propose a framework to construct maps representing the dynamics of indistinguishable particles reduced state, in particular fermions, which are always correlated, and for which the usual tensor product structure between 'system' and 'environment' is absent.

4.1 Indistinguishable particles

In classical systems it is feasible, in principle, to keep track of individual particles, even the particles being identical. We can always label them and follow their paths at each instant of time. In quantum mechanics, however, identical particles are truly indistinguishable. This is because quantum systems are characterized by vectors in a complex vector space, from which we can only obtain expectation values of observables, then there exists an intrinsic uncertainty about the position of the particles at each instant of time, which makes unfeasible to label the particles and follow their trajectories. For simplicity, let us assume two particles, 1 and 2, with the corresponding Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Consider orthonormal basis $\{|\alpha\rangle_1\}$ and $\{|\beta\rangle_j\}$ in each space $\mathcal{H}_1$ and $\mathcal{H}_2$. We can write a generic pure state for the composite system as

$$|\psi\rangle = \sum_{\alpha,\beta} c_{\alpha,\beta} |\alpha\rangle_1 \otimes |\beta\rangle_2. \tag{4.1}$$

Now, define the permutation operator P_{12} that represents particle exchange in quantum mechanics and is given by the relation $P_{12}\left(|\alpha\rangle_1 \otimes |\beta\rangle_2\right) = |\beta\rangle_1 \otimes |\alpha\rangle_2$. Its action in a two-particle state is

$$|\psi'\rangle = \sum_{\alpha,\beta} c_{\alpha,\beta} |\beta\rangle_1 \otimes |\alpha\rangle_2, \tag{4.2}$$

note that $P_{12}|\psi'\rangle = |\psi\rangle$. Therefore, P_{12} is its own inverse, Hermitian and unitary, that is

$$P_{12}^{-1} = P_{12}, \quad P_{12}^{\dagger} = P_{12}, \quad P_{12}^{\dagger} P_{12} = P_{12} P_{12}^{\dagger} = \mathbb{I}. \tag{4.3}$$

A pair of states that differ only by the exchange of indistinguished particles cannot be distinguished by any observation. Then, any observable O must obey:

$$\langle\psi|O|\psi\rangle = \langle\psi'|O|\psi'\rangle = \langle\psi|P_{12}OP_{12}^{\dagger}|\psi\rangle. \tag{4.4}$$

From the unitarity and hermiticity of P_{12}, Eq.(4.3), it is easy to show that observables on the space of the indistinguishable particles have to commute with the permutation operator, $[P_{12}, O] = 0$, that is, all observables must be permutation-invariant. Obviously this is also true for Hamiltonians, which tells us that P_{12} is a constant of motion. Since P_{12} has eigenvalues ± 1, a direct consequence of relations Eq.(4.3), states that are initially symmetric or anti-symmetric stays in their symmetric($\mathcal{H}_{1,2}^{S}$) or anti-symmetric($\mathcal{H}_{1,2}^{A}$) subspaces at all times. The projectors in the symmetric and anti symmetric spaces, respectively, can be defined as:

$$\mathcal{S} = \frac{\mathbb{I} + P_{12}}{2}, \quad \mathcal{A} = \frac{\mathbb{I} - P_{12}}{2}, \tag{4.5}$$

where $\mathcal{S} = \mathcal{S}^{\dagger} = \mathcal{S}^2$, $\mathcal{A} = \mathcal{A}^{\dagger} = \mathcal{A}^2$ and $\mathcal{SA} = \mathcal{AS} = 0$. Ultimately, states of indistinguishable particles, which are physically realizable, are either symmetric or anti-symmetric under permutations. Projecting the state in Eq.(4.1) in such spaces and normalizing, we can write

$$\begin{aligned} \mathcal{S}|\psi\rangle &= |\psi\rangle_S = \frac{1}{\sqrt{2}}\sum_{\alpha,\beta} c_{\alpha,\beta}\left(|\alpha\rangle_1 \otimes |\beta\rangle_2 + |\beta\rangle_1 \otimes |\alpha\rangle_2\right), \\ \mathcal{A}|\psi\rangle &= |\psi\rangle_A = \frac{1}{\sqrt{2}}\sum_{\alpha,\beta} c_{\alpha,\beta}\left(|\alpha\rangle_1 \otimes |\beta\rangle_2 - |\beta\rangle_1 \otimes |\alpha\rangle_2\right). \end{aligned} \tag{4.6}$$

The states from the subspaces $\mathcal{H}_{1,2}^{S}$ and $\mathcal{H}_{1,2}^{A}$ describe two different types of particles: bosons and fermions, respectively. Note that the antisymmetric state agrees with Pauli's exclusion principle, which states that indistinguishable fermions cannot be found in the same state. In this work, our main focus is to study the reduced dynamics of fermionic systems. The antisymmetrization of the fermionic state imposes correlations between the fermions, the well know exchange contributions from the Hartree-Fock theory, which leads to constraints on the reduced dynamic map construction, as discussed in the Sec.(3.2).

We begin by characterizing states where the only correlation present is exchange, for example, a two-fermion state represented by a single Slater determinant $|\phi\rangle = \frac{1}{\sqrt{2}}\left(|\alpha\rangle_1 \otimes |\beta\rangle_2 - |\beta\rangle_1 \otimes |\alpha\rangle_2\right)$, or as we will see in second quatization description $|\phi\rangle = a_{\alpha}^{\dagger}a_{\beta}^{\dagger}|0\rangle$, where $a_j^{\dagger}$ is the typical fermionic creation operator. In a composition of distinguishable quantum systems with associated Hilbert space $\mathcal{H}_{1,\cdots,N} = \mathcal{H}_1^{L_1} \otimes \cdots \otimes \mathcal{H}_N^{L_N}$, where N is the number of subsystems and L_i is the dimension of i'th subsystem, the tensor product structure between the subsystems plays an important role for the characterization of correlations as entanglement [50] and quantumness [51, 52]. However, as discussed earlier, the state space of N indistinguishable fermions is described by the antisymmetrized composed Hilbert space $\mathcal{F}_N^L = \mathcal{A}(\mathcal{H}_1^L \otimes \cdots \otimes \mathcal{H}_N^L)$, Fig. 1, where N is the number of

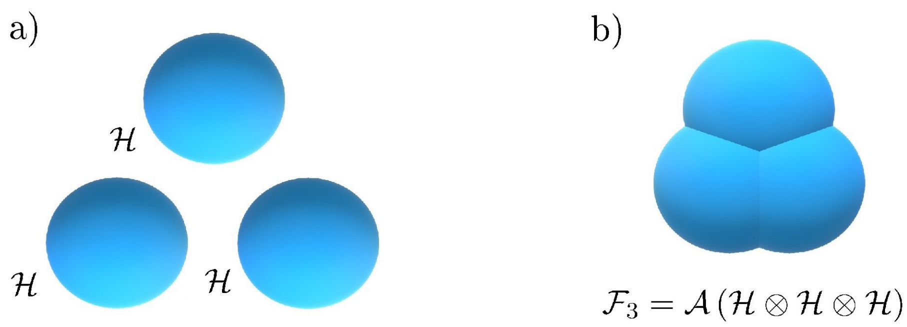

Figure 1 – Pictorial view of Hilbert space with (a) tensor product structure ($\mathcal{H}\otimes\mathcal{H}\otimes\mathcal{H}$), and (b) antisymmetric space without tensor product structure, where the particle states overlap. A partial trace over a subsystem in the antisymmetric space has information about the whole system, since the particles are indistinguishable.

fermions and L is the number of accessible modes. Note that this space does not support a tensor product structure and have a more suitable description in the second quantization formalism. A base in this subspace can be constructed out of fermionic operators $\{a_k\}_{k=1}^{L}$, satisfying the usual anti-commutation relations:

$$\{a_l, a_k^\dagger\} = \delta_{k,l}, \qquad \{a_k, a_l\} = \{a_k^\dagger, a_l^\dagger\} = 0, \tag{4.7}$$

where a_k and $a_k^\dagger$ are annihilation and creation operators for the k'th mode, respectively. A single particle orthonormal basis is formed by the set of states $\{a_k^\dagger|0\rangle\}_{k=1}^{L}$, where $|0\rangle$ is the vacuum state in the fermionic Fock space [1] defined as the absence of particles, $a_j|0\rangle = 0$ for all j.

As previously mentioned, the correlation of indistinguishable particles, mostly entanglement, was study by many groups [38–46], giving rise to many definitions that agree with each other in the fermionic case, in the sense that the exchange correlations generated by mere antisymmetrization of the state, due to indistinguishability of their fermions, does not result in entanglement [38–46], that is, the set of unentangled states can be written as a convex sum of Slater determinants. More generally, with studies in quantumness [47, 48], we can define states where the only non-classical correlation present is exchange. A fermionic state $\omega \in \mathcal{D}\left(\mathcal{F}_N^L\right)$ has no quantumness of correlation if it can be decomposed as a convex combination of orthogonal Slater determinants, namely,

$$\omega = \sum_{\vec{k}} p_{\vec{k}} a_{\vec{k}}^\dagger |0\rangle\langle 0| a_{\vec{k}}, \tag{4.8}$$

where $\vec{k} = (k_1, \ldots, k_N)$, with $k_i = 1, ..., L$, denotes the modes occupied by the fermions, $a_{\vec{k}}^\dagger|0\rangle \equiv a_{k_1}^\dagger \cdots a_{k_N}^\dagger|0\rangle$, and p is a probability distributions, with $\sum_{\vec{k}} p_{\vec{k}} = 1$. Since, we are interested in exploring the role of initial exchange correlations in the reduced dynamics

[1] Given a system with L modes its fermionic Fock space is $\mathcal{F}^L = |0\rangle\langle 0| \oplus \mathcal{H}_1^L \oplus \mathcal{F}_2^L \cdots \mathcal{F}_L^L$, where $\oplus$ is the direct sum and $\mathcal{F}_j^L = \mathcal{A}\left(\mathcal{H}_1^L \otimes \cdots \otimes \mathcal{H}_j^L\right)$.

$$
\begin{tikzcd}
\rho(0) \arrow[r, "U_t"] \arrow[d, "\mathrm{Tr}_{N-1}"'] & \rho(t) \arrow[d, "\mathrm{Tr}_{N-1}"] \\
\rho_{r_1}(0) \arrow[r, "\Phi_t"] & \rho_{r_1}(t)
\end{tikzcd}
$$

Figure 2 – Schematic diagram characterizing the dynamics of indistinguishable fermions. Suppose an initial N-fermion state $\rho(0)$ evolving under the unitary U_t. The reduced one-fermion state $\rho_r(0) = Tr_{N-1}(\rho(0))$ evolves under the dynamical map Φ_t.

of fermionic systems, we will choose the initial global fermionic state in the set with no quantumnes.

4.2 Dynamical Maps for Reduced States of Fermionic Systems

In this section we introduce the formalism to describe the dynamics of a single fermion in a closed system of N fermions. More precisely, given a system of N indistinguishable fermions in the state $\rho(0)$, evolving under the unitary U_t, which preserves the total number of particles, we want to obtain the dynamical map Φ_t, which evolves the one-particle reduced state $\rho_r = Tr_{N-1}(\rho(0))$, see Fig.2. Since the fermionic states are restricted to the antisymmetric sector of the Hilbert space, it is not possible to start with initial states in the tensor product form. In section (3.2), we discussed that one way to deal with the problem of obtaining completely positive maps characterizing the dynamics of states initially correlated with an external system, is to restrict the domain of the map. Using the fact that the Kraus representation assures completely positivity (Sec.(2.18)), we will show that for some sets of initial states with no quantumness of correlations, we can construct completely positive maps for the reduced state.

The construction of the single-fermion dynamical map, in the simplest scenario of a closed system of two fermions initially in a pure state, $\rho(0) = |\psi\rangle\langle\psi|$, gives us a good grasp on the general features of the formalism, and includes all the technical problems of the general case. The generalisation to N-fermion mixed states is straightforward and performed in Appendix A. Let us consider a set of states in the antisymmetric space of 2 fermions and $L+1$ modes, that can be written in a given basis of Slater determinants as:

$$\mathcal{D}_2^{\mu,pure} \equiv \left\{ a_\mu^\dagger a_k^\dagger |0\rangle\langle 0| a_k a_\mu \right\}_{k=0}^{L}, \tag{4.9}$$

where μ is a fixed mode. Note that μ labels a reference mode, and different values of μ lead to distinct sets. We can compute the one-particle reduced state by tracing out one fermion from Eq.(4.9). Assuming that $\{f_k^\dagger\}_{k=0}^L$ is an orthonormal basis of fermionic creation operators for the space of a single fermion ($\mathcal{F}_1^{L+1}$), thus $f_k^\dagger = \sum_l V_{kl} a_l^\dagger$, V is a unitary matrix of dimension $L+1$. The partial trace over one particle is given by $\rho_r = \frac{1}{2}\sum_{k=0}^L f_k \rho f_k^\dagger$. The explicit calculation of the matrix element $(\rho_r)_{i,j}$ goes as follows:

$$\begin{aligned}(\rho_r)_{i,j} &= \langle 0| f_j \left(\tfrac{1}{2}\textstyle\sum_{k=0}^L f_k \rho f_k^\dagger\right) f_i^\dagger |0\rangle \\ &= \tfrac{1}{2}\textstyle\sum_{k=0}^L \langle 0| f_k \left(f_j \rho f_i^\dagger\right) f_k^\dagger|0\rangle \\ &= \tfrac{1}{2} Tr(f_i^\dagger f_j \rho),\end{aligned} \tag{4.10}$$

where we used the fermionic anti-commutation relations and the cyclicality of the trace. Now we can write the set of single-fermion reduced states of Eq.(4.9):

$$\begin{aligned}\mathcal{D}_{r(2)}^{\mu,pure} &= Tr_1\left(\mathcal{D}_2^{\mu,pure}\right) \\ &= \left\{\frac{1}{2} a_k^\dagger |0\rangle\langle 0| a_k + \frac{1}{2} a_\mu^\dagger |0\rangle\langle 0| a_\mu\right\}_{k=0}^L,\end{aligned} \tag{4.11}$$

with μ a fixed mode. Assuming the dynamics of $\rho(0) \in \mathcal{D}_2^{\mu,pure}$ is given by the unitary U_t, we can define a CP map Φ_t^μ for the dynamics of the single-fermion reduced state $\rho_r(0) \in \mathcal{D}_{r(2)}^{\mu,pure}$, *i.e.*, a CP map $\Phi_t^\mu : \mathcal{D}_{r(2)}^{\mu,pure} \to \mathcal{D}(\mathcal{F}_1^{L+1})$ as follows:

Definition 1. *A dynamical map Φ_t^μ for the single-fermion reduced state $\rho_r(0) \in \mathcal{D}_{r(2)}^{\mu,pure}$, of a 2-fermion pure state initially with no quantumness of correlations, $\rho(0) \in \mathcal{D}_2^{\mu,pure}$, evolving under the global unitary U_t, has the operator sum representation $\Phi_t^\mu[\rho_r] = \sum_{j=0}^L K_j^\mu \rho_r K_j^{\dagger\mu}$, with the Kraus operators*

$$K_l^\mu = f_l U_t a_\mu^\dagger. \tag{4.12}$$

Proof. If the 2-fermion state evolves according to $\rho(t) = U_t \rho(0) U_t^\dagger$, the reduced density matrix is:

$$\begin{aligned}\rho_r(t) &= Tr_1(U_t a_\mu^\dagger a_k^\dagger |0\rangle\langle 0| a_k a_\mu U_t^\dagger) \\ &= \sum_{l=0}^L f_l U_t a_\mu^\dagger \left(\frac{1}{2} a_k^\dagger |0\rangle\langle 0| a_k\right) a_\mu U_t^\dagger f_l^\dagger,\end{aligned} \tag{4.13}$$

where in the last equation we used the definition of fermionic partial trace, Eq.(4.10), and the anti-commutation relations. Using the fact that we cannot create more than one fermion in the same mode, Pauli exclusion principle, we can add a second null term in Eq.(4.13), in order to recover the reduced state in the form of Eq.(4.11),

$$\begin{aligned}\rho_r(t) = &\sum_{l=0}^L f_l U_t a_\mu^\dagger \left(\frac{1}{2} a_k^\dagger |0\rangle\langle 0| a_k\right) a_\mu U_t^\dagger f_l^\dagger \\ &+ \sum_{l=0}^L f_l U_t a_\mu^\dagger \left(\frac{1}{2} a_\mu^\dagger |0\rangle\langle 0| a_\mu\right) a_\mu U_t^\dagger f_l^\dagger,\end{aligned} \tag{4.14}$$

which can be written as,

$$\begin{aligned}\rho_r(t) &= \sum_{l=0}^{L} f_l U_t a_\mu^\dagger \left(\rho_r(0)\right) a_\mu U_t^\dagger f_l^\dagger \\ &= \sum_{l=0}^{L} K_l^\mu \rho_r(0) K_l^{\mu\dagger},\end{aligned} \tag{4.15}$$

with $K_l^\mu = f_l U_t a_\mu^\dagger$. □

Due to the restriction of the map domain, Eq.(4.11), the relation between Kraus operators and trace preservation can be written as

$$\sum_l K_l^{\mu\dagger} K_l^\mu = \mathrm{diag}\left(\lambda_0, \lambda_1, ..., \lambda_L\right), \tag{4.16}$$

with $\lambda_{i\neq\mu} = 2$ and $\lambda_\mu = 0$, one can see that

$$Tr\left(\rho_r(t)\right) = Tr\left[\mathrm{diag}\left(\lambda_0, \lambda_1, ..., \lambda_L\right)\rho_r(0)\right] = 1, \tag{4.17}$$

where $\rho_r(0) \in \mathcal{D}_{r(2)}^{\mu,pure}$. This can be checked by computing the matrix elements of $\sum_l K_l^{\mu\dagger} K_l^\mu$, in the basis $\{a_k^\dagger|0\rangle\}_{k=0}^{L}$, namely:

$$\begin{aligned}\sum_{l=0}^{L}\left(K_l^{\mu\dagger}K_l^\mu\right)_{i,j} &= \langle 0|a_i \sum_{l=0}^{L} K_l^{\mu\dagger}\left(\sum_{k=0}^{L} a_k^\dagger|0\rangle\langle 0|a_k\right) K_l^\mu a_j^\dagger|0\rangle \\ &= \langle 0|a_i a_\mu U_t^\dagger \left(\sum_{k,l} f_l^\dagger a_k^\dagger|0\rangle\langle 0|a_k f_l\right) \\ &\quad \times U_t a_\mu^\dagger a_j^\dagger|0\rangle,\end{aligned} \tag{4.18}$$

where we used in the first line the identity $\sum_k a_k^\dagger|0\rangle\langle 0|a_k = \mathbb{I}_{\mathcal{F}_1^{L+1}}$. Since $\{a_i\}$ and $\{f_i\}$ are both orthonormal bases, there exists a unitary V, of dimension $L+1$, which performs the single particle transformation $f_l^\dagger = \sum_m V_{lm} a_m^\dagger$, we can simplify the term

$$\begin{aligned}&\left(\sum_{k,l} f_l^\dagger a_k^\dagger|0\rangle\langle 0|a_k f_l\right) = \\ &= \left(\sum_{k,l,m,n} V_{m,l}V_{n,l}^* a_m^\dagger a_k^\dagger|0\rangle\langle 0|a_k a_n\right) \\ &= \left(\sum_{k,m} a_m^\dagger a_k^\dagger|0\rangle\langle 0|a_k a_m\right) = 2\mathbb{I}_{\mathcal{F}_2^{L+1}},\end{aligned} \tag{4.19}$$

therefore,we have:

$$\begin{aligned}\sum_{l=0}^{L}\left(K_l^{\mu\dagger}K_l^\mu\right)_{i,j} &= 2\langle 0|a_i a_\mu a_\mu^\dagger a_j^\dagger|0\rangle \\ &= \begin{cases} 2, & \text{if } i=j,\ i\neq\mu,\ j\neq\mu \\ 0, & \text{otherwise}\end{cases}.\end{aligned} \tag{4.20}$$

As mentioned before, fixing different values of the reference mode μ, generates distinct maps Φ_t^μ with domain $\mathcal{D}_{r(2)}^{\mu,pure}$. Now let us compare these distinct maps. We know that given two sets $\mathcal{D}_2^{\mu,pure}$ and $\mathcal{D}_2^{\nu,pure}$, with fixed modes μ and ν, there exists a unitary $V \in \mathcal{U}(\mathcal{F}_2^{L+1})$ such that $a_\nu^\dagger a_k^\dagger|0\rangle = Va_\mu^\dagger a_k^\dagger|0\rangle$. Therefore, any pair of maps Φ_t^μ and Φ_t^ν have the Kraus operators $\{K_j^\mu = f_j U_t a_\mu^\dagger\}_j$ and $\{E_j^\nu = f_j U_t V a_\mu^\dagger\}_j$, respectively. We can compute an upper bound to the norm difference of the (Choi-Jamiolkowski) dynamical matrices $D_{\Phi_t^\mu}$ and $D_{\Phi_t^\nu}$, associated with the maps, which is proved in Appendix B.1 :

$$\begin{aligned}&\|D_{\Phi_t^\mu} - D_{\Phi_t^\nu}\|_1 \leq \\ &d^2L^2 \sup_{a_{\vec{k}}^\dagger|0\rangle\langle 0|a_{\vec{k}'} \in \mathcal{F}_2^{L+1}} \| \left(a_{\vec{k}}^\dagger|0\rangle\langle 0|a_{\vec{k}'} - V^T a_{\vec{k}}^\dagger|0\rangle\langle 0|a_{\vec{k}'}V^* \right) \|_1,\end{aligned} \tag{4.21}$$

where d is the dimension of $\mathcal{F}_2^{L+1}$ and $\|\cdot\|_1$ is the well know trace norm given by the relation, $\|A\|_1 = Tr\left(\sqrt{A^\dagger A}\right)$ for all operators A. It is illustrative to compare this bound with its counterpart in the case of distinguishable particles, where we have initially uncorrelated system S and environment E forming a closed global system, whose dynamics is described by a unitary U_{SE}. Assuming two dynamical maps, Φ_t and Λ_t, constructed from different initial states of the environment, we have the two sets of Kraus operators $\{K_a = \langle a|U_{SE}|0\rangle\}_a$ and $\{E_a = \langle a|U_{SE}(\mathbb{I}_S \otimes V_E)|0\rangle\}_a$, respectively. Then the following inequality, which is proved in Appendix B.2, holds:

$$\|D_\Phi - D_\Lambda\|_1 \leq d_S^2 \| |0\rangle\langle 0| - V_E|0\rangle\langle 0|V_E^\dagger\|_1, \tag{4.22}$$

where d_S is the dimension of the Hilbert space of the system S. It is important to emphasize that the two frameworks are completely different. A tensor product structure between system and environment is absent in our context of indistinguishable fermions. Another remark is that the two maps in the distinguishable particles case have the same domain, which in general is not true in the case of indistinguishable fermions.

4.3 Examples of One-Particle Dynamical Maps of Indistinguishable Fermions

In this section we illustrate our formalism, deriving the Kraus operators for the dynamics of one-fermion reduced state of two distinct two-particle Hamiltonians. To simplify the discussion, we assume initial pure global state, such that the Kraus operators $\{K_l^\mu = f_l U_t a_\mu^\dagger\}$ have domain given by Eq.(4.11).

4.3.1 Non-interacting Hamiltonian

Our first example, consisting of a non-interacting Hamiltonian, shows the consistency of our formalism. As no correlation can be created, and the initial global state is pure, it is expected the one-particle evolution be unitary. The Hamiltonian can be written in terms of fermionic operators as $H = \sum_{i,j} M_{i,j} a_i^\dagger a_j$, and has the following diagonal form: $H = \sum_k \lambda_k b_k^\dagger b_k$, where

$$b_k^\dagger = \sum_i V_{k,i} a_i^\dagger, \tag{4.23}$$

$$a_j^\dagger = \sum_k V_{k,j}^* b_k^\dagger, \tag{4.24}$$

λ_k are the single particle energy excitations and V is the unitary that diagonalizes M. The dynamical evolution is given by the unitary $U_t = exp\Big(-it \sum_k \lambda_k b_k^\dagger b_k\Big)$. Now, we form the Kraus operators using Eq.(4.12), with the choice $\{f_k^\dagger\}_{k=0}^L = \{b_k\}_{k=0}^L$, namely: $K_l^\mu = b_l U_t a_\mu$. The matrix elements of the Kraus operator are explicitly:

$$\begin{aligned} (K_l^\mu)_{m,n} &= \langle 0|b_m b_l U_t a_\mu^\dagger b_n^\dagger|0\rangle \\ &= \langle 0|b_m b_l U_t \left(\sum_k V_{k,\mu}^* b_k^\dagger\right) b_n^\dagger|0\rangle \\ &= \sum_k V_{k,\mu}^* e^{-it(\lambda_k+\lambda_n)} \left(\delta_{l,k}\delta_{m,n} - \delta_{m,k}\delta_{l,n}\right), \end{aligned} \tag{4.25}$$

thus

$$K_l^\mu = \sum_m e^{-it(\lambda_l+\lambda_m)} \Big(V_{l,\mu}^* b_m^\dagger|0\rangle\langle 0|b_m - V_{m,\mu}^* b_m^\dagger|0\rangle\langle 0|b_l\Big).$$

The map acts on its domain (Eq.(4.11)) as the unitary U_t:

$$\begin{aligned} \rho_r(t) &= \frac{1}{2}\sum_{m,n} \Big(V_{m,k}^* V_{n,k} + V_{m,\mu}^* V_{n,\mu}\Big) \\ &\quad \times e^{-it(\lambda_m-\lambda_n)} b_m^\dagger|0\rangle\langle 0|b_n \\ &= U_t \rho_r(0) U_t{}^\dagger. \end{aligned} \tag{4.26}$$

4.3.2 Four Level Interacting System

Consider two spin-1/2 fermions, in a lattice of two sites, whose dynamics is given by the following Hamiltonian:

$$H = -\sum_{\sigma=\uparrow\downarrow} \Big(a_{1\sigma}^\dagger a_{2\sigma} + h.c\Big) + u\sum_{j=1}^{2} n_{j\uparrow}n_{j\downarrow} + v n_1 n_2, \tag{4.27}$$

where $a_{j\sigma}^\dagger$ and $a_{j\sigma}$ are creation and annihilation operators, respectively, of a fermion at site j with spin σ, $n_{j\sigma} = a_{j\sigma}^\dagger a_{j\sigma}$ and $n_j = n_{j\uparrow} + n_{j\downarrow}$ are the number operators. The first term of the Hamiltonian characterizes hopping (tunnelling) between sites, while the second and third terms characterize the on-site and intersite interactions, parametrized by u and v, respectively. In the basis $a_{\vec{k}}^\dagger|0\rangle \in \mathcal{F}_2^4$, where $\vec{k} = (k_1, k_2)$ has six possible configurations,

$$\begin{aligned} \vec{k} \in \; &\{(1\uparrow, 1\downarrow), (1\uparrow, 2\uparrow), (1\uparrow, 2\downarrow), (1\downarrow, 2\uparrow), \\ &(1\downarrow, 2\uparrow), (2\uparrow, 2\downarrow)\}, \end{aligned} \tag{4.28}$$

we obtain the following matrix representation for the Hamiltonian:

$$H = \begin{pmatrix} u & 0 & -1 & 1 & 0 & 0 \\ 0 & v & 0 & 0 & 0 & 0 \\ -1 & 0 & v & 0 & 0 & -1 \\ 1 & 0 & 0 & v & 0 & 1 \\ 0 & v & 0 & 0 & v & 0 \\ 0 & 0 & -1 & 1 & 0 & u \end{pmatrix}. \tag{4.29}$$

Now we form the Kraus operators $K_j^\mu = a_j U_t a_\mu^\dagger$, with the choice $\{f_k^\dagger\}_{k=0}^L = \{a_k^\dagger\}_{k=0}^L$. If the unitary V diagonalizes the Hamiltonian, $D = VHV^\dagger$, we can write U_t as:

$$U_t = \sum_{\vec{l}} e^{-iD_{\vec{l},\vec{l}}t} \sum_{\vec{k},\vec{k}'} V_{\vec{l},\vec{k}} V^*_{\vec{l},\vec{k}'} a^\dagger_{\vec{k}} |0\rangle\langle 0| a_{\vec{k}'}. \tag{4.30}$$

According to Eq.4.12 we have:

$$\begin{aligned} K_j^\mu &= a_j U_t a_\mu^\dagger \\ &= \sum_{\vec{l}} e^{-iD_{\vec{l},\vec{l}}t} \sum_{k_1,k_2,k'_1,k'_2} V_{\vec{l},k_1k_2} V^*_{\vec{l},k'_1k'_2} \times \\ & \quad a_j a^\dagger_{k_1} a^\dagger_{k_2} |0\rangle\langle 0| a_{k'_2} a_{k'_1} a^\dagger_\mu. \end{aligned} \tag{4.31}$$

Using the anti-commutation relations, the last line of Eq.(4.31) reduces to:

$$\begin{aligned} & a_j a^\dagger_{k_1} a^\dagger_{k_2} |0\rangle\langle 0| a_{k'_2} a_{k'_1} a^\dagger_\mu = \\ & = \left(\delta_{j,k_1} a^\dagger_{k_2} - \delta_{j,k_2} a^\dagger_{k_1}\right) |0\rangle\langle 0| \left(a_{k'_2}\delta_{k'_1,\mu} - a_{k'_1}\delta_{k'_2,\mu}\right), \end{aligned} \tag{4.32}$$

and finally,

$$\begin{aligned} K_j^\mu &= \sum_{\vec{l}} e^{-iD_{\vec{l},\vec{l}}t} \sum_{k,k'} \left[V_{\vec{l},jk} \left(V^*_{\vec{l},k'\mu} - V^*_{\vec{l},\mu k'} \right) + \right. \\ & \quad \left. V_{\vec{l},kj} \left(V^*_{\vec{l},kj} - V^*_{\vec{l},\mu k'} \right) \right] a^\dagger_k |0\rangle\langle 0| a_{k'}. \end{aligned} \tag{4.33}$$

The unitary V can now be written explicitly as

$$V = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ a(u,v) & 0 & b(u,v) & -b(u,v) & 0 & a(u,v) \\ b(u,v) & 0 & -a(u,v) & a(u,v) & 0 & b(u,v) \end{pmatrix}, \tag{4.34}$$

while the explicit form of D is:

$$\begin{aligned} D &= \operatorname{diag}\left(u, v, v, v, \frac{1}{2}\left[(u+v) - \sqrt{\Delta(u,v)^2 + 16}\right], \right. \\ & \quad \left. \frac{1}{2}\left[(u+v) + \sqrt{\Delta(u,v)^2 + 16}\right]\right), \end{aligned} \tag{4.35}$$

with $\Delta(u,v) = v - u$,

$$a(u,v) = \frac{\Delta(u,v) + \sqrt{\Delta(u,v)^2 + 16}}{\sqrt{2\left[\left(\Delta(u,v) + \sqrt{\Delta(u,v)^2 + 16}\right)^2 + 16\right]}},$$

and

$$b(u,v) = \frac{4}{\sqrt{2\left[\left(\Delta(u,v) + \sqrt{\Delta(u,v)^2 + 16}\right)^2 + 16\right]}}.$$

In summary, we recognized conditions for the validity of quantum subsystems dynamics in the presence of exchange correlation. More specifically, we show that it is possible to write maps characterizing the dynamics of one or a few fermions that are part of a system of N indistinguishable particles whose dynamics is given by a unitary evolution. These results adds another class of states in recent discussions about describing the dynamics of initially correlated systems associated with the important problem of clarifying the boundary between completely positive and not completely positive maps [3–10, 34, 35]. It is worth mentioning that a possible unfolding of the formalism to be investigated would be the possibility of computations gains with its use. Since it is well know that many properties of many-body Hamiltonian can be deduced from the single particle reduced state. As an example, we can study the dynamical map of one particle obtained from the initial state of the N fermions in the ground state of a Hamiltonian without interaction, consequently a state of one slater determinant that can be obtained analytically, undergoing an adiabatic evolution leading to the ground state of the target Hamiltonian, with ground state presenting phase transition of interest.

5 Non-Markovianity of open quantum systems

The need to fight decoherence, to guarantee the proper working of the quantum enhanced technologies of information and computation [2], has renovated the motivation for the in-depth study of system-environment interaction dynamics. In particular, the Markovian or non-Markovian nature of the dynamics is of great interest [53]. Several witnesses and quantifiers have been proposed in order to characterize the non-Markovianity of a quantum processes [18, 19, 21]. For instance, the information flow between system and environment, quantified by the distinguishability of any two quantum states [22–24, 54], or by the Fisher information [25], or mutual information [26]. The entanglement based measure of non-Markovianity [27], grounded on the principle that entanglement cannot be produced by a local CP map. In this chapter, we shall present the notion of Markovianity. We first introduce this concept in the classical theory of stochastic processes showing analogies and differences with the quantum case. We define the divisibility criterion for measures of non-Markovianity.

5.1 Markovianity in classical stochastic processes

The supposition of Markovianity can be translated directly into a rigorous mathematical definition for classical stochastic processes. Consider a stochastic process defined as a family of random variables $\{X(t)|t \in [t_0, t_f] \in \mathbb{R}^+\}$, where the parameter t represents time, taking values in a discrete set $\{x_0(t_0), x_1(t_1), \ldots, x_n(t_n)\}$ with ordered set of times $t_0 \leq t_1 \leq \cdots \leq t_n$, we may describe this dynamical process through joint distributions of the form $p\left(x_n, t_n|x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right)$. In general, the probability that the random variable X acquire a value x_n at an arbitrary time t_n is conditioned to the entire history of the dynamics, as can be seen from Bayes' theorem,

$$p\left(x_n, t_n|x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right) = \frac{p\left(x_n, t_n; x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right)}{p\left(x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right)}. \tag{5.1}$$

However, if the process is Markovian we just need to provide that it took the value x_{n-1} at some previous time $t_{n-1} < t_n$ to uniquely determine the condition probability, and does not have the influence of the values of X for previous times to t_{n-1}, which can be formulated in terms of conditional probabilities as

$$p\left(x_n, t_n|x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right) = p\left(x_n, t_n|x_{n-1}, t_{n-1}\right). \tag{5.2}$$

In the sense described above, Markovian process is said to lack memory. The quantum analogues of random variables of classical processes are operators characterizing system observables, therefore the definition of Markovianity given by Eq.(5.2) has no satisfactory direct parallel to quantum mechanics because quantum theory is based on noncommutative algebras. A different approach, known as the divisibility criterion, focused on the study of dynamical maps acting on single-time probabilities $p(x_0, t_0)$, gives a sufficient condition for a classical stochastic process to be non-Markovian. Similarly, we can define the divisibility criterion for the quantum case, now investigating the dynamical map on quantum states.

Consider a classical stochastic process, such that the single-time probability distribution at time t is a probability vector $\mathbf{p}(t)$, with elements $p(j,t)$ satisfying $p(j,t) \geq 0$ for all j and $\sum_j p(j,t) = 1$. Consider a linear map $\Lambda(t, t_0)$ that performs the time evolution of the probability vector $\mathbf{p}(t_0)$:

$$\mathbf{p}(t) = \Lambda(t, t_0)\mathbf{p}(t_0). \tag{5.3}$$

The map Λ that associates probability vectors to probability vectors satisfy the following conditions:

$$\begin{aligned} \sum_{j=1}^{N} (\Lambda)_{jk} &= 1 \quad \forall k, \\ (\Lambda)_{jk} &\geq 0 \quad \forall j, k. \end{aligned} \tag{5.4}$$

A map that respects the properties described in Eq.(5.4) is named stochastic matrix. For a stochastic process, not necessary Markovian, we can define the relation

$$p\left(k, t\right) = \sum_{j} p\left(k, t | j, t_0\right) p\left(j, t_0\right), \tag{5.5}$$

obtained from the definition of the probability condition Eq.(5.1). Each element of the probability vector defined in Eq.(5.3) can be written as $p\left(i, t\right) = \sum_j \left(\Lambda(t, t_0)\right)_{ij} p\left(j, t_0\right)$, comparing with the expression Eq.(5.5), we can conclude that $\left(\Lambda(t, t_0)\right)_{ij} = p(i, t|j, t_0)$. However, this is not necessarily true for an intermediate time $t_1 > t_0$, that is, we may have $\left(\Lambda(t, t_1)\right)_{ij} \neq p(i, t|j, t_1)$. In general the conditional probability $p(i, t|j, t_1)$ is not uniquely defined due to the dependency of the initial condition, i.e. $p(i, t|j, t_1; k, t_0)$ can be distinct of $p(i, t|j, t_1; k', t_0)$ to $k \neq k'$, an exception to this fact would be Makovian processes that satisfy Eq.(5.2), and therefore the relation $\left(\Lambda(t, t_1)\right)_{ij} = p(i, t|j, t_1)$ is valid. The Markov condition Eq.(5.2) implies that the conditional probability $p\left(x, t|x_0, t_0\right)$ satisfies the discrete version of the so-called Chapman-Kolmogorov equation

$$p\left(x, t|x_0, t_0\right) = \sum_{x_1} p\left(x, t|x_1, t_1\right) p\left(x_1, t_1|x_0, t_0\right), \quad t_0 < t_1 < t. \tag{5.6}$$

One can see this by applying the definition of conditional probability Eq.(5.1), and the Markovian condition Eq.(5.2) on a joint probability for the three consecutive times, $p(x, t; x_1, t_1; x_0, t_0) = p(x, t|x_1, t_1)p(x_1, t_1|x_0, t_0)p(x_0, t_0)$, dividing both sides by $p(x_0, t_0)$ and summing over x_1.

Provided that the map $\Lambda(t,t_0)$ is invertible for all $t > t_0$, we can compute maps for intermediate times as follows:

$$\Lambda(t,t_1) = \Lambda(t,t_0)\Lambda(t_1,t_0)^{-1}, \tag{5.7}$$

where $t > t_1 > t_0$. The map $\Lambda(t,t_1)$ is not necessarily stochastic, i.e., it does not satisfy the relations in Eq.(5.4). The class of maps that has stochastic intermediate maps for any $t > t_1 > t_0$ is called P-divisible. Intermediate map $\Lambda(t,t_1)$ violates P-divisibility only in the case of non-Markovian processes, this gives a sufficient condition to detect non-Markovianity.

5.2 Quantum Dynamical Maps and the Divisibility Criterion

The standard description of the evolution of an open quantum system can be written in the well known operator sum representation [2, 33] (see section 2.3):

$$\rho(t) = \sum_j K_j\left(t,t_0\right)\rho(t_0)K_j^\dagger\left(t,t_0\right), \qquad \sum_j K_j^\dagger K_j = \mathbb{I}, \tag{5.8}$$

where the K_j are the Kraus operators and $\rho(t_0)$ is the state of the open system at initial time t_0. We can conveniently rewrite the dynamic process (Eq.5.8) in the natural representation as (Eq.2.26):

$$|\rho(t)\rangle = \Phi\left(t,t_0\right)|\rho(t_0)\rangle, \;\; \Phi\left(t,t_0\right) = \sum_j K_j\left(t,t_0\right)\otimes K_j^*\left(t,t_0\right), \tag{5.9}$$

where $|\rho\rangle \equiv vec(\rho)$. Consider the evolution of the system from an initial time t_0 to a final time t_f,

$$|\rho(t_f)\rangle = \Phi(t_f,t_0)|\rho(t_0)\rangle. \tag{5.10}$$

Suppose this evolution is broken in two steps with an intermediate time, $t_f > t_m > t_0$, namely:

$$|\rho(t_f)\rangle = \Phi(t_f,t_m)\Phi(t_m,t_0)|\rho(t_0)\rangle. \tag{5.11}$$

Whereas $\Phi(t_f,t_0)$ is a completely positive (CP) map for arbitrary t_f [33], the map corresponding to the intermediate step, $\Phi(t_f,t_m)$, may be non-CP for some t_m. As realizable maps are always CP, $\Phi(t_f,t_m)$ being non-CP for the particular time t_m witnesses the fact that such a division is not possible. A trivial case in which any intermediate division is possible corresponds to unitary evolution. Markovian evolutions also admit arbitrary intermediate steps. The intermediate map may fail to be CP only in the case of non-Markovian evolution. This *divisibility criterion* [27] is therefore a sufficient condition to detect non-Markovianity.

In order the check the complete positivity of a map, we use the well known duality between CP maps and positive operators, expressed by the Choi's theorem [33, 55]. First we define the unique dynamical matrix associated to the map:

$$D^{mn}_{\mu\nu} = \Phi^{m\mu}_{n\nu} = \langle m\mu|\Phi|n\nu\rangle, \tag{5.12}$$

where Latin and Greek indices correspond to system and environment Hilbert spaces, respectively. The Choi's theorem states that the map (Φ) is CP if and only if its dynamical matrix (D) is a positive semi-definite operator. Finally, to check the complete positivity of the intermediate map, we form the matrix of its super-operator by means of the product:

$$\Phi(t_f, t_m) = \Phi(t_f, t_0)\Phi^{-1}(t_m, t_0). \tag{5.13}$$

Note that $\Phi(t, t_0)$ is the matrix representation of the map that evolves the system from the initial time t_0 to any time t. $\Phi^{-1}(t_m, t_0)$ is the pseudo-inverse of $\Phi(t_m, t_0)$, and thus evolves the system from t_m to t_0. Therefore the matrix product in Eq.5.13 defines a matrix representation for the intermediate map. While the dynamical matrix ($D(t, t_0)$) corresponding to $\Phi(t, t_0)$ is always positive semi-definite, the one ($D(t_f, t_m)$) related to $\Phi(t_f, t_m)$ may happen to be non-positive, and in this case it witnesses a non-Markovian evolution.

6 Non-Markovian Dynamics of One and Two Qubits in an Ising Model Environment

In this chapter, we present our results on the topic of non-Markovianity [Eur. Phys. J. D 71, 119 (2017)]. We obtained explicitly the Choi representation of the quantum map of an arbitrary quadratic fermionic Hamiltonian acting on qubits, and performed a comparative exploration of its dynamics from the point of view of (non-)divisibility [30,31]. After obtaining the analytical expression of the dynamical matrix, we specialized to the case of an environment represented by the quantum one-dimensional Ising model acting on one central qubit, which in the case of finite size lattices can be solved analytically by means of the well known Jordan-Wigner and Bogoliubov transformations [56,57]. The divisibility criterion consists in checking if an intermediate quantum map is not Complete Positive (CP) for some time instant, which amounts to checking the non-positivity of the corresponding dynamical matrix [33]. We showed that the non-positivity of the dynamical matrix, measured by its eigenvalues, in this case is a simple function of the Loschmidt echo [58], a quantity that indicates decoherence induced by perturbations. We also investigated the action of a trivial extension of the map on the decay of entanglement of the system coupled to an ancilla. We saw that the intermediate map is not contractive, and entanglement is again a function of the Loschmidt echo which is not monotonically decreasing, signaling non-Markovianity and information flux from the environment to the system [28]. Finally, we wished to know if the number of particles in the system has some influence on the dynamics of the environment. Thus we derived the map acting on a system composed of two qubits, concluding that the results do not have any change.

6.1 Dynamical Matrix for a General Fermionic Quadratic Hamiltonian

In previous chapters, we reviewed the formalism of quantum maps and the divisibility criterion. We now apply such formalism to environments described by general fermionic quadratic Hamiltonians, interacting with a qubit. We will show how to obtain the exact expression for the Kraus decomposition of the dynamical matrix. Let us then consider a general fermionic quadratic Hamiltonian, namely,

$$H_g = \sum_{m,n=1}^{L} (x_{m,n} a_m^\dagger a_n + y_{m,n} a_m^\dagger a_n^\dagger + h.c.). \tag{6.1}$$

where L is the lattice size, and $x_{m,n}, y_{m,n}$ are arbitrary complex numbers. $a_j^\dagger(a_j)$ is the creation (annihilation) operator, satisfying the usual anti-commutation relations:

$$\{a_i, a_j^\dagger\} = \delta_{ij},\ \{a_i, a_j\} = 0. \tag{6.2}$$

For the interaction of the qubit with this environment, we consider the following Hamiltonian:

$$H_{int} = -\delta|e\rangle\langle e| \otimes V_e, \tag{6.3}$$

where $|g\rangle$ and $|e\rangle$ are the qubit ground and excited states, respectively, and V_e is a fermionic quadratic Hamiltonian. We consider that the qubit and environment are initially uncorrelated, and they are in an arbitrary pure initial state,

$$|\psi(0)\rangle = |\chi(0)\rangle \otimes |\varphi(0)\rangle = (c_g|g\rangle + c_e|e\rangle) \otimes |\varphi(0)\rangle, \tag{6.4}$$

where $|\chi(0)\rangle = c_g|g\rangle + c_e|e\rangle$, with $|c_g|^2 + |c_e|^2 = 1$, is the initial qubit state. The evolution under the total Hamiltonian,

$$H = H_g + H_{int}, \tag{6.5}$$

is given by:

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\chi(0)\rangle \otimes |\varphi(0)\rangle, \tag{6.6}$$

$$|\psi(t)\rangle = c_g|g\rangle \otimes \underbrace{e^{-iH_gt/\hbar}|\varphi(0)\rangle}_{|\varphi_g(t)\rangle} + c_e|e\rangle \otimes \underbrace{e^{-iH_et/\hbar}|\varphi(0)\rangle}_{|\varphi_e(t)\rangle}, \tag{6.7}$$

where

$$H_e = H_g - \delta V_e. \tag{6.8}$$

Such Hamiltonians, H_e and H_g, can be easily diagonalized by a Bogoliubov transformation [56], where we introduce to the problem new fermionic operators $B_{\pm k}$ and $A_{\pm k}$, constructed as a linear combination of operators $a_{\pm k}$,

$$B_{\pm k} \equiv \cos\left(\frac{\theta_g^k}{2}\right) a_{\pm k} \mp i \sin\left(\frac{\theta_g^k}{2}\right) a_{\mp k}^\dagger, \tag{6.9}$$

$$A_{\pm k} \equiv \cos\left(\frac{\theta_e^k}{2}\right) a_{\pm k} \mp i \sin\left(\frac{\theta_e^k}{2}\right) a_{\mp k}^\dagger. \tag{6.10}$$

The index k is associated with the reciprocal space arising from a Fourier transformation. The θ_g^k and θ_e^k parameters are dependent on the Hamiltonian parameters, in the next section we will define them explicitly for the Ising model [56, 57]. These new fermionic operators are related according to

$$B_{\pm k} = \cos(\alpha_k)A_{\pm k} \mp i\sin(\alpha_k)A_{\mp k}^\dagger, \tag{6.11}$$

where $\alpha_k = (\theta_g^k - \theta_e^k)/2$. The Hamiltonians in diagonal form read:

$$H_g = \sum_k \epsilon_g^k(B_k^\dagger B_k + C_g),\ H_e = \sum_k \epsilon_e^k(A_k^\dagger A_k + C_e), \tag{6.12}$$

where C_g and C_e are both real constants, and $\epsilon^k_{g(e)}$ are the single-particle eigenvalues. The ground states of H_g (G_g) and H_e (G_e) are related by:

$$|G_g\rangle = \prod_{k>0}\left[\cos(\alpha_k) + i\sin(\alpha_k)A^\dagger_k A^\dagger_{-k}\right]|G_e\rangle. \tag{6.13}$$

Now we derive the Kraus decomposition of the map super-operator (Φ). The Kraus operators of the evolution are:

$$K_i = (\mathbb{I}_S \otimes \langle i|)\, e^{-iHt/\hbar}\, (\mathbb{I}_S \otimes |\varphi(0)\rangle), \tag{6.14}$$

with $\mathbb{I}_S = |g\rangle\langle g| + |e\rangle\langle e|$. Assuming, without loss of generality (the map does not depend on the initial states of the qubit-environment), that the environment is initially in its ground state , $|\varphi(0)\rangle = |G_g\rangle$, and using Eq.(6.7), we obtain:

$$K_i = \mathbb{I}_S \otimes \langle i|\left[|g\rangle\langle g| \otimes |\varphi_g(t)\rangle + |e\rangle\langle e| \otimes |\varphi_e(t)\rangle\right]. \tag{6.15}$$

The environment states $|\varphi_g(t)\rangle$ and $|\varphi_e(t)\rangle$ are given by:

$$\begin{gathered}|\varphi_g(t)\rangle = e^{-iH_g t/\hbar}|G_g\rangle = e^{-iE_g t/\hbar}|G_g\rangle = \\ e^{-iE_g t/\hbar}\prod_{k>0}\left[\cos(\alpha_k) + i\sin(\alpha_k)A^\dagger_k A^\dagger_{-k}\right]|G_e\rangle,\end{gathered} \tag{6.16}$$

where E_g is the ground state energy of H_g. Likewise, using Eq.(6.13), we obtain:

$$\begin{gathered}|\varphi_e(t)\rangle = e^{-iH_e t/\hbar}\times \\ \prod_{k>0}\left[\cos(\alpha_k) + i\sin(\alpha_k)A^\dagger_k A^\dagger_{-k}\right]|G_e\rangle = \\ \prod_{k>0}\left[\cos(\alpha_k) + e^{-i(\epsilon^k_e+\epsilon^{-k}_e)t/\hbar} i\sin(\alpha_k)A^\dagger_k A^\dagger_{-k}\right]\times \\ e^{-iE_e t/\hbar}|G_e\rangle.\end{gathered} \tag{6.17}$$

In order to obtain the Kraus operators, it is enough to calculate the overlaps $\langle i|\varphi_g(t)\rangle$ and $\langle i|\varphi_e(t)\rangle$, for a given environment basis $\{|i\rangle\}$, as shown in Eq.(6.15). A convenient basis is formed by the eigenstates of H_e, namely:

$$\{|i\rangle\} = \{|G_e\rangle, A^\dagger_{\vec{k}_N}|G_e\rangle\}, \tag{6.18}$$

where $\vec{k}_N = (k_1, k_2, ..., k_N)$ is the vector representing the momentum of the $N(=1,\ldots,L)$ excitations, and $A^\dagger_{\vec{k}} = A^\dagger_{k_1}A^\dagger_{k_2}...A^\dagger_{k_N}$. It is easy to see that the only non null elements for "$\langle i|\varphi_g(t)\rangle$", using Eq.(6.16), are given by,

$$\langle G_e|\varphi_g(t)\rangle = e^{-iE_g t/\hbar}(\prod_{k>0}\cos(\alpha_k)), \tag{6.19}$$

and

$$\begin{gathered}a_{\vec{k}_N}(t) \equiv \langle G_e|A_{-\vec{k}_N}A_{\vec{k}_N}|\varphi_g(t)\rangle = \\ e^{-iE_g t/\hbar}\prod_{k\in\vec{k}_N}(i\sin(\alpha_k))(\prod_{k>0,\, k\notin\vec{k}_N}\cos(\alpha_k)),\end{gathered} \tag{6.20}$$

where N varies from 1 to $L/2$. Analogously, the non null terms for "$\langle i|\varphi_e(t)\rangle$", using Eq.(6.17), are given by,

$$\begin{gathered} b_{\vec{k}_N}(t) \equiv \langle G_e|A_{-\vec{k}_N}A_{\vec{k}_N}|\varphi_e(t)\rangle = \\ e^{-iE_e t/\hbar}\prod_{k\in\vec{k}_N}\left[i\sin(\alpha_k)\exp(-i(\epsilon_e^k+\epsilon_e^{-k})t/\hbar)\right]\times \\ (\prod_{k>0,\,k\notin\vec{k}_N}\cos(\alpha_k)). \end{gathered} \tag{6.21}$$

It is easy to check the following relation:

$$b_{\vec{k}_N}(t) = a_{\vec{k}_N}(t)f_{\vec{k}_N}(t), \tag{6.22}$$

where

$$f_{\vec{k}_N}(t) \equiv e^{-i(E_e-E_g)t/\hbar}\exp(-i\sum_{k\in\vec{k}_N}^{N}(\epsilon_e^k+\epsilon_e^{-k})t/\hbar). \tag{6.23}$$

Finally, we reach the first result of this work, obtaining a simple expression for the Kraus operators of the quantum map,

$$K_{\vec{k}_N} = a_{\vec{k}_N}(t)(|g\rangle\langle g| + f_{\vec{k}_N}(t)|e\rangle\langle e|). \tag{6.24}$$

Note that $\left|a_{\vec{k}_N}(t)\right|^2$ is not a time dependent variable, and

$$\sum_{\{\vec{k}_N\}}\left|a_{\vec{k}_N}(t)\right|^2 = Tr(|\varphi_g(t)\rangle\langle\varphi_g(t)|) = 1. \tag{6.25}$$

By using this fact, we can then write the quantum map in terms of the Kraus operators as follows,

$$\begin{aligned} \Phi(t,0) &= \sum_{\{\vec{k}_N\}} K_{\vec{k}_N}\otimes K^*_{\vec{k}_N} \\ &= |g\rangle\langle g|\otimes|g\rangle\langle g| + |e\rangle\langle e|\otimes|e\rangle\langle e| + \\ &\quad |g\rangle\langle g|\otimes|e\rangle\langle e|\sum_{\{\vec{k}_N\}}\left|a_{\vec{k}_N}(t)\right|^2 f_{\vec{k}_N}(t)^* + \\ &\quad |e\rangle\langle e|\otimes|g\rangle\langle g|\sum_{\{\vec{k}_N\}}\left|a_{\vec{k}_N}(t)\right|^2 f_{\vec{k}_N}(t). \end{aligned} \tag{6.26}$$

If we define the following variable,

$$x(t) \equiv \sum_{\{\vec{k}_N\}}\left|a_{\vec{k}_N}(t)\right|^2 f_{\vec{k}_N}(t), \tag{6.27}$$

the quantum map can be rewritten as,

$$\begin{aligned} \Phi(t,0) = {} & [|g\rangle\langle g|\otimes|g\rangle\langle g| + |e\rangle\langle e|\otimes|e\rangle\langle e| + \\ & |g\rangle\langle g|\otimes|e\rangle\langle e|x(t)^* + |e\rangle\langle e|\otimes|g\rangle\langle g|x(t)]\,. \end{aligned} \tag{6.28}$$

As expected, the quantum map consists in a decoherence channel, and thus we can identify the variable "$x(t)$" with the known Loschmidt echo $\mathcal{L}(t)$ [24, 54, 59],

$$\mathcal{L}(t) = |x(t)|^2 = |\langle\varphi_g(t)|\varphi_e(t)\rangle|^2. \tag{6.29}$$

The above relation follows just by noticing that the qubit reduced state, $\rho_S(t) = Tr_E(|\psi(t)\rangle\langle\psi(t)|)$, taking the partial trace of Eq.(6.4), is given by $\rho_S(t) = |c_g|^2|g\rangle\langle g|+|c_e|^2|e\rangle\langle e|+c_g^*c_e\mu(t)|e\rangle\langle g|+ H.c.$, where $\mu(t) = \langle\varphi_g(t)|\varphi_e(t)\rangle$ is the decoherence factor. The quantum map corresponding to such an evolution is the decoherence channel, as described before.

From Eq.(5.13), we have the following expression for the intermediate map:

$$\begin{aligned}\Phi(t_f, t_m) = [&|g\rangle\langle g| \otimes |g\rangle\langle g| + |e\rangle\langle e| \otimes |e\rangle\langle e| + \\ &|g\rangle\langle g| \otimes |e\rangle\langle e| y(t_f, t_m)^* + \\ &|e\rangle\langle e| \otimes |g\rangle\langle g| y(t_f, t_m)]\,,\end{aligned} \tag{6.30}$$

where

$$y(t_f, t_m) \equiv \frac{x(t_f)}{x(t_m)}. \tag{6.31}$$

The dynamical matrix of this quantum map is

$$D_{\Phi(t_f,t_m)} = \begin{pmatrix} 1 & 0 & 0 & y(t_f,t_m)^* \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ y(t_f,t_m) & 0 & 0 & 1 \end{pmatrix}. \tag{6.32}$$

Computing the minimum eigenvalue, we arrive at the following simple sufficient condition for the positive-semi-definiteness of the dynamical matrix:

$$1 - |y(t_f, t_m)| \geq 0. \tag{6.33}$$

Therefore we have obtained a simple function capable to witness the non-Markovianity of the dynamics, *i.e.*, Φ is non-Markovian if $|y(t_f, t_m)| > 1$.

6.2 Ising model as an environment for a system of one qubit

In the previous section, we derived the dynamical matrix for an arbitrary quadratic fermionic Hamiltonian. In this section we focus on an environment described by the Ising Hamiltonian in a transverse field (H_{ising}), with periodic boundary conditions ($L + 1 = 1$).

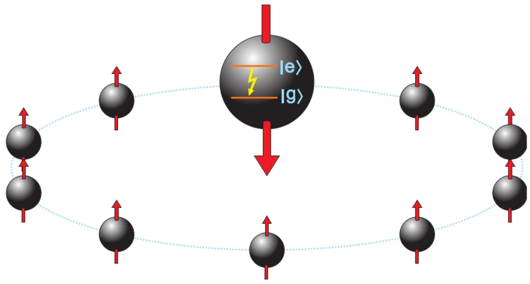

Figure 3 – Schematic view of spins forming a ring array, representing the environment governed by the Ising Hamiltonian (Eq.(6.34)). The central spin is the qubit interacting with the environment according to Eq.(6.35).

The interaction with the environment (H_{int}) is by means of the transverse magnetic field in the Z direction (see Fig.3), more precisely,

$$H_{Ising} = -J\sum_{j=1}^{L}(\sigma_j^x\sigma_{j+1}^x + \lambda\sigma_j^z), \tag{6.34}$$

$$H_{int} = -\delta|e\rangle\langle e|\otimes\sum_{j=1}^{L}\sigma_j^z. \tag{6.35}$$

In order to employ the previous section's results, we first do the identification:

$$H_e = H_{ising} - \delta\sum_{j=1}^{L}\sigma_j^z, \tag{6.36}$$

$$H_g = H_{ising}. \tag{6.37}$$

We now diagonalize the Ising Hamiltonian [57]. First we use the usual Jordan-Wigner transformation,

$$\sigma_j^+ = \exp{(i\pi\sum_{l<j}a_l^\dagger a_l)} = \prod_{l<j}(1-2a_l^\dagger a_l)a_j, \tag{6.38}$$

$$a_j = (\prod_{l<j}\sigma_l^z)\sigma_j^+. \tag{6.39}$$

The Ising Hamiltonian can then be rewritten in terms of quadratic fermionic operators:

$$H_{ising} = J\left[-\sum_{j=1}^{L-1}(a_j^\dagger a_{j+1} + a_j^\dagger a_{j+1}^\dagger + h.c.)\right.$$
$$\left.+e^{(i\pi)\hat{N}}(a_L^\dagger a_1 + a_L^\dagger a_1^\dagger + h.c.) + 2\lambda\hat{N} - \lambda L\right], \tag{6.40}$$

where $\hat{N} = \sum_j a_j^\dagger a_j$. The Hamiltonian conserves the parity, $\left[H, e^{(i\pi)\hat{N}}\right] = 0$. Thus we can analyze its *odd/even* subspaces separately. The gap between the ground state energy of these two subspaces closes in the thermodynamic limit. For simplicity, we shall proceed the analysis in the *even* sector, which leads to a simple quadratic Hamiltonian with anti-periodic boundary conditions. Using the momentum eigenstates,

$$a_k = \frac{1}{\sqrt{L}}\sum_j e^{(-ikj)}a_j, \tag{6.41}$$

with $k = \frac{2\pi}{L}q,\ q = \pm 1/2, \pm 3/2, ..., \pm(L-1)/2$, for L even, and the Bogoliubov transformation (Eq.(6.10)), with phases

$$\theta_e^k(\delta) = \arctan\left[\frac{-\sin(k)}{\cos(k) - (\lambda + \delta)}\right], \tag{6.42}$$

the Hamiltonian assumes the desired diagonal form:

$$H_e = \sum_k \epsilon_e^k \, (A_k^\dagger A_k - 1/2), \tag{6.43}$$

with eigenvalues given by:

$$\epsilon_e^k(\delta) = J\sqrt{1 + (\lambda+\delta)^2 - 2(\lambda+\delta)\cos(k)}. \tag{6.44}$$

6.3 Ising model as an environment for a system of two qubits

Now we determine the exact expression for the quantum map(Φ), in the case of two qubits interacting with an environment described by an arbitrary quadratic fermionic Hamiltonian H_g (Eq.(6.1)). The motivation is to investigate how the number of particles in the system affects the environment. We assume the two qubits described by the Hamiltonian

$$H_S = -J_S\left[\sigma_1^z\sigma_2^z + \lambda_S\left(\sigma_1^z + \sigma_2^z\right)\right], \tag{6.45}$$

where $\sigma^z = |g\rangle\langle g| - |e\rangle\langle e|$, with $|g\rangle$ and $|e\rangle$ being the qubit ground and excited states. For the interaction with the environment, we consider the following Hamiltonian:

$$\begin{aligned} H_{int} &= -\left[\delta_1|gg\rangle\langle gg| + \delta_2\left(|ge\rangle\langle ge|\right.\right. \\ &\qquad \left.\left. + |eg\rangle\langle eg|\right)\right] \otimes V, \end{aligned} \tag{6.46}$$

where V is a fermionic quadratic Hamiltonian. We assume that the two qubits and the environment are initially uncorrelated, and they are in an arbitrary pure initial state,

$$|\psi(0)\rangle = |\chi(0)\rangle \otimes |\varphi(0)\rangle,$$

where $|\chi(0)\rangle = c_{gg}|gg\rangle + c_{ge}|ge\rangle + c_{eg}|eg\rangle + c_{ee}|ee\rangle$ ($|c_{gg}|^2 + |c_{ge}|^2 + |c_{eg}|^2 + |c_{ee}|^2 = 1$) is the initial two-qubit state. Therefore, the state of the composite system, at an arbitrary time t, can be written as:

$$\begin{aligned} |\Psi(t)\rangle &= e^{-i(H_g + H_{int} + H_S)t/\hbar}|\chi(0)\rangle \otimes |\varphi(0)\rangle \\ &= e^{-iJ_S t/\hbar}\left(c_{ge}|ge\rangle + c_{eg}|eg\rangle\right)|\varphi_2(t)\rangle + \\ &\quad c_{gg}e^{iJ_S(1+2\lambda)t/\hbar}|gg\rangle|\varphi_1(t)\rangle + \\ &\quad c_{ee}e^{iJ_S(1-2\lambda)t/\hbar}|ee\rangle|\varphi_0(t)\rangle, \end{aligned} \tag{6.47}$$

where $|\varphi_a(t)\rangle = e^{-iH_a t/\hbar}|\varphi(0)\rangle$, with Hamiltonian $H_a = H_0 - \delta_a V_e$, $a = (0,1,2)$, and $\delta_0 = 0$. With this notation, we have $H_0 \equiv H_g$. The Hamiltonian $H_a(a = (0,1,2))$ can be diagonalized by a Bogoliubov transformation,

$$\eta_a^{\pm k} = \cos\left(\frac{\theta_a^k}{2}\right) a_{\pm k} \mp i \sin\left(\frac{\theta_a^k}{2}\right) a_{\mp k}^{\dagger}. \tag{6.48}$$

These fermionic operators are related by:

$$\eta_a^{\pm k} = \cos\left(\alpha_{a,b}^k\right) \eta_b^{\pm k} \mp i \sin\left(\alpha_{a,b}^k\right) \eta_b^{\mp k\dagger}, \tag{6.49}$$

where $\alpha_{a,b}^k = (\theta_a^k - \theta_b^k)/2$. The Hamiltonian in diagonal form reads:

$$H_a = \sum_k \epsilon_a^k \left(\eta_a^{k\dagger}\eta_a^k + C_a\right), \tag{6.50}$$

where C_0, C_1 and C_2 are real constants, ϵ_0^k, ϵ_1^k and ϵ_2^k are the single-particle eigenvalues. The ground states of H_0 (G_0), H_1 (G_1) and H_2 (G_2) are related according to:

$$|G_a\rangle = \prod_{k>0} \left[\cos\left(\alpha_{a,b}^k\right) + i \sin\left(\alpha_{a,b}^k\right) \eta_b^{k\dagger}\eta_b^{-k\dagger}\right] |G_b\rangle. \tag{6.51}$$

Using the definition of Kraus operators in Eq.(6.14), and the Eq.(6.47), we can write:

$$\begin{aligned} K_i \;=\; & \langle i|\varphi_2\rangle e^{-iJt/\hbar} \left(|ge\rangle\langle ge| + |eg\rangle\langle eg|\right) + \\ & \langle i|\varphi_1\rangle e^{iJ(1+2\lambda)t/\hbar}|gg\rangle\langle gg| + \\ & \langle i|\varphi_0\rangle e^{iJ(1-2\lambda)t/\hbar}|ee\rangle\langle ee|, \end{aligned} \tag{6.52}$$

where $\{|i\rangle\}$ is an environment basis. Finally we obtain the quantum map:

$$\begin{aligned} \Phi(t,0) \;=\; & \sum_i K_i \otimes K_i^* \\ =\; & [|gg\rangle\langle gg| \otimes |gg\rangle\langle gg| + |ee\rangle\langle ee| \otimes |ee\rangle\langle ee| + \\ & |ge\rangle\langle ge| \otimes |ge\rangle\langle ge| + |eg\rangle\langle eg| \otimes |eg\rangle\langle eg| + \\ & |ge\rangle\langle ge| \otimes |eg\rangle\langle eg| + |eg\rangle\langle eg| \otimes |ge\rangle\langle ge| + \\ & (|ee\rangle\langle ee| \otimes |eg\rangle\langle eg| + |ee\rangle\langle ee| \otimes |ge\rangle\langle ge|) \times \\ & x_{0,2}(t)^* e^{i\phi_- t} + \\ & (|eg\rangle\langle eg| \otimes |ee\rangle\langle ee| + |ge\rangle\langle ge| \otimes |ee\rangle\langle ee|) \times \\ & x_{0,2}(t) e^{-i\phi_- t} + \\ & (|gg\rangle\langle gg| \otimes |eg\rangle\langle eg| + |gg\rangle\langle gg| \otimes |ge\rangle\langle ge|) \\ & x_{1,2}(t)^* e^{i\phi_+ t} + \\ & (|eg\rangle\langle eg| \otimes |gg\rangle\langle gg| + |ge\rangle\langle ge| \otimes |gg\rangle\langle gg|) \\ & x_{1,2}(t) e^{-i\phi_+ t} + \\ & |ee\rangle\langle ee| \otimes |gg\rangle\langle gg| x_{0,1}(t)^* e^{-i\phi_0 t} + \\ & \left. |gg\rangle\langle gg| \otimes |ee\rangle\langle ee| x_{0,1}(t) e^{i\phi_0 t} \right], \end{aligned} \tag{6.53}$$

with, $\phi_\pm = 2J_S(1 \pm \lambda_S)/\hbar$ and $\phi_0 = 4J_S\lambda_S/\hbar$, and $x_{a,b}(t) = \langle\varphi_b|\varphi_a\rangle$. Choosing the environment in its initial ground state, $|\varphi(0)\rangle = |G_0\rangle$, and using equations (6.49-6.51), we have:

$$\begin{aligned}
x_{a,b}(t) &= \langle\varphi_b|\varphi_a\rangle \\
&= \prod_{k>0} \left\{ \cos\left(\alpha_{0,a}^k\right)\cos\left(\alpha_{0,b}^k\right)\cos\left(\alpha_{a,b}^k\right) + \right. \\
&\quad \left[\cos\left(\alpha_{0,a}^k\right)\sin\left(\alpha_{0,b}^k\right)e^{i(\epsilon_b^k+\epsilon_b^{-k})t/\hbar} - \right. \\
&\quad \left. \cos\left(\alpha_{0,b}^k\right)\sin\left(\alpha_{0,a}^k\right)e^{-i(\epsilon_a^k+\epsilon_a^{-k})t/\hbar}\right] \times \\
&\quad \sin\left(\alpha_{a,b}^k\right) + \sin\left(\alpha_{0,a}^k\right)\sin\left(\alpha_{0,b}^k\right)\cos\left(\alpha_{a,b}^k\right) \times \\
&\quad \left. e^{-i\left[(\epsilon_a^k+\epsilon_a^{-k})-(\epsilon_b^k+\epsilon_b^{-k})\right]t/\hbar}\right\} e^{-i(E_a-E_b)t/\hbar},
\end{aligned} \tag{6.54}$$

where E_a is the ground state energy of H_a. Finally, we obtain the dynamical matrix of the intermediate map, namely:

$$\begin{aligned}
D_{\Phi(t_f,t_m)} &= [|gg\rangle\langle gg| \otimes |gg\rangle\langle gg| + |ee\rangle\langle ee| \otimes |ee\rangle\langle ee| + \\
&\quad |ge\rangle\langle ge| \otimes |ge\rangle\langle ge| + |eg\rangle\langle eg| \otimes |eg\rangle\langle eg| + \\
&\quad |ge\rangle\langle eg| \otimes |ge\rangle\langle eg| + |eg\rangle\langle ge| \otimes |eg\rangle\langle ge| + \\
&\quad (|ee\rangle\langle eg| \otimes |ee\rangle\langle eg| + |ee\rangle\langle ge| \otimes |ee\rangle\langle ge|) \times \\
&\quad y_{0,2}(t_f,t_m)^* e^{i\phi_-(t_f-t_m)} + \\
&\quad (|eg\rangle\langle ee| \otimes |eg\rangle\langle ee| + |ge\rangle\langle ee| \otimes |ge\rangle\langle ee|) \times \\
&\quad y_{0,2}(t_f,t_m) e^{-i\phi_-(t_f-t_m)} + \\
&\quad (|gg\rangle\langle eg| \otimes |gg\rangle\langle eg| + |gg\rangle\langle ge| \otimes |gg\rangle\langle ge|) \times \\
&\quad y_{1,2}(t_f,t_m)^* e^{i\phi_+(t_f-t_m)} + \\
&\quad (|eg\rangle\langle gg| \otimes |eg\rangle\langle gg| + |ge\rangle\langle gg| \otimes |ge\rangle\langle gg|) \times \\
&\quad y_{1,2}(t_f,t_m) e^{-i\phi_+(t_f-t_m)} + \\
&\quad |ee\rangle\langle gg| \otimes |ee\rangle\langle gg| y_{0,1}(t_f,t_m)^* e^{-i\phi_0(t_f-t_m)} + \\
&\quad \left. |gg\rangle\langle ee| \otimes |gg\rangle\langle ee| y_{0,1}(t_f,t_m) e^{i\phi_0(t_f-t_m)}\right],
\end{aligned} \tag{6.55}$$

where

$$y_{a,b}(t_f,t_m) = \frac{x_{a,b}(t_f)}{x_{a,b}(t_m)}. \tag{6.56}$$

Unlike the case of one qubit, where we presented a very simple expression for the minimum eigenvalue of the dynamical matrix (Eq.(6.33)), directly related to the well know Loschmidt echo, in the case of two qubits the minimum eigenvalue is a non-trivial function of the parameters $y_{a,b}(t_f,t_m)$. However, working numerically we learn that the two-qubit case does not present any new characteristic that would result in a different behavior of the non-Markovianity in relation to the one-qubit case.

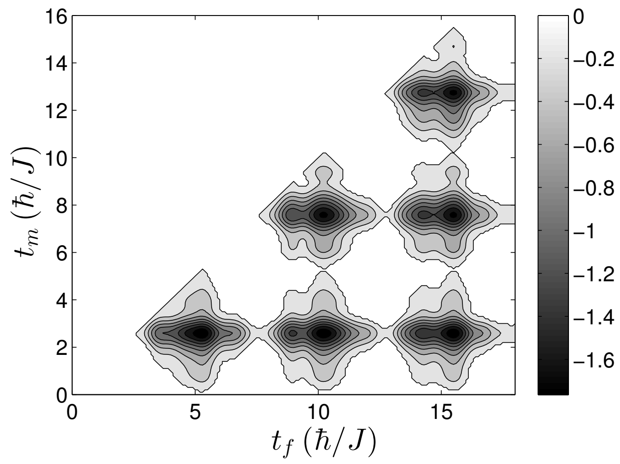

Figure 4 – Manifestation of the non-Markovianity by means of the most negative eigenvalue of the intermediate quantum map $D_{\Phi(t_f,t_m)}$ (greyscale), as a function of t_f and t_m, for a lattice with parameters $L = 10$, $\lambda = 0.5$ and $\delta = 0.5$.

6.4 Witnessing the non-Markovianity in the Ising Model: Finite size effects

Now we are equipped to characterize the dynamics of a qubit interacting with an environment governed by the Ising model (Fig.3). We consider lattices up to $L = 5 \times 10^5$ sites, and investigate the non-Markovianity in the vicinity of the critical point of the quantum Ising model, which is well known to be equal to $\lambda^* \equiv \lambda + \delta = 1$. Let us define a measure (η) of non-Markovianity as the minimum of the eigenvalues for the intermediate quantum dynamical matrix $D_{\Phi(t_t,t_m)}$ over all final times t_f and over all time partitions t_m, precisely:

$$\eta = \min_{\{t_f\}} \min_{\{t_m<t_f\}} eig\{D_{\Phi(t_t,t_m)}\}, \tag{6.57}$$

where eig is the set of eigenvalues of the intermediate dynamical matrix $D_{\Phi(t_f,t_m)}$. In order to exemplify such a non-Markovianity measure, we plot, in Fig.4, the smallest eigenvalue of the intermediate map as a function of the final (t_f) and intermediate (t_m) times, at the critical point of the Ising model, for a lattice with $L = 10$ sites. As the values of t_m and t_f are swept, the non-Markovian regions of the dynamics are revealed. Notice that the previously defined non-Markovianity measure is only based on the minimum eigenvalue of the dynamical matrix. One might expect, however, that the number of negative eigenvalues could influence the strength of the non-Markovianity. For our models under analysis, however, it seems not play any relevant effect: i) in the case of a single qubit it becomes trivial, since one can only have a single negative eigenvalue for the dynamical matrix; ii) and in the case of two-qubits we found that indeed there are cases where the dynamical matrix presents more than one negative eigenvalue, but its absolute value is always at least two orders of magnitude smaller than the absolute value of the minimum

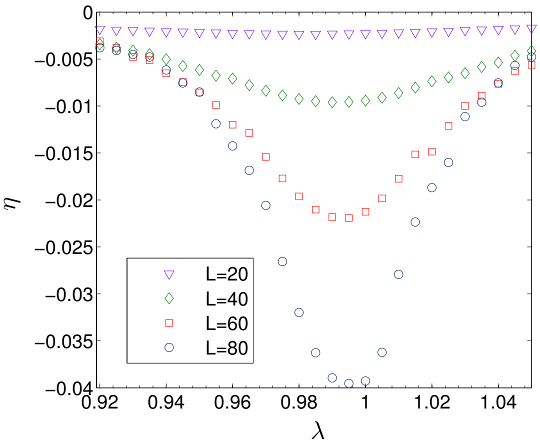

Figure 5 – The non-Markovianity measure η (Eq. (6.57)) in function of the transverse field λ, for $\delta = 0.01$, and for different lattice sizes (L), in the vicinity of the Ising model critical point.

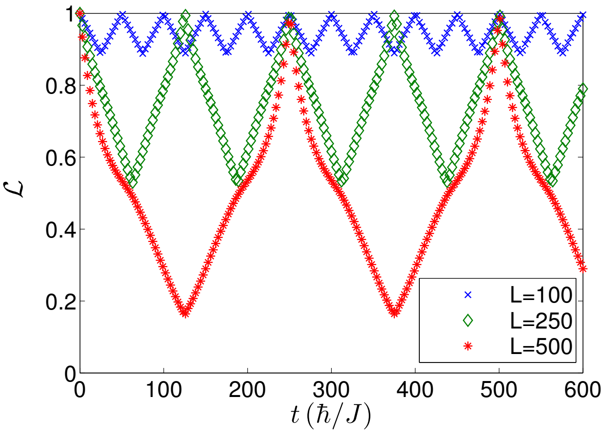

Figure 6 – The Loschmidt echo $\mathcal{L}$ (Eq. (37)) as a function of the time, at the critical point $\lambda^* = \lambda + \delta = 1$, with $\delta = 10^{-2}$, for different lattice sizes.

eigenvalue, and thus could be neglected. In Fig. 5, the non-Markovianity, quantified by η (Eq.(6.57)), is plotted against the transverse field (λ), in the vicinity of the Ising model critical point, for a fixed interaction coupling constant $\delta = 0.01$. We see that the larger the lattice, the larger the non-Markovianity. The most interesting feature shown in this figure is the maximum of non-Markovianity occurring precisely at the Ising model critical point. The behavior of this measure for larger lattice sizes, and in the thermodynamic limit, for the particular model studied in this section could also be inferred by the Loschmidt echo [24, 54, 59], from Eqs.(6.29) and (6.33). Note, however, that this equivalence between η and the Loschmidt echo is not necessarily true in general. In Fig. 6 ,we see the behavior of the Loschmidt echo, for different lattice sizes, at the critical point ($\lambda^* = 1$). We highlight some of its features: (i) the Loschmidt echo has an abrupt decay followed by a revival, with a time period "τ", which is proportional to the lattice size, $\tau \propto L$; (ii)

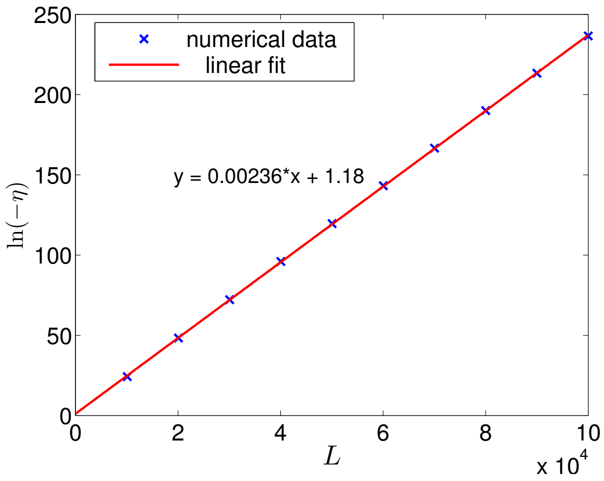

Figure 7 – Finite size scaling analysis: $ln(-\eta)$ as a function of L, for $L = 100$ to $L = 10^5$ sites, at the critical point $\lambda^* = 1$, with $\delta = 10^{-2}$. The linear fit reveals an exponential divergence of the non-Markovianity with the lattice size.

the difference between the minimum value of the decay (which we shall denote by $\mathcal{L}_{dec}$) and the maximal of the revival ($\mathcal{L}_{rev}$) becomes higher as we increase the lattice size. In this way, the non-Markovianity measure is simply given by $\eta = \mathcal{L}_{rev}/\mathcal{L}_{dec}$. Performing a finite-size scaling analysis, we see, in Fig. 7, that such a measure grows exponentially with lattice size, $\eta(\lambda^*) \propto exp(\alpha_* L)$, with $\alpha_* \sim 2.36 \times 10^{-3}$. Notice however that, despite such exponentially increasing behavior, at the thermodynamic limit the period τ diverges, and there is no revival of the function, consequently, the non-Markovianity pointed by this measure must be null: $\eta(\lambda^*) = 0$ for $L \to \infty$. It should be clear by now, that the non-Markovianity we have observed so far is due to the finite size of the lattice and the periodical dynamical revivals thereof. The behavior of the Loschmidt echo outside of the critical point is plotted in Fig. 8. We highlight some of its features: (i) due to finite size effects, we see that after a certain time (Γ), which increases with the lattice size ($\Gamma \propto L$), the function has a chaotic behavior; (ii) the "shape" of the function before the chaotic behavior is invariant with the lattice size, only its amplitude is changed. Performing then a finite-size scaling analysis, we see, in Fig. 9, that the non-Markovianity measure grows exponentially with lattice size, $\eta(\lambda^* - 0.1) \propto exp(\beta_l L)$, with $\beta_l \sim 1.43 \times 10^{-5}$, and $\eta(\lambda^* + 0.1) \propto exp(\beta_r L)$, with $\beta_r \sim 1.29 \times 10^{-5}$. Notice that although the measure also has an exponential scaling, as in the critical point, its exponential factors are much smaller, namely, $\beta_{l(r)}/\alpha_* \sim 10^{-2}$. In summary, we see that the non-Markovianity measure, for finite size systems, reaches its maximal at the critical point, whereas in the thermodynamic limit it is zero exactly at the critical point, and it diverges outside of the critical point. Assuming the environment described by the Ising Hamiltonian, the measure (η) (Eq.6.57) and the witness ($\mathcal{N}$) (Eq.6.60) for the non-Markovian dynamics for the two qubits have exactly the same behavior of the non-Markovian dynamics for one qubit. Here we will just

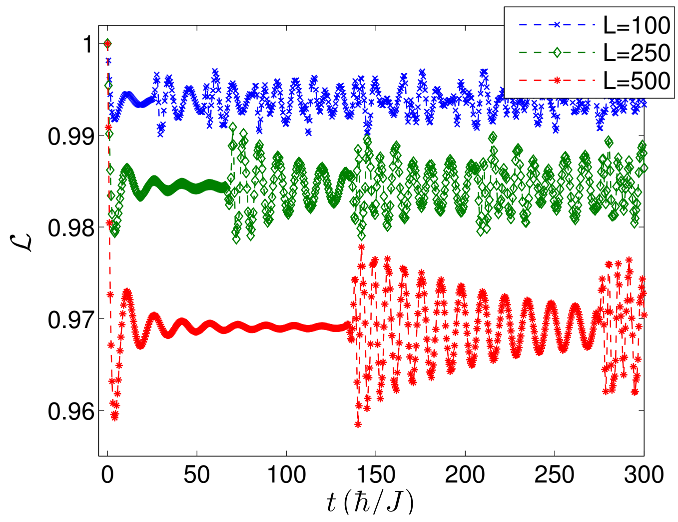

Figure 8 – The Loschmidt echo $\mathcal{L}$ (Eq. (37)) as a function of the time, outside of the critical point; more precisely, for $\lambda = \lambda^* - 0.1$, and $\delta = 10^{-2}$. The behavior for $\lambda = \lambda^* + 0.1$ is completely similar to this one.

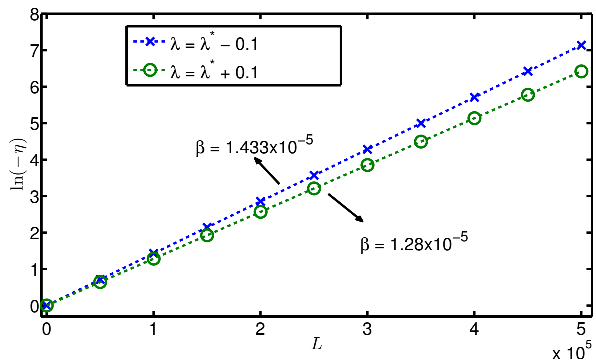

Figure 9 – Finite size scaling analysis: $ln(-\eta)$ as a function of L, for $L = 100$ to $L = 5\times10^5$ sites, outside of the critical point, more precisely, for $\lambda = \lambda^* \pm 0.1$, and $\delta = 10^{-2}$. The linear fit reveals an exponential divergence of the non-Markovianity with the lattice size, $(-\eta) \propto e^{\beta L}$.

highlight that the results do not depend on the parameters J_S and λ_S, and the choice of a Hamiltonian H_S for the open system (two spins) just adds a relative phase in its initial state, $|\chi(0)\rangle$, do not affecting (η) nor $(\mathcal{N})$.

6.5 Entanglement as a witness of non-Markovianity in the Ising model: Beyond finite size effects

In the previous section, we characterized the non-Markovianity by means of the non-positivity of the dynamical matrix expressed as a simple function of the Loschmidt echo. Now we will further explore the dynamics using a witness of non-Markovianity. Different non-Markovianity witnesses based on entanglement, or on bipartite correlations, have recently appeared in the literature [60–62]. We based our witness on the entanglement between the central qubit coupled to an ancilla. Our main concern shall be to detect the non-Markovianity that is not due to the finite lattice size. To see how this works, we assume a system S, with dynamics described by a map Φ, and a static ancillary system A. The system-ancilla evolution is given by,

$$\rho_{SA}(t_f) = \Phi(t_f, t_0) \otimes \mathbb{I}_A \left[\rho_{SA}(t_0)\right]. \tag{6.58}$$

Note that we have trivially extended the map to a separable one, with no local action over the ancilla. Entanglement cannot be generated by a local CP map. Assuming that the map $(\Phi(t_f, t_0))$ is divisible, in the sense discussed in section II, i.e., the intermediate map $(\Phi(t_f, t_m))$ is CP, $t_f > t_m > t_0$, we have:

$$\begin{aligned} E\left[\rho_{SA}(t_f)\right] &= E\left[(\Phi(t_f, t_m)\Phi(t_m, t_0) \otimes \mathbb{I}_A \left[\rho_{SA}(t_0)\right]\right] \\ &= E\left[(\Phi(t_f, t_m) \otimes \mathbb{I}_A \left[\rho_{SA}(t_m)\right]\right] \\ &\leq E\left[\rho_{SA}(t_m)\right], \end{aligned} \tag{6.59}$$

where $E\left[\rho_{SA}(t)\right]$ is some quantifier of bipartite entanglement. The above equation expresses the fact that entanglement is monotonically decreasing under local CP maps. In order to simplify notation, from now on we shall write $E\left[\rho_{SA}(t)\right] = E_{SA}(t)$. From Eq.(6.59) we have that a local CP divisible map leads to a monotonic decrease $\left(\frac{d}{dt}E_{SA}(t) \leq 0\right)$ of an entanglement measure of the system and ancilla. Therefore any violation of this monotonicity $\left(\frac{d}{dt}E_{SA}(t) > 0\right)$ is a sufficient criterion to witness non-Markovianity. Based on this idea, we can consider a witness $(\mathcal{N})$ of non-Markovianity in the form [60]:

$$\mathcal{N} = \int_{(d/dt)E_{SA}>0} \frac{d}{dt}E_{SA}(t), \tag{6.60}$$

such that $\mathcal{N} > 0$ for non-Markovian dynamics. Now consider system and ancilla as two qubits in an initial maximally entangled state, $|\phi^+\rangle = (|gg\rangle + |ee\rangle)/\sqrt{2}$. The system is under the action of the map given by Eq.(6.28), and the ancilla is let alone. We resume the study of our problem (Fig.3) under this new perspective. In Fig.6, we saw that at the critical point $\lambda^* = 1$, the revival of the Loschmidt echo, *i.e.* the revival of the coherence (recoherence), occurs in a time τ proportional to the lattice size. This non-Markovianity, due to the finite size of the lattice, allows for the open system to regain coherence and information from the environment. It is shown in Fig.10, where the entanglement measure (E_{SA}) is the negativity, for different lattice sizes at the critical point. The period of time in which the negativity increases is proportional to the lattice size, as expected. However, looking at outside of the critical point, in a time before the detection of non-Markovianity due to the size effect, we can witness non-Markovianity related to the characteristic features

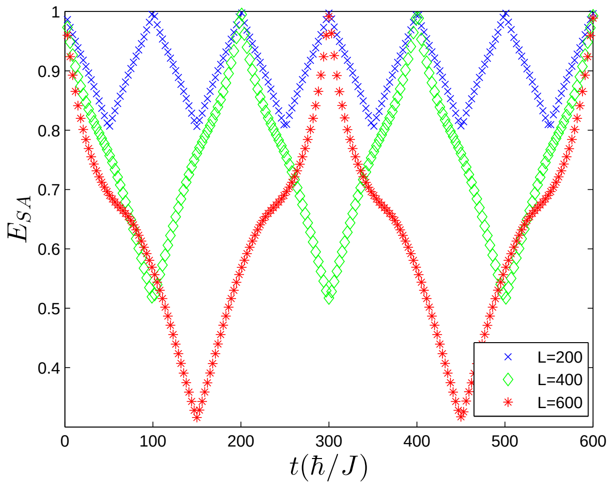

Figure 10 – The entanglement measure E_{SA}, quantified by the negativity as a function of time, at the critical point $\lambda^* = \lambda + \delta = 1$, and $\delta = 10^{-2}$, for different lattice sizes.

of the environment. This fact was observed before by means of the distinguishability of two quantum states [24, 54]. In Fig.11, we plot the negativity, for different lattice sizes, outside of the critical point, with fixed interaction coupling constant $\delta = 0.01$, in a time interval excluding the finite size effect. We see that even for different lattice sizes the negativity presents the same behavior, *i.e.* the period of time in which E_{SA} monotonically increases is the same. The degree of non-Markovianity, quantified by $\mathcal{N}$ (Eq.(6.60)), becomes higher as we increase the lattice size, $\mathcal{N} = \sum_n \left(E_{SA}(\tau_n^{max}) - E_{SA}(\tau_n^{min})\right)$, where $E_{SA}(\tau_n^{max})$ and $E_{SA}(\tau_n^{min})$ are the set of local maximum and minimum values of $E_{SA}(t)$. At this point one can note that the behavior of the negativity is similar to the Loschmidt echo, more precisely, in this specific case we have the interesting result:

$$E_{SA} = \sqrt{\mathcal{L}}. \tag{6.61}$$

The above equation follows from the definition of negativity, $E_{SA} = \sum_i \left(|p_i| - p_i\right)$, where the p_i are the four eigenvalues $\frac{1}{2}(-|x(t)|, |x(t)|, 1, 1)$ of $\rho_{SA}^{\Gamma}(t)$, which is the partial trace of $\rho_{SA}(t) = \Phi(t,0) \otimes \mathbb{I}_A \left[|\phi^+\rangle\langle\phi^+|\right] = (|g\rangle\langle g| \otimes |g\rangle\langle g| + |e\rangle\langle e| \otimes |e\rangle\langle e| + |g\rangle\langle e| \otimes |g\rangle\langle e| x(t)^* + |e\rangle\langle g| \otimes |e\rangle\langle g| x(t))/2$. In Fig.12, we see the witness of non-Markovianity, against the effective transverse field ($\lambda_{ef} = \lambda + \delta$), for two different lattice sizes, in an interval that avoids finite size effects. Increasing the field from small values, the witness decreases, until it gets close to the critical point, where it starts to increase, and suddenly drops to zero, exactly at the critical point ($\mathcal{N}(\lambda^*) = 0$). This is a very nice result to conclude this section, for the dynamics is known to be Markovian at the critical point.

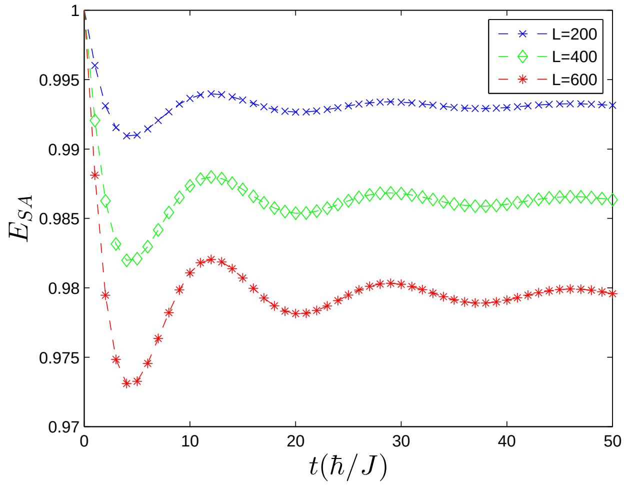

Figure 11 – The negativity E_{SA} as a function of time, outside of the critical point, for $\lambda = \lambda^* - 0.1$, and $\delta = 10^{-2}$, for different lattice sizes.

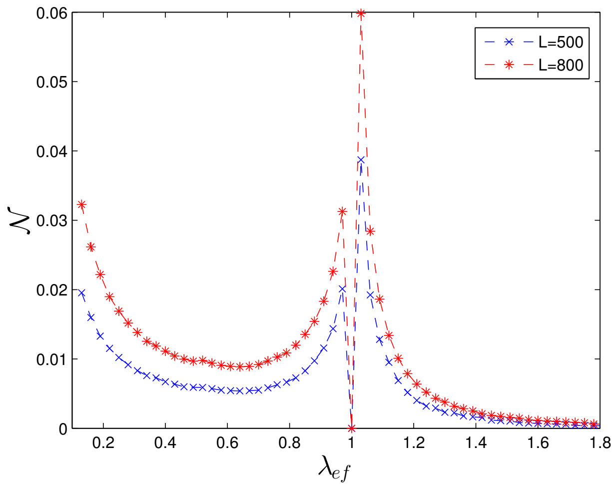

Figure 12 – The witness of non-Markovianity $\mathcal{N}$ as a function of the effective field $\lambda_{ef} = \lambda + \delta$, for $\delta = 0.01$, and in a time window excluding finite size effects.

7 Conclusion

In this thesis, we investigated subjects in two main topics of the theory of open quantum systems: we characterized the reduced dynamics of an initially correlated systems composed of indistinguishable fermions, we explored the concept of non-Markovianity in an open system (one or two qubits) under the influence of an environment modeled by the Ising model with transverse field.

In systems of indistinguishable fermions, antisymmetrization eliminates the notion of separability, and the very concept of correlation, which is an important ingredient in obtaining CP maps for open systems, becomes subtle. We showed that it is possible to write a CP map for a single fermion, which is part of a system on N indistinguishable particles, for sets of initial global states with no quantumness of correlation. We also illustrated our formalism with examples of maps corresponding to a non-interacting and an interacting Hamiltonian of two fermions. The extension of our formalism to subsystems with more than one indistinguishable particle, and for the case of bosons, presents no difficulty. As many properties of many-body Hamiltonians can be inferred from the single particle reduced state, an interesting investigation would be if any computational gain could be obtained by the employment of the formalism developed in chapter 4. As an example, in order to study the phase transition of a given model we may explore the dynamical map of one particle obtained from the initial state of the N fermions in the ground state of a Hamiltonian without interaction, consequently a state of one slater determinant that can be obtained analytically, undergoing an adiabatic evolution leading to the ground state of the target Hamiltonian, with ground state presenting phase transition of interest.

We derived the analytical expression for the Kraus representation of the map corresponding to the evolution of one and two qubits interacting with an environment represented by a general quadratic fermionic Hamiltonian. We concluded that the non-Markovian dynamics of two qubits interacting with the Ising environment does not present any new feature in relation to the dynamics of one qubit. We introduced simple functions to check the non-Markovianity of the dynamics. For the particular case of the Ising environment, we investigated the dynamics of one qubit interacting with lattices up to 10^5 sites. We quantified the non-Markovianity by the most negative eigenvalue (η - Eq.6.57) of the dynamical matrix, and obtained that, for finite size systems, it reaches its maximum at the critical point, whereas in the thermodynamic limit it is zero exactly at the critical point, diverging outside of the critical point. We also quantified the non-Markovianity using an entanglement based approach ($\mathcal{N}$ - Eq.6.60). We showed, in the case of one qubit interacting with Ising model, that the non-Markovianity measures we introduced are simple functions of the Loschmidt echo. Finally, we clearly identified two kinds of non-Markovianity, one due to the finite size of the environment, and another intrinsic of the Ising Hamiltonian, and we were able to quantify both.

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Appendix

APPENDIX A – Dynamical Map for Single-Fermion Reduced State - General Case with Initial Mixed States

A.1 System of Two Fermions

Consider a set of mixed quantum states in the antisymmetric space of $L+1$ modes and two fermions, $\rho(0) \in \mathcal{D}(\mathcal{F}_2^{L+1})$, written in a basis of Slater determinants:

$$\mathcal{D}_2^p = \left\{ \rho(0) = \sum_{\mu\in\Sigma, k\in\Gamma} p_\mu q_k a_\mu^\dagger a_k^\dagger |0\rangle\langle 0| a_\mu a_k \;\middle|\; p \text{ fixed} \right\}, \tag{A.1}$$

where $\sum_{\mu\in\Sigma} p_\mu = \sum_{k\in\Gamma} q_k = 1$, with both Σ and Γ finite, and disjoint, $\Sigma \cap \Gamma = \emptyset$. Let $|\Sigma| = d$, $|\Gamma| = L+1-d$, and $\mathbb{Z}_{L+1} = \{0, 1, \ldots, L\}$, we took the d elements of Σ from $\mathbb{Z}_{L+1}$, and the set Γ as $\mathbb{Z}_d \setminus \Sigma$. Tracing out one fermion from $\mathcal{D}_2^p$, we obtain a set of single-fermion reduced state,

$$\mathcal{D}_{r(2)}^p = \left\{ \rho_r(0) = \frac{1}{2}\sum_{k\in\Gamma} q_k a_k^\dagger |0\rangle\langle 0| a_k + \frac{1}{2}\sum_{\mu\in\Sigma} p_\mu a_\mu^\dagger |0\rangle\langle 0| a_\mu \;\middle|\; p \text{ fixed} \right\}. \tag{A.2}$$

Definition 2. *A CP map Φ_t^p, describing the dynamics of the single particle reduced state $\rho_r(0) \in \mathcal{D}_{r(2)}^p$, can be written in Kraus representation as:*

$$\Phi_t^p[\rho_r(0)] = \sum_{j=0}^{L} \sum_{\mu\in\Sigma} K_{j,\mu}^p \rho_r(0) K_{j,\mu}^{p\dagger}, \tag{A.3}$$

with the Kraus operators:

$$K_{l,\mu}^p = f_l U_t {a_\mu}^\dagger \sqrt{p_\mu} \prod_{m\in\Sigma} \left(1 - a_m^\dagger a_m\right), \tag{A.4}$$

Proof. The one-particle reduced dynamics can be expressed as $\rho_r(t) = Tr_1(U_t\rho(0)U_t^\dagger)$:

$$\begin{aligned}
&\rho_r(t) = \\
&= \frac{1}{2}\sum_{k=0}^{L} f_l U_t \left(\sum_{\mu\in\Sigma,k\in\Gamma} p_\mu q_k a_\mu^\dagger a_k^\dagger |0\rangle\langle 0| a_\mu a_k\right) U_t^\dagger f_l^\dagger \\
&= \sum_{l=0}^{L}\sum_{\mu\in\Sigma} \sqrt{p_\mu} f_l U_t a_\mu^\dagger \left(\frac{1}{2}\sum_{k\in\Gamma} q_k a_k^\dagger |0\rangle\langle 0| a_k\right) \times \\
&\sqrt{p_\mu} a_\mu U_t^\dagger f_l^\dagger .
\end{aligned} \tag{A.5}$$

Defining an operator $\prod_{m\in\Sigma}\left(1 - a_m^\dagger a_m\right)$ that annihilates fermions in Σ, and leaves states unchanged otherwise, we can write

$$\begin{aligned}
&\rho_r(t) = \\
&= \sum_{l=0}^{L}\sum_{\mu\in\Sigma} \sqrt{p_\mu} f_l U_t a_\mu^\dagger \prod_{m\in\Sigma}\left(1 - a_m^\dagger a_m\right) \times \\
&\left(\frac{1}{2}\sum_{k\in\Gamma} q_k a_k^\dagger |0\rangle\langle 0| a_k\right) \prod_{m\in\Sigma}\left(1 - a_m^\dagger a_m\right) a_\mu U_t^\dagger f_l^\dagger \sqrt{p_\mu} .
\end{aligned} \tag{A.6}$$

Note that

$$\prod_{m\in\Sigma}\left(1 - a_m^\dagger a_m\right)\left(\frac{1}{2}\sum_{j\in\Sigma} p_j a_j^\dagger |0\rangle\langle 0| a_j\right) = 0. \tag{A.7}$$

Adding Eq.(A.7) to Eq.(A.6), Definition 2 is proven:

$$\begin{aligned}
\rho_r(t) &= \sum_{l=0}^{L}\sum_{\mu\in\Sigma} f_l U_t a_\mu^\dagger \sqrt{p_\mu} \prod_{m\in\Sigma}\left(1 - a_m^\dagger a_m\right) \\
&\quad \times \left(\frac{1}{2}\sum_{k\in\Gamma} q_k a_k^\dagger |0\rangle\langle 0| a_k + \frac{1}{2}\sum_{j\in\Sigma} p_j a_j^\dagger |0\rangle\langle 0| a_j\right) \\
&\quad \times \prod_{m\in\Sigma}\left(1 - a_m^\dagger a_m\right) \sqrt{p_\mu} a_\mu U_t^\dagger f_l^\dagger \\
&= \sum_{l=0}^{L}\sum_{\mu\in\Sigma} K_{l,\mu}^{p} \rho_r(0) K_{l,\mu}^{\dagger p} .
\end{aligned} \tag{A.8}$$

□

A.2 System of N-Fermions

Consider a set of states $\rho \in \mathcal{D}(\mathcal{F}_N^{L+1})$, with no quantumness,

$$\mathcal{D}_N^p = \left\{ \rho(0) = \sum_{\vec{\mu}\in\vec{\Sigma}} \sum_{k\in\Gamma} p_{\vec{\mu}} q_k \times a_{\vec{\mu}} a_k |0\rangle\langle 0| a_k a_{\vec{\mu}} \;\middle|\; p \text{ fixed} \right\}, \tag{A.9}$$

where $\vec{\mu} = (\mu_1, \ldots, \mu_{N-1})$, $\vec{\Sigma} = (\Sigma_1, \ldots, \Sigma_{N-1})$ are $N-1$-tuples, and $p_{\vec{\mu}}$, q_k are probability distributions. The sets Σ_j and Γ are finite, and disjoint $\Sigma_j \cap \Gamma = \emptyset\ \forall j$. With $\left|\vec{\Sigma} = \cup_{i=1}^{N-1}\Sigma_i\right| = d$, $|\Gamma| = L+1-d$, and $\mathbb{Z}_{L+1} = \{0, 1, \ldots, L\}$, we took the d elements of $\cup_{i=1}^{N-1}\Sigma_i$ from $\mathbb{Z}_{L+1}$, and the set Γ as $\mathbb{Z}_d \setminus \cup_{i=1}^{N-1}\Sigma_i$. Note that d is the number of accessible modes for $N-1$ fermions, thus $d \geq N-1$.

Tracing $N-1$ fermions out from (A.9), we obtain the set of single-fermion reduced states $\{\rho_r(0)\}$:

$$\mathcal{D}_{r(N)}^p = \left\{ \rho_r(0) = \frac{1}{N}\sum_{k\in\Gamma} q_k a_k^\dagger |0\rangle\langle 0| a_k + \frac{1}{N}\sum_{j=1}^{N-1}\sum_{\mu_j\in\Sigma_j} p_{\mu_j} a_{\mu_j}^\dagger |0\rangle\langle 0| a_{\mu_j} \;\middle|\; p \text{ fixed} \right\}, \tag{A.10}$$

where $p_{\mu_j} = \sum_{\vec{\mu}\setminus\mu_j} p_{\vec{\mu}}$ is the marginal distribution.

Definition 3. *A CP map Φ_t^p describing the dynamics of the single particle reduced state $\rho_r(0) \in \mathcal{S}_{r(N)}^p$, can be written in Kraus representation as:*

$$\Phi_t^p[\rho_r(0)] = \sum_{\vec{l},\vec{\mu}}^{L} K_{\vec{l},\vec{\mu}}^p \rho_r(0) K_{\vec{l},\vec{\mu}}^{p\dagger}, \tag{A.11}$$

with the Kraus operators:

$$K_{\vec{l},\vec{\mu}}^p = \sqrt{p_\mu} f_{\vec{l}}\, U a_{\vec{\mu}}^\dagger \prod_{m\in\cup_{i=1}^{N-1}\Sigma_i} \left(1 - a_m^\dagger a_m\right). \tag{A.12}$$

The proof of Definition 3 is *mutatis mutandis* the same performed for Definition 2.

APPENDIX B – Norm Bound

B.1 Fermionic System

Theorem 1. *Consider two maps Φ and Λ, with Kraus operators $K_j = f_j U a_\mu$ and $E_j = f_j U V a_\mu$, respectively. Then the following inequality holds:*

$$\begin{aligned}&\|D_\Phi - D_\Lambda\|_1 \leq \\ &d^2 L^2 \sup_{a^\dagger_{\vec{k}}|0\rangle\langle 0|a_{\vec{k}'} \in \mathcal{F}_2^{L+1}} \| \left(a^\dagger_{\vec{k}}|0\rangle\langle 0|a_{\vec{k}'} - V^T a^\dagger_{\vec{k}}|0\rangle\langle 0|a_{\vec{k}'} V^* \right) \|_1,\end{aligned} \tag{B.1}$$

where d is the dimension of $\mathcal{F}_2^{L+1}$, $\vec{k} = (k_1, k_2)$ is a 2-tuple indicating the modes occupied by a pair of fermions, with $k_i = 0, \cdots, L$, and V is a unitary operator, $V : \mathcal{D}(\mathcal{F}_2^{L+1}) \to \mathcal{D}(\mathcal{F}_2^{L+1})$.

Proof. Writing the dynamical matrix of a map Φ in terms of the Kraus operators $\{K_j\}$:

$$D_\Phi = \sum_j \mathrm{vec}(K_j)\,\mathrm{vec}(K_j)^\dagger\,, \tag{B.2}$$

where the vec operation is defined by $\mathrm{vec}(|x\rangle\langle y|) = |x\rangle \otimes |y\rangle$, we obtain:

$$\begin{aligned}&\|D_\Phi - D_\Lambda\|_1 = \\ &= \| \sum_j \left(\mathrm{vec}(K_j)\,\mathrm{vec}(K_j)^\dagger - \mathrm{vec}(E_j)\,\mathrm{vec}(E_j)^\dagger \right) \|_1 \\ &= \| \sum_j \left(\mathrm{vec}(f_j U a_\mu)\,\mathrm{vec}(f_j U a_\mu)^\dagger - \right. \\ &\quad \left. \mathrm{vec}(a_j U V a_\mu)\,\mathrm{vec}(f_j U V a_\mu)^\dagger \right) \|_1.\end{aligned} \tag{B.3}$$

Using the following identity for matrices:

$$\mathrm{vec}(ABC) = \left(A \otimes C^T \right) \mathrm{vec}(B)\,, \tag{B.4}$$

we have,

$$\begin{aligned}&\|D_\Phi - D_\Lambda\|_1 = \\ &= \| \sum_j \left(f_j \otimes a^*_\mu \mathrm{vec}(U)\,\mathrm{vec}(U)^\dagger\, f^\dagger_j \otimes a^T_\mu - \right. \\ &\quad \left. f_j \otimes a^*_\mu V^T \mathrm{vec}(U)\,\mathrm{vec}(U)^\dagger\, f^\dagger_j \otimes V^* a^T_\mu \right) \|_1.\end{aligned} \tag{B.5}$$

With the unitary operator U written as,

$$U = \sum_{\vec{k},\vec{k}'} u_{\vec{k},\vec{k}'} a^{\dagger}_{\vec{k}} |0\rangle\langle 0| a_{\vec{k}'} \tag{B.6}$$

where $\vec{k} = (k_1, k_2)$, Eq.(B.5) becomes:

$$\begin{aligned}
&\|D_\Phi - D_\Lambda\|_1 = \\
&= \| \sum_j \sum_{\vec{k},\vec{k}'\vec{l},\vec{l}'} u_{\vec{k},\vec{k}'} u^*_{\vec{l},\vec{l}'} \left[\left(f_j a^{\dagger}_{\vec{k}} |0\rangle \otimes a^*_\mu a^{\dagger}_{\vec{k}'} |0\rangle \right) \times \right. \\
&\left(\langle 0| a_{\vec{l}} f^{\dagger}_j \otimes \langle 0| a_{\vec{l}'} a^T_\mu \right) - \left(f_j a^{\dagger}_{\vec{k}} |0\rangle \otimes a^*_\mu V^T a^{\dagger}_{\vec{k}'} |0\rangle \right) \times \\
&\left. \left(\langle 0| a_{\vec{l}} f^{\dagger}_j \otimes \langle 0| a_{\vec{l}'} V^* a^T_\mu \right) \right] \|_1 \\
&= \| \sum_{\vec{k},\vec{k}'\vec{l},\vec{l}'} u_{\vec{k},\vec{k}'} u^*_{\vec{l},\vec{l}'} \left[\sum_j \left(f_j a^{\dagger}_{\vec{k}} |0\rangle\langle 0| a_{\vec{l}} f^{\dagger}_j \right) \otimes \right. \\
&\left. \left(a^*_\mu a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} a^T_\mu - a^*_\mu V^T a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} V^* a^T_\mu \right) \right] \|_1 .
\end{aligned} \tag{B.7}$$

Using some norm properties, as triangle inequality ($\|A + B\| \leq \|A\| + \|B\|$), positive scalability ($\|\alpha A\| = |\alpha| \|A\|,\ \alpha \in \mathbb{C}$), and tensor product ($\|A_1 \otimes A_2\| = \|A_1\| \|A_2\|$) and the definition of fermionic partial trace of one particle, we can write:

$$\begin{aligned}
&\|D_\Phi - D_\Lambda\|_1 \leq \\
&\sum_{\vec{k},\vec{k}'\vec{l},\vec{l}'} \left| u_{\vec{k},\vec{k}'} u^*_{\vec{l},\vec{l}'} \right| \|Tr_1 \left(a^{\dagger}_{\vec{k}} |0\rangle\langle 0| a_{\vec{l}} \right) \|_1 \times \\
&\|a^*_\mu \left(a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} - V^T a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} V^* \right) a^T_\mu \|_1 .
\end{aligned} \tag{B.8}$$

As the trace norm is non-increasing under partial trace ($\|Tr_{\mathcal{H}_{A_2}}(A)\|_1 \leq \|A\|_1$), is sub-multiplicative ($\|AB\|_1 \leq \|A\|_1 \|B\|_1$), and we also have $\|A\|_1 = \|A^\dagger\|_1 = \|A^T\|_1 = \|A^*\|_1$:

$$\|D_\Phi - D_\Lambda\|_1 \leq \tag{B.9}$$

$$\begin{aligned}
&\sum_{\vec{k},\vec{k}'\vec{l},\vec{l}'} \left| u_{\vec{k},\vec{k}'} u^*_{\vec{l},\vec{l}'} \right| \|a^{\dagger}_{\vec{k}} |0\rangle\langle 0| a_{\vec{l}} \|_1 \times \\
&\| \left(a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} - V^T a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} V^* \right) \|_1 \|a_\mu\|_1^2 .
\end{aligned} \tag{B.10}$$

As $\|a^{\dagger}_{\vec{k}} |0\rangle\langle 0| a_{\vec{l}}\|_1 = Tr\sqrt{a^{\dagger}_{\vec{l}} |0\rangle\langle 0| a_{\vec{l}}} = 1$, and $\|a_\mu\|_1 = Tr\sqrt{n_\mu} = L$ is the number of states $\{a^{\dagger}_{\vec{k}} |0\rangle\}$ with occupied mode μ:

$$\begin{aligned}
&\|D_\Phi - D_\Lambda\|_1 \leq \\
&L^2 \sum_{\vec{k},\vec{k}'\vec{l},\vec{l}'} \sqrt{u_{\vec{k},\vec{k}'} u^*_{\vec{l},\vec{l}'} u^*_{\vec{k},\vec{k}'} u_{\vec{l},\vec{l}'}} \times \\
&\| \left(a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} - V^T a^{\dagger}_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} V^* \right) \|_1 .
\end{aligned} \tag{B.11}$$

From the definition of unitary operators we have, $\sum_k u^*_{i,k} u_{j,k} = \sum_k u^*_{k,i} u_{k,j} = \delta_{i,j}$, therefore:

$$\begin{aligned} &\|D_\Phi - D_\Lambda\|_1 \leq \\ &L^2 \sum_{\vec{k}'\vec{l}'} \| \left(a^\dagger_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} - V^T a^\dagger_{\vec{k}'} |0\rangle\langle 0| a_{\vec{l}'} V^* \right) \|_1. \end{aligned} \tag{B.12}$$

Finally,

$$\begin{aligned} &\|D_\Phi - D_\Lambda\|_1 \leq \\ &d^2 L^2 \sup_{a^\dagger_{\vec{k}}|0\rangle\langle 0|a_{\vec{k}'} \in \mathcal{F}_2^{L+1}} \| \left(a^\dagger_{\vec{k}} |0\rangle\langle 0| a_{\vec{k}'} - V^T a^\dagger_{\vec{k}} |0\rangle\langle 0| a_{\vec{k}'} V^* \right) \|_1. \end{aligned} \tag{B.13}$$

□

B.2 System of Distinguishable Particles

Theorem 2. *Assume two maps* Φ *and* Λ*, with Kraus operators* $\{K_a = \langle a|U_{SE}|0\rangle\}_a$ *and* $\{E_a = \langle a|U_{SE}(\mathbb{I}_S \otimes V_E)|0\rangle\}_a$*, respectively. Then the following inequality holds:*

$$\|D_\Phi - D_\Lambda\|_1 \leq d_S^2 \||0\rangle\langle 0| - V_E|0\rangle\langle 0|V_E^\dagger\|_1, \tag{B.14}$$

where d_S *is the dimension of the Hilbert space of the system* S*.*

Proof. Writing the dynamical matrix of a map Φ in the Choi representation:

$$D_\Phi = \sum_{i,j=1}^{d_S} \Phi(|i\rangle\langle j|) \otimes |i\rangle\langle j|, \tag{B.15}$$

we obtain:

$$\begin{aligned} &\|D_\Phi - D_\Lambda\|_1 = \\ &= \frac{1}{d_S^2} \| \sum_{i,j=1}^{d_S} \Phi(|i\rangle\langle j|) \otimes |i\rangle\langle j| - \sum_{i,j=1}^{d_S} \Lambda(|i\rangle\langle j|) \otimes |i\rangle\langle j| \|_1 \\ &= \| \sum_{i,j=1}^{d_S} \left\{ \sum_a K_a |i\rangle\langle j| K_a^\dagger - E_a |i\rangle\langle j| E_a^\dagger \right\} \otimes |i\rangle\langle j| \|_1 \\ &\leq \sum_{i,j=1}^{d_S} \| \left\{ \sum_a K_a |i\rangle\langle j| K_a^\dagger - E_a |i\rangle\langle j| E_a^\dagger \right\} \otimes |i\rangle\langle j| \|_1. \end{aligned} \tag{B.16}$$

Thus, by the definition of Kraus operators above:

$$\begin{aligned} &K_a |i\rangle\langle j| K_a^\dagger - E_a |i\rangle\langle j| E_a^\dagger = \\ &= \langle a|_E \left\{ U_{SE} |i\rangle\langle j|_S \otimes (|0\rangle\langle 0|_E - V|0\rangle\langle 0|_E V^\dagger) U_{SE}^\dagger \right\} |a\rangle_E, \end{aligned} \tag{B.17}$$

substituting in Eq.(B.16), and using $\|A \otimes B\| = \|A\|\|B\|$:

$$\begin{aligned}
&\|D_\Phi - D_\Lambda\|_1 \leq \\
&d_S^2 \| \left\{ \sum_a \langle a| \left[U_{SE}|i\rangle\langle j| \otimes (|0\rangle\langle 0| - V|0\rangle\langle 0|V^\dagger) U_{SE}^\dagger \right] |a\rangle \right\} \|_1 \\
&= d_S^2 \| \left\{ \left[U_{SE}|i\rangle\langle j| \otimes (|0\rangle\langle 0| - V|0\rangle\langle 0|V^\dagger) U_{SE}^\dagger \right] \right\} \|_1,
\end{aligned} \tag{B.18}$$

where we used that $\sum_a \langle a|A|a\rangle = \mathrm{Tr}_E(A)$. Finally, as trace distance is invariant under unitary operations, the statement is proved:

$$\|D_\Phi - D_\Lambda\|_1 \leq d_S^2 \|(|0\rangle\langle 0| - V|0\rangle\langle 0|V^\dagger)\|_1. \tag{B.19}$$

$\square$