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The Theory of Non-Markovian Open Quantum Systems

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The Theory of Non-Markovian Open Quantum Systems

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The Theory of Non-Markovian Open Quantum Systems

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We study the role of correlations with the environment as the source of non-Markovian quantum evolutions. We first focus on the impact that correlations with the environment can have on the dynamical map that evolve the system. We expand the set of initial states of a system and its environment that are known to guarantee completely positive reduced dynamics for the system when the combined state evolves unitarily. We characterize the correlations in the initial state in terms of its quantum discord. The induced maps can be not completely positive when quantum correlations including, but not limited to, entanglement are present. We discuss the implications and limitations of the Markov approximation necessary to derive the Kossakowski-Lindblad master equation. A generalized non-Markovian master equation is derived from the dynamical map of systems correlated with their environment. The physical meaning of not completely positive maps is studied to obtain a

consistent theory of non-Markovian quantum dynamics. These are associated to inverse maps necessary to establish correlations and they give rise to a canonical embedding map that is local in time. This master equation goes beyond the Kossakowski-Lindblad master equation. Non-equilibrium quantum thermodynamics can be be studied within this theory. Through out this discussion, the general dynamics of two interacting qubits is used as an example for illustrations.

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Chapter 1

Introduction

It is natural to follow our classical mechanical intuition, with particles and trajectories and full knowledge of their position and momentum. On the other hand, quantum mechanical phenomena dominate in the realm of scales smaller than our daily experience. Quantum entanglement, where correlations go beyond what is described by the sampling assumption of classical probability theory, is the iconic concept that illustrates the counter-intuitive aspect of quantum mechanics. How can both worlds, the classical and quantum world, be connected?

To go from the realm where quantum effects are of major importance to the macroscopic world we can consider the phenomena of decoherence. Decoherence is the loss of quantum mechanical information. Quantum information seems to be inherently more fragile than classical information. For example, although classical information can be copied at will, as it is done in personal computers for its storage and transmission, quantum information cannot be copied as a consequence of the linearity of quantum mechanics.

The interdisciplinary field of quantum computation has applied algorithm analysis from computer science to a new kind of computer that would

exploit quantum mechanical effects in order to get algorithms that are in principle faster than anything that can be done by a classical computer. This challenges current encryption schemes, while also suggests stronger encryption protocols. A quantum computer will impact our lives by revolutionizing digital communication and information security.

However, the fragility of quantum mechanical systems against decoherence has proven to be a difficult challenge to overcome. This has provided the motivation to reexamine fundamental quantum mechanical phenomena. Without the understanding of decoherence, it cannot be controlled. Without harnessing decoherence, a quantum computer cannot be build.

A main approach to the study of decoherence is to assume that it is not possible to know all the parameters necessary to represent the evolution of a state. The known part is treated as a system and the unknown parameters as the environment. Thus, the system is treated as an open quantum system, where information can go outside it and into the environment. This is a reasonable model; in practice it is impossible to fully isolate a system from its environment. The evolution is now given by a dynamical map, first introduced in 1961 by Sudarshan et al. [1].

The Kossakowski-Lindblad master equation approach to open quantum system uses the Markov approximation to describe irreversibility in quantum systems [2]. The Markov approximation implies that to know the state of the system at a later time it is only necessary to know the state at the present time. This requires that the environment, and correlations with it, do not change.

In this work we study open quantum systems beyond this approximation, allowing for correlations with the environment that evolve in time.

1.1 Arrangement of this Dissertation

The fundamentals of stochastic processes are discussed in Chapter 2. We review the theory of classical stochastic processes and the definitions of Markovian and non-Markovian stochastic processes. The theory of quantum dynamical maps is treated in a similar context. Different forms for the dynamical map and their properties are reviewed, including the role of states uncorrelated with their environment. A simple example of a dynamical map is studied.

The general interaction between two initially uncorrelated qubits (two-dimensional quantum systems), is studied in Chapter 3. The total evolution of the state, as well as the partial evolution of each of the qubits is calculated using the dynamical maps formalism.

In Chapter 4 we review two models of decoherence. First we discuss the Rau refreshing model inspired after Boltzmann's collision model. We study the effects of the approximations that yield the much simpler Markovian Kossakowksi-Lindblad master equation. We derive this master equation from the dynamical maps formalism and discuss all the necessary approximations and assumptions made and how they restrict its validity.

Chapter 5 is about the consequences of having correlations with the

environment and the mathematical properties of the dynamical maps that come from them. The correlations limit the valid domain where the dynamical map can act on. We study examples of initially correlated states. We also show how different kinds of correlations, either classical or quantum, can lead to maps with positive or negative eigenvalues correspondingly.

In Chapter 6 we define a consistent way to treat dynamics that come from initially correlated states, and their relationship to the history of the evolution. We discuss the significance of inverse maps and how they give an interpretation to the reduced valid domain of a map. A canonical dynamical map is defined in order to treat dynamical map and their inverses on an equal level. With the canonical dynamical map, a canonical embedding map can be defined that connects the dynamics of the total system-environment state with the reduced state and vice-versa, properly accounting for correlations with the environment at all times. An example is computed.

Chapter 7 contains the derivation of a non-Markovian master equation. With the aid of the canonical dynamical map and the embedding map, a consistent way of defining a master equation for correlated systems is described. This is more general than the Kossakowski-Lindblad master equation since no approximation is needed in order to derive it. This equation is fully reversible. An example is discussed, and its relationship to other master equation is studied.

In Chapter 8 we study the role of approximations to the non-Markovian master equation, and show how irreversibility can arise from them. Quantum

mechanical decays that deviate from exponential decay are described by means of an example and the connection to non-equilibrium quantum thermodynamics discussed.

The experimental implications of this work, concluding remarks and future directions are included in Chapter 9.

Chapter 2

Stochastic Processes

Physics is the study of matter and its motion; it is the study of the structure of space and time. To describe the change in time of physical variables we use equations of motion. An example is Hamilton's equations of motion in classical mechanics, where the change of the position and momentum variables is fully deterministic.

Probability theory, on the other hand, is suitable for phenomena where in principle or in practice the partial knowledge of the evolution makes it impossible to describe by a deterministic equation. Probability theory is applied to situations where it is not possible to exactly predict the outcome of a variable. Instead, all different possible outcomes are weighted by proper probabilistic weights that represent their likelihood. In this case, if the change of this probabilistic variable is desired, instead of a dynamical process a *stochastic process* is used.

The stochastic process approach to quantum mechanics was originated and developed by Sudarshan [1, 3–6]. The evolution is represented by a dynamical map and it is the most general form of a process that takes density

matrices into density matrices,

$$\rho_{rs} \rightarrow \rho'_{r's'} = \sum_{r,s} \mathfrak{B}_{r'r,s's}\ \rho_{rs}.$$

The dynamical map is of fundamental importance in the study of open quantum systems, and is central to the research presented in this dissertation.

In this chapter we review the theory of stochastic processes for quantum variables, focusing on the theory of dynamical maps and its connection to the reduced dynamics of a state.

2.1 Classical Stochastic Processes

We first review the properties of a classical stochastic process. We describe a classical probalistic variable with a vector $\overrightarrow{p}$, that in order to have a proper probabilistic interpretation must be composed of real parameters p_j where $\sum_j p_j = 1$. A classical probability vector $\overrightarrow{p}(i)$ can be evolved into another one, $\overrightarrow{p}(f)$, by means of a matrix $\mathfrak{M}$ using the equation

$$\overrightarrow{p}(i) \rightarrow \overrightarrow{p}(f) = \mathfrak{M} \cdot \overrightarrow{p}(i).$$

The probability vectors form a convex set; for a finite number of nonzero components it is a simplex. If the vectors are written in tensor notation, the evolution is fully determined by

$$p(f)_{r'} = \mathfrak{M}_{r',r} p(i)_r.$$

In this dissertation we will often use the convention that repeated indices imply a summation over them. Both $\overrightarrow{p}(i)$ and $\overrightarrow{p}(f)$ have the sum of their

nonnegative elements equal unity. Hence,

$$\sum_r \mathfrak{M}_{r',r} = 1.$$

If $\mathfrak{M}$ is treated as a map, it must have as its domain all probability vectors $\{\overrightarrow{p}(i)\}$, and as its image a subset of the domain. Matrices with these properties are called stochastic matrices. The only stochastic maps that are invertible for the whole domain are the permutations of the vertices of the simplex. These stochastic matrices whose inverse happen to be also a stochastic matrix correspond to maps whose domain and image are the whole set $\{\overrightarrow{p}\}$ and form a special subclass called bi-stochastic matrices. If an inverse is desired for more general cases, caution must be taken on where it acts. The inverse of a stochastic matrix $\widetilde{\mathfrak{M}}$, such that

$$\widetilde{\mathfrak{M}} \cdot \mathfrak{M} = \mathbb{I},$$

might itself not be a stochastic matrix. $\widetilde{\mathfrak{M}}$ is properly defined only on the subset of probability vectors of the form $\mathfrak{M} \cdot \overrightarrow{p}$ for all $\{\overrightarrow{p}\}$.

The probability vectors can be evolved as a process in time with a stochastic map,

$$\overrightarrow{p}(t_f) = \mathfrak{M}_{(t_f|t_i)} \cdot \overrightarrow{p}(t_i).$$

If $\overrightarrow{p}(t_f)$ depends only on the particular state $\overrightarrow{p}(t_i)$, it is said to be a Markov process. Markovian processes correspond to the loss of information in a mononotonic fashion. If to define the process $\mathfrak{N}$ for a time interval $[t_i \to t_f]$

other variables $\overrightarrow{r}(t_i)$ are needed, such that

$$\overrightarrow{p}(t_f) = \mathfrak{N}_{(t_f|t_i)}\Big(\overrightarrow{r}(t_i)\Big) \cdot \overrightarrow{p}(t_i),$$

the process is said to be non-Markovian. These additional variables can represent the state $\overrightarrow{p}(t)$ at other times $t \neq t_i$, and may be referred to as memory effects. In such a case, the knowledge of $\overrightarrow{p}(t)$ is the history needed to consistently define $\mathfrak{N}$.

A Markovian process in $\overrightarrow{q}$ can be made non-Markovian in $\overrightarrow{p}$ by reducing the space of known parameters:

$$\begin{aligned} &\textit{Markovian:} \qquad \overrightarrow{q}(t_f) = \mathfrak{M}_{(t_f|t_i)} \cdot \overrightarrow{q}(t_i) \\ &\qquad\quad \downarrow \\ &\textit{Non-Markovian:} \quad \overrightarrow{p}(t_f) = \mathfrak{N}_{(t_f|t_i)}\Big(\overrightarrow{r}(t_i)\Big) \cdot \overrightarrow{p}(t_i). \end{aligned}$$

On the other hand, a non-Markovian process $\mathfrak{N}$ may be mapped into a Markovian process $\mathfrak{M}$ by extending the space from $\overrightarrow{p}(t)$ to

$$\overrightarrow{q}(t) \equiv \Big\{\overrightarrow{p}(t), \overrightarrow{r}(t_i)\Big\}.$$

A physical example of this is the process of classical multiple scattering of particles. This is a Markovian evolution in position and momentum variables; if integrated over momentum variables, correlations with them are now folded into a memory kernel that leads to non-Markovian effects. A method that extends the space to get from non-Markovian phenomena to Markovian

by studying the direct time evolution of the motion of the particles was computed for scattering particles in [7]. In this dissertation we will study how to perform such extensions to open quantum systems.

2.2 Quantum Stochastic Processes

In order to generalize the notion of classical probability vectors to quantum mechanics we use the density matrix [8, 9]. A finite-dimensional density matrix ρ must have the following properties:

$$\mathrm{Tr}\,[\rho] = 1 \qquad \text{(Unit-trace)}, \tag{2.1a}$$

$$\rho = \rho^{\dagger} \qquad \text{(Hermiticity)}, \tag{2.1b}$$

$$u^{*}\,\rho\,u \geq 0 \qquad \text{(Non Negativity)}. \tag{2.1c}$$

which are necessary to ascribe a physical interpretation to a density matrix. Hermiticity guarantees real eigenvalues, non negativity that they are not negative, the unit-trace condition that the real eigenvalues add up to one and can be associated with probability weights.

If a density matrix is idem-potent, such that:

$$\rho = \rho^{2},$$

then it can be written using Dirac's notation [8],

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

and its said to be a *pure* state. $|\psi\rangle$ follows Schrödinger's equation of motion,

$$H(t)|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle.$$

This is the differential form of the equation:

$$|\psi(t)\rangle = U_{(t,0)}|\psi(0)\rangle, \quad U_{(t,0)} = \mathcal{T}_{\rightharpoonup}\ \exp\Big(-i\hbar\int_0^t H(s)ds\Big)$$

where $\mathcal{T}_{\rightharpoonup}$ is the time-ordering operator.[1]

In the density matrix formalism, similar equations can be written for the evolution,

$$\rho(t) = U_{(t,0)}\,\rho(0)\,U^{\dagger}_{(t,0)}$$

and its differential form,

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

is known as the von Neumann equation [9]. This formalism is analogous to the deterministic evolution from Hamilton's equations of motion. However, since we introduced density matrices as a generalization of a probability vector, we can also study their dynamics as a stochastic process [1, 3, 5]. Quantum stochastic processes can be represented in different forms with different mathematical properties.

2.2.1 $\mathfrak{A}$ Form

The most general quantum mechanical state is described by its density matrix ρ that must have unit-trace, Hermiticity, and non negative eigenvalues [9]. All these are modeled after the properties of classical probability vectors and allow us to interpret the expectation values of density matrices as physical

[1]For compactness, from now on we will use units such that $\hbar = 1$.

observables. Just like in the classical case, a quantum stochastic supermatrix $\mathfrak{A}$ can be defined to describe the most general linear evolution of an initial density matrix $\rho(i)$ to a final density matrix $\rho(f)$. This was first proposed by Sudarshan [1].

If we write the density matrices in terms of their indices, the quantum stochastic process can be made to act like its classical analogue by writing the density matrix as a vector $\overrightarrow{\rho}$ with two indices:

$$\rho(i)_{rs} \rightarrow \rho(f)_{r's'} = \mathfrak{A}_{r's',rs}\ \rho(i)_{rs}.$$

The quantum stochastic supermatrix has the properties:

$$\mathfrak{A}_{r'r',rs} = \delta_{r,s}, \tag{2.2a}$$

$$\mathfrak{A}_{s'r',sr} = \mathfrak{A}^*_{r's',rs}, \tag{2.2b}$$

$$x^*_{r'} x_{s'} \mathfrak{A}_{r's',rs} y_r y^*_s \geq 0. \tag{2.2c}$$

The first property guarantees the preservation of the trace, the second property preserves Hermiticity, while the last property imposes the condition that positive density matrices are mapped into positive density matrices and may be referred to as *positivity* [1]. In Chapter 5 we will study physical situations where the positivity condition will need to be relaxed. We observe that in this form the composition of two maps, $\mathfrak{A}' \star \mathfrak{A}$, is simply the matrix multiplication of their super matrices $\mathfrak{A}'_{r's',r''s''}\mathfrak{A}_{r''s'',rs}$.

Just like in the classical case, the inverse $\widetilde{\mathfrak{A}}$ can be defined. The matrix $\widetilde{\mathfrak{A}}$ is positive only on a convex domain; it should act only on a subset of all

density matrices. Its action is only well-behaved on the subset of density matrices of the form $\mathfrak{A} \cdot \overrightarrow{\rho}$ for all $\{\overrightarrow{\rho}\}$ and is defined only when $\mathfrak{A}$ is nonsingular. This subset is called the *compatibility domain* [10, 11]. Outside the compatibility domain the positivity (non negativity) of the density matrix need not be preserved by the inverse map.

2.2.2 $\mathfrak{B}$ Form

The properties of $\mathfrak{A}$ appear to be somewhat complicated; a simple redefinition (index exchange) can be used $\mathfrak{B}_{r'r,s's} \equiv \mathfrak{A}_{r's',rs}$ to obtain:

$$\mathfrak{B}_{r'r,r's} = \delta_{r,s}, \tag{2.3a}$$

$$\mathfrak{B}_{r'r,s's} = \mathfrak{B}^*_{s's,r'r}, \tag{2.3b}$$

$$x^*_{r'} y^*_r \mathfrak{B}_{r'r,s's} x_{s'} y_s \geq 0, \tag{2.3c}$$

corresponding to trace preservation, Hermiticity and positivity [1]. This simplifies the properties significantly; preserving Hermiticity is now guaranteed by the map $\mathfrak{B}$ itself being Hermitian. However, in this form the action of the superoperator $\mathfrak{B}$ is not as simple as matrix multiplication on a vector $\overrightarrow{\rho}$ as it was in the $\mathfrak{A}$ form. Instead, the map $\mathfrak{B}$ acts in the following manner:

$$\rho(i)_{rs} \rightarrow \rho(f)_{r's'} = \mathfrak{B}_{r'r,s's} \rho(i)_{rs},$$

or just

$$\rho(i) \rightarrow \rho(f) = \mathfrak{B} \rho(i)$$

for short. In this form, the composition of two maps $\mathfrak{B}' \star \mathfrak{B}$ is $\mathfrak{B}'_{r'r'',s's''} \mathfrak{B}_{r''r,s''s}$, which is not just matrix multiplication as it was in the $\mathfrak{A}$ form. The inverse

$\widetilde{\mathfrak{B}}$ can be calculated from $\widetilde{\mathfrak{A}}$ by exchanging the indices and inherits its compatibility domain.

2.2.3 Choi Form

Finally, the Choi representation of the map, as developed in [5, 12, 13], highlights some other properties. This form is obtained by decomposing $\mathfrak{B}$ into its eigenmatrices and real eigenvalues,

$$\mathfrak{B}_{r'r,s's}\rho(i)_{rs} = \sum_{\alpha} \lambda(\alpha)\, \mathrm{C}(\alpha)_{r'r}\, \rho(i)_{rs}\, \mathrm{C}^*(\alpha)_{ss'},$$

which expresses the action of the map as:

$$\rho(f) \equiv \sum_{\alpha} \lambda_\alpha \mathrm{C}_\alpha\, \rho(i)\, \mathrm{C}_\alpha^\dagger. \tag{2.4}$$

Note that $\mathrm{Tr}[\mathrm{C}_\alpha^\dagger \mathrm{C}_\beta] = 0$ for $\alpha \neq \beta$. Hermiticity of ρ is automatically preserved by the multiplication on the left and right. With the condition:

$$\sum_{\alpha} \lambda_\alpha \mathrm{C}_\alpha^\dagger \mathrm{C}_\alpha = \mathbb{I},$$

the trace of ρ is also preserved. The positivity condition is still only implicit. A stronger condition, *complete positivity*, is very natural now. Complete positivity is defined as having all non-negative eigenvalues $\lambda_\alpha \geq 0$ [5, 12, 13]. Complete positivity is a condition on the map itself, while positivity is a condition on the action of the map on density matrices. Much attention has been given to this class of maps, but confining quantum evolution to them has proven to be too restrictive [10, 11, 14–18]. Inverse maps are in general not positive, much less completely positive. In this dissertation we will use the $\mathfrak{A}$ and $\mathfrak{B}$

forms to show how the complete positivity condition is in general incompatible with non-Markovian open quantum systems.

2.2.4 Dynamical Maps of Open Quantum Systems

The evolution of the state of a closed quantum system is generated by a unitary operator[2],

$$U_{(t_f|t_i)} = e^{-i(t_f - t_i)H}.$$

The differential form of this evolution is given by the von Neumann equation,

$$\dot{\rho}(t) = -i\left[H, \rho(t)\right].$$

It can also be viewed as a stochastic evolution through a unitary map,

$$\mathfrak{U}_{(t_f|t_i)}\rho(t_i) \equiv U_{(t_f|t_i)}\ \rho(t_i)\ U^{\dagger}_{(t_f|t_i)} = \rho(t_f). \tag{2.5}$$

This map is completely positive. The inverse of this map,

$$\widetilde{\mathfrak{U}_{(t_i|t_f)}} \equiv \mathfrak{U}^{\dagger}_{(t_f|t_i)} = \mathfrak{U}_{(t_i|t_f)},$$

has as its compatibility domain the whole set of density matrices, making it bi-stochastic, that is, a map that preserves positivity for the whole domain and whose inverse does also the same.

We are interested in the evolution of an open quantum system where the total state might depend on variables that are accessible to us, the system

[2]For compactness, we assume a time independent Hamiltonian H, but the results also apply to the time dependent case.

$\mathcal{S}$, and some that are inaccessible, a finite-dimensional environment $\mathcal{E}$ [1]. The density matrix of the system space is found by tracing-out the environmental variables [5],

$$\eta^{\mathcal{S}} = \mathrm{Tr}_{\mathcal{E}} \left[\rho^{\mathcal{S}\mathcal{E}}\right].$$

From now on the total system-environment space will be denoted by ρ, while the reduced system state by η. Superscripts to indicate the system $\mathcal{S}$ and environment $\mathcal{E}$ will be suppressed when its meaning is clear.

If we only monitor the evolution of the system, it is in general non-unitary and best described by a dynamical map of the form:

$$\mathfrak{B}_{(t_f|t_i)}\eta(t_i) \equiv \mathrm{Tr}_{\mathcal{E}} \left[U_{(t_f|t_i)}\rho(t_i)U^{\dagger}_{(t_f|t_i)}\right] = \eta(t_f), \tag{2.6}$$

where $\eta(t_i) = \mathrm{Tr}_{\mathcal{E}}\left[\rho(t_i)\right]$. In the full space, the evolution is given by the unitary map $\mathfrak{U}$, while in the reduced space we get a more complicated evolution:

$$\begin{array}{ccc} \rho(t_i) & \longmapsto & \rho(t_f) = U_{(t_f|t_i)}\rho(t_i)U^{\dagger}_{(t_f|t_i)} \\ \downarrow & & \downarrow \\ \eta(t_i) & \dashrightarrow & \eta(t_f) = \mathrm{Tr}_{\mathcal{E}}\left[\rho(t_f)\right]. \end{array} \tag{2.7}$$

To go to the reduced space, or "down" $\downarrow$, we use the trace map

$$\mathfrak{T}\rho^{\mathcal{S}\mathcal{E}} \equiv \mathrm{Tr}_{\mathcal{E}}\rho^{\mathcal{S}\mathcal{E}} = \eta.$$

To go "up" to the higher dimensional total space, a map that inverts the trace such that,

$$\widetilde{\mathfrak{T}} \star \mathfrak{T}\rho^{\mathcal{S}\mathcal{E}} = \rho^{\mathcal{S}\mathcal{E}},$$

will need to be implemented. But, $\mathfrak{T}$ has a kernel, so defining $\widetilde{\mathfrak{T}}$ will need to account for it. Studying the physical implication of such a map is one of the main themes of this paper. With such a map, the dynamical map for the process from $\eta(t_i) \to \eta(t_f)$ can be expressed as the composition of three maps,

$$\mathfrak{B}_{(t_f|t_i)} \equiv \mathfrak{T} \star \mathfrak{U}_{(t_f|t_i)} \star \widetilde{\mathfrak{T}}. \tag{2.8}$$

First, the trace is inverted to go to the total space, then a unitary map evolves it and finally a trace reduces it to the system space. If $t_f = t_i$, there is no evolution and the map is just unity. Since the density matrices are restricted to a compact region, all linear maps have near recurrences in time. These are called Poincaré recurrences.

2.2.5 Initially Uncorrelated States and Complete Positivity

A standard assumption for the evolution of an open system of the form Eq. (2.6) is that the system and environment are in a Kronecker product,

$$\rho^{\mathcal{SE}}(t_i) = \eta^{\mathcal{S}}(t_i) \otimes \tau^{\mathcal{E}},$$

at the initial time. Uncoupling a system from its environment is in practice very difficult, and is not accomplished in many experiments [19]. It has been shown that completely positive maps can be seen as a contraction of the dynamics of $\eta^{\mathcal{S}}(t_i) \otimes \tau^{\mathcal{E}}$ [20]. If η is $N \times N$, the dimension of τ need be only $N^2 \times N^2$ or less, and lead to a map of the form Eq. (2.4) with non negative eigenvalues. This was first shown in [1, 5, 20], but here we follow a slightly different approach.

We can break the corresponding dynamical map into the composition, as in Eq. (2.8), of several completely positive maps. The reduction at the end of the evolution, $\mathfrak{T}$, and the unitary map $\mathfrak{U}$ are both completely positive. With the knowledge that at the initial time the system is uncorrelated from its environment, the map $\widetilde{\mathfrak{T}}$ can be defined as an embedding map $\mathfrak{E}$ [20] that takes the system state at the initial time, and embeds it into a system-environment space:

$$\widetilde{\mathfrak{T}}\Big(\eta(t_i)\Big) \equiv \mathfrak{E}_{t_i}\Big(\eta(t_i)\Big) = \eta(t_i) \otimes \tau. \tag{2.9}$$

Since τ has non negative eigenvalues, it can be written as

$$\mathfrak{E}\left(\eta\right) = \left(\mathbb{I}^{\mathcal{S}} \otimes \sqrt{\tau^{\mathcal{E}}}\right) \eta^{\mathcal{S}} \left(\mathbb{I}^{\mathcal{S}} \otimes \sqrt{\tau^{\mathcal{E}}}\right)^{\dagger},$$

which is of the form of Eq. (2.4) with non negative eigenvalues. The dynamical map from a state that is initially uncorrelated from its environment is the composition of three completely positive maps: embedding, unitary evolution, and reduction. Initially uncorrelated states are not the only states that can give rise to completely positive maps [17]. This will be discussed in Chapter 5 in detail. The embedding map presented here is only applicable to the system at time t_i. At other times it might have developed correlations with the environment and not be of the simply-separable (product) form. A generalization of this map for all times will be presented in Chapter 7.

2.2.6 Example

To illustrate the relationship between the different forms of the map, we compute a simple example of a two level system represented by the Bloch vector $\overrightarrow{a}$. Its most general transformation in the affine form [21] is:

$$\overrightarrow{a}(t_f) = \overline{R}_{(t_f|t_i)} \cdot \overrightarrow{a}(t_i) + \overrightarrow{r}, \tag{2.10}$$

where the matrix $\overline{R}$ represents a squeezing and rotation of the Bloch vector, and the vector $\overrightarrow{r}$ a translation. For this example. we will focus on the particular case where the system interacts with a two-level uncorrelated environment $\tau = \frac{1}{2}\mathbb{I}$, such that the total initial state is:

$$\rho(t_0)^{\mathcal{S}\mathcal{E}} = \frac{1}{2}\Big(\mathbb{I}^{\mathcal{S}} + a_j(t_0)\sigma_j^{\mathcal{S}}\Big) \otimes \frac{1}{2}\mathbb{I}^{\mathcal{E}}, \tag{2.11}$$

where summation over the repeated index j is implied. Also, $\mathbb{I}$ is the unit matrix in two dimensions,

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and σ_j are the Pauli spin matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The system $\mathcal{S}$ is described by the Bloch vector $\overrightarrow{a}$, while the environment at the initial time is fully mixed. If we assume a unitary operator that depends on the Hamiltonian,

$$H = \sum_j \frac{1}{2}\sigma_j^{\mathcal{S}} \otimes \sigma_j^{\mathcal{E}},$$

the evolution of the Bloch vector is:

$$\overrightarrow{a}(t) = \cos(t - t_0)^2 \, \overrightarrow{a}(t_0), \tag{2.12}$$

which is a uniform squeezing with no translation [22]. The full calculation will be carried out in detail in Chapter 3.

This interaction was chosen because it swaps the system with the environment at periodic intervals, thus providing an environment that stores the system information, and then returns it. As time changes, the state is pinned down to the fully mixed state (from the initial environment) and grows again into the full state (from the memory of the environment) periodically.

The evolution can be treated as a map from $\eta(t_0) \rightarrow \eta(t)$ with the form from Eq. (2.6). If the density matrix,

$$\eta(t) = \sum_j \frac{1}{2}\Big(\mathbb{I} + a_j(t)\sigma_j\Big),$$

is written as a vector,

$$\overrightarrow{\eta}(t) = \frac{1}{2}\begin{pmatrix} 1 + a_3(t) \\ a_1(t) - ia_2(t) \\ a_1(t) + ia_2(t) \\ 1 + a_3(t) \end{pmatrix},$$

the evolution is a stochastic matrix transformation,

$$\overrightarrow{\eta}(t) = \mathfrak{A}_{(t|t_0)} \cdot \overrightarrow{\eta}(t_0),$$

where

$$\mathfrak{A}_{(t|t_0)} = \frac{1}{2}\begin{pmatrix} 1 + c^2 & 0 & 0 & 1 - c^2 \\ 0 & 2c^2 & 0 & 0 \\ 0 & 0 & 2c^2 & 0 \\ 1 - c^2 & 0 & 0 & 1 + c^2 \end{pmatrix},$$

with the convention that $c \equiv \cos(t - t_0)$. By index exchange, we get the map in its Hermitian form:

$$\mathfrak{B}_{(t|t_0)} = \frac{1}{2}\begin{pmatrix} 1+c^2 & 0 & 0 & 2c^2 \\ 0 & 1-c^2 & 0 & 0 \\ 0 & 0 & 1-c^2 & 0 \\ 2c^2 & 0 & 0 & 1+c^2 \end{pmatrix}.$$

By rewriting the map in terms of its eigenvalues and eigenmatrices,

$$\eta(t) = \sum_{\alpha=0}^{3} \lambda_\alpha(t - t_0) \mathrm{C}_\alpha \, \eta(t_0) \, \mathrm{C}_\alpha^\dagger$$

with

$$\lambda_0(t - t_0) = \frac{1}{2}\left(1 + 3c^2\right), \qquad \mathrm{C}_0 = \frac{1}{\sqrt{2}}\mathbb{I},$$
$$\lambda_{1,2,3}(t - t_0) = \frac{1}{2}\left(1 - c^2\right), \qquad \mathrm{C}_{1,2,3} = \frac{1}{\sqrt{2}}\sigma_{1,2,3},$$

we confirm that it is completely positive and trace preserving.

The process is reversible. Also, note that even if this map is expanded in a Taylor series for $t \approx t_0$, where:

$$c^2 = \cos(t - t_0)^2 = 1 - (t - t_0)^2 + \ldots,$$

there are no terms of first order. This is because the interaction was chosen to be only for the "kickback" of the environment on the system.

In the next chapter, we study the evolution of two qubits by means of a more general interaction.

Chapter 3

Dynamics of Two Qubits

Universal, two qubit quantum gates are the basic units from which quantum information processing devices may be constructed [23, 24]. Physical implementations of two qubit gates depend on understanding and controlling the possible interactions between the individual qubits. Zhang *et al.* [25] have obtained the most general form for non local two-qubit interactions. A complete picture of the dynamical possibilities allowed by this interaction is yet to be pieced together, although some numerical efforts have started to scratch the surface [26].

In this chapter we compute the most general evolution of the interaction of two qubits.

3.1 Evolution for two initially simply-separable qubits

Consider a qubit ρ^A interacting with another qubit ρ^B:

$$\rho^A = \frac{\mathbb{I}^A + \sum_i a_i \sigma_i^A}{2}, \quad \rho^B = \frac{\mathbb{I}^B + \sum_i b_i \sigma_i^B}{2}, \tag{3.1}$$

with σ_i^A and σ_i^B being the Pauli spin matrices for each of them. The Bloch vectors $\overrightarrow{a} = (a_1, a_2, a_3)$ and $\overrightarrow{b} = (b_1, b_2, b_3)$ provide a convenient way of

parameterizing single qubit states that we will use in this section. Together, ρ^A and ρ^B form the initially simply-separable (Kronecker product) 4×4 state,

$$\begin{aligned} \rho^{AB}(0) &= \rho^A \otimes \rho^B \\ &= \sum_{i,j} \frac{1}{4} \left[\mathbb{I}^A \otimes \mathbb{I}^B + \left(a_i \sigma_i^A \otimes \mathbb{I}^B + b_i \mathbb{I}^A \otimes \sigma_i^B \right) + a_i b_j \sigma_i^A \otimes \sigma_j^B \right], \end{aligned}$$

where subscripts take values from $\{1, 2, 3\}$. The most general Hamiltonian for two qubits is:

$$H = \sum_i \alpha_i \sigma_i^A \otimes \mathbb{I}^B + \sum_i \beta_i \mathbb{I}^A \otimes \sigma_i^B + \sum_{i,j} \Gamma_{ij} \sigma_i^A \otimes \sigma_j^B. \tag{3.2}$$

In the interaction picture, it becomes,

$$H \to \widehat{H}(t) = \sum_{i,j} \widehat{\Gamma}_{ij}(t) \sigma_i^A \otimes \sigma_j^B, \tag{3.3}$$

which has nine parameters. Using local unitary transformations with three parameters each, the number of parameters can be brought down to three [6, 25, 27, 28]:

$$\widehat{H}(t) \to H(t) = \sum_i \gamma_i(t) \sigma_i^A \otimes \sigma_i^B. \tag{3.4}$$

The time evolution of the overall state ρ^{AB} is given by,

$$\rho^{AB}(t) = U \rho^{AB}(0) U^\dagger,$$

where $U = \mathcal{T} e^{-i \int H(t) dt}$. For simplicity, we will assume that there is no free evolution for individual qubits, making $\gamma_i(t) \to \gamma_i$ and

$$U = \prod_{j=1}^{3} \left[\cos(\gamma_j t) \mathbb{I}^A \otimes \mathbb{I}^B - i \sin(\gamma_j t) \sigma_j^A \otimes \sigma_j^B \right]. \tag{3.5}$$

To calculate $\rho^{AB}(t)$, we use the property that

$$\sigma_1^A \otimes \sigma_1^A, \quad \sigma_2^B \otimes \sigma_2^B, \quad \sigma_3^A \otimes \sigma_3^B,$$

all commute with each other. For each of the terms of $\rho^{AB}(0)$ we obtain:

$$\begin{aligned} U\mathbb{I} \otimes \mathbb{I}U^\dagger &= \mathbb{I} \otimes \mathbb{I}, \\ U\sigma_i \otimes \sigma_i U^\dagger &= \sigma_i \otimes \sigma_i, \\ U\mathbb{I} \otimes \sigma_i U^\dagger &= \mathbb{I} \otimes \sigma_i e^{2it(\gamma_j \sigma_j \otimes \sigma_j + \gamma_k \sigma_k \otimes \sigma_k)}, \\ U\sigma_i \otimes \sigma_j U^\dagger &= \sigma_i \otimes \sigma_j e^{2it(\gamma_i \sigma_i \otimes \sigma_i + \gamma_j \sigma_j \otimes \sigma_j)}, \end{aligned} \tag{3.6}$$

Using Eq. (3.6), the evolution generated by Eq. (3.5) of the two qubit density matrix is:

$$\begin{aligned} \rho^{AB}(t) = \frac{1}{4} \sum_{i=1}^{3} \big[& \mathbb{I}^A \otimes \mathbb{I}^B + a_i b_i \sigma_i^A \otimes \sigma_i^B \\ & a_i \left(c_j c_k \sigma_i^A \otimes \mathbb{I}^B + s_j s_k \mathbb{I}^A \otimes \sigma_i^B + c_k s_j \sigma_k^A \otimes \sigma_j^B - c_j s_k \sigma_j^A \otimes \sigma_k^B \right) \\ & + b_i \left(c_j c_k \mathbb{I}^A \otimes \sigma_i^B + s_j s_k \sigma_i^A \otimes \mathbb{I}^B + c_k s_j \sigma_j^A \otimes \sigma_k^B - c_j s_k \sigma_k^A \otimes \sigma_j^B \right) + \\ & + a_i b_j \left(c_i c_j \sigma_i^A \otimes \sigma_j^B + s_i s_j \sigma_j^A \otimes \sigma_i^B + c_i s_j \sigma_k^A \otimes \mathbb{I}^B - c_j s_i \mathbb{I}^A \otimes \sigma_k^B \right) \\ & + a_j b_i (c_i c_j \sigma_j^A \otimes \sigma_i^B + s_i s_j \sigma_i^A \otimes \sigma_j^B + c_i s_j \mathbb{I}^A \otimes \sigma_k^B - c_j s_i \sigma_k^A \otimes \mathbb{I}^B) \big], \end{aligned} \tag{3.7}$$

where $c_i \equiv \cos(2t\gamma_i)$, $s_i \equiv \sin(2t\gamma_i)$ and i, j, k are cyclic. In other words, the coefficients of the Pauli matrices in Eq. (3.2) transform as follows:

$$\left\{ \begin{array}{c} a_k \\ b_k \end{array} \right\} \mapsto \left\{ \begin{array}{c} a_k \\ b_k \end{array} \right\} c_i c_j + \left\{ \begin{array}{c} b_k \\ a_k \end{array} \right\} s_i s_j + \left\{ \begin{array}{c} a_i b_j \\ a_j b_i \end{array} \right\} c_i s_j - \left\{ \begin{array}{c} a_j b_i \\ a_i b_j \end{array} \right\} c_j s_i,$$

where $\{i, j, k\}$ are cyclic. We also have

$$a_i b_j \mapsto a_i b_j c_i c_j + a_j b_i s_i s_j + \epsilon_{ijk}(b_k c_j s_i - a_k c_i s_j), \tag{3.8}$$

where it is not required for $\{i, j, k\}$ to be cyclic or distinct.

3.2 Reduced dynamics of two initially simply separable qubits

To find the reduced dynamics of the system, ρ^A, we just need to carry out the partial trace from Eq. (2.6). Using Eqs. (3.7), (3.8) and the fact that σ_i^B are traceless, this is quite straightforward:

$$\rho^A(t) = \frac{1}{2}\begin{pmatrix} 1+a_3(t) & a_1(t)-ia_2(t) \\ a_1(t)+ia_2(t) & 1-a_3(t) \end{pmatrix}, \tag{3.9}$$

where

$$a_i(t) = a_i c_j c_k + b_i s_j s_k + a_j b_k c_j s_k - a_k b_j c_k s_j.$$

This can be thought of as an evolution along elliptical orbits in the Bloch sphere [29].

The time evolution of ρ^A can be described using the dynamical map from Eq. (2.6). The mapping matrix can be explicitly calculated to be [1]:

$$\mathfrak{B}_{(t,0)} = \frac{1}{2}\begin{pmatrix} 1+b_3s_1s_2+c_1c_2 & b_2c_1s_2-ib_1c_2s_1 & (b_1s_3-b_2c_3)\,s_2 & (c_1+c_2) \\ & & -i\,(b_2s_3+b_1c_3)\,s_1 & \times(c_3+ib_3s_3) \\ b_2c_1s_3+ib_1c_2s_1 & 1+b_3s_1s_2-c_1c_2 & (c_2-c_1) & (b_1s_3+b_2c_3)\,s_2 \\ & & \times(c_3-ib_3s_3) & -i\,(b_2s_3-b_1c_3)\,s_1 \\ (b_1s_3-b_2c_3)\,s_2 & (c_2-c_1) & & \\ +i\,(b_2s_3+b_1c_3)\,s_1 & \times(c_3+ib_3s_3) & 1-b_3s_1s_2-c_1c_2 & -b_2c_1s_2+ib_1c_2s_1 \\ (c_1+c_2) & (b_1s_3+b_2c_3)\,s_2 & & \\ \times(c_3-ib_3s_3) & +i\,(b_2s_3-b_1c_3)\,s_1 & -b_2c_1s_2-ib_1c_2s_1 & 1-b_3s_1s_2+c_1c_2 \end{pmatrix}.$$

Note how the dynamical map carries the influence of ρ^B through the parameters $b_1,\ b_2,\ b_3$. Thus, given any known initial state ρ^A and sufficiently detailed evolution $\rho^A(t)$, its interaction with another unknown ρ^B can be reconstructed, and even used to determine the parameters for the unknown state.

The most general map on a qubit can be implemented as the contraction of the unitary evolution of the given qubit coupled to at most two other qubits.

We have restricted to the case where there is only one other qubit, thereby excluding certain maps. When ρ^B is allowed to be a mixed state, the family of dynamical maps we are excluding by choosing a one qubit environment is very small [30].

This map is quasi periodic, as it depends on time on trigonometric functions. Even if parameters from the contracted space go into the other subspace for a time, they can be recovered at a later time. There is no dissipation. In the next chapter we review some approaches to introduce dissipation into such dynamics.

Chapter 4

Decoherence and Irreversibilty

We have so far studied Hamiltonian dynamics on quantum systems where no information is lost. In the previous chapter, we considered an open system evolution that, since the environment was finite-dimensional, there were Poincaré recurrences.

However, in practice a system interacts with an environment in a seemingly irreversible manner; no recurrences are observed. This is the same issue that bothered Boltzmann: how can irreversible, thermodynamic, behavior be derived from purely Hamiltonian dynamics? He was interested in the statistical mechanics of gases as derived from the Hamiltonian dynamics of the individual particles that form the gas. The answer Boltzmann chose was to make the approximation that the particle of interest, the system, interacts with other particles in sequence, the environment, each of them only for such short time that the environmental particles cannot affect back the system.

He considered the system particle $\mathbb{S}$ to move in a straight line until it collides with an environmental particle. Some energy is exchanged in this collision, but the total energy is conserved. However, the environmental particle is now discarded and with it the energy it had. This depends directly

on the assumption that the probability of an interaction of this environmental particle with the system $\mathcal{S}$ is very low. The system $\mathcal{S}$ continues with its new energy until it collides with a new environmental particles, where they interact, and the environmental energy discarded successively. An infinite number of collisions of this type make the system reach thermodynamic equilibrium and is called the collision model.

The biggest challenge to scalable quantum computation is the loss of quantum information to the environment in an irreversible manner. How can such irreversibility be derived from a unitary evolution? In this chapter we review the quantum version of Boltzmann's collision model, the Rau refreshing model. We show how in the limit of very short time interactions the refreshing model leads to the Kossakowski-Lindblad master equation. We also study the approximations that must be made to a stochastic process described by a dynamical map in order to obtain the Kossakowski-Lindblad master equation,

$$\frac{\partial \eta}{\partial t} = \mathfrak{L}\eta \equiv -i[H,\eta] + \sum_{\alpha} \frac{1}{2}\left(2\mathrm{L}_{\alpha}\eta\mathrm{L}_{\alpha}^{\dagger} - \mathrm{L}_{\alpha}^{\dagger}\mathrm{L}_{\alpha}\eta - \eta\mathrm{L}_{\alpha}^{\dagger}\mathrm{L}_{\alpha}\right).$$

We discuss the implications of these approximations, and the limitations of the Kossakowski-Lindblad master equation.

4.1 Rau Refreshing Model

A quantum mechanical version of the Boltzmann collision model was developed by Rau [31]. We review her approach by means of an example, related to the one discussed in previous chapters. Consider the case where the

system is a qubit described by the Bloch vector $\overrightarrow{a}$ which first interacts with a two level environment $\tau = \frac{1}{2}\mathbb{I}$, such that the total initial state is:

$$\rho(t_0)^{\mathcal{SE}} = \frac{1}{2}\left(\mathbb{I}^{\mathcal{S}} + a_j(t_0)\sigma_j^{\mathcal{S}}\right) \otimes \frac{1}{2}\mathbb{I}^{\mathcal{E}}, \tag{4.1}$$

where summation over the repeated index j is implied. By means of unitary operation given by the Hamiltonian $H = \sum_j \sigma_j^{\mathcal{S}} \otimes \sigma_j^{\mathcal{E}}$, the evolution of the Bloch vector is:

$$\overrightarrow{a}(t) = \cos\left(2(t-t_0)\right)^2 \overrightarrow{a}(t_0), \tag{4.2}$$

such that the system part of the toal density matrix,

$$\eta(t) = \mathrm{Tr}_{\mathcal{E}}\left[\rho(t)\right],$$

evolves according to:

$$\eta(t) = \frac{1}{2}\left(\mathbb{I}^{\mathcal{S}} + a_j(t)\sigma_j^{\mathcal{S}}\right) = \frac{1}{2}\left(\mathbb{I}^{\mathcal{S}} + \cos\left(2(t-t_0)\right)^2 a_j(t_0)\sigma_j^{\mathcal{S}}\right).$$

This interaction exchanges the system with the environment at periodic intervals and has no decoherence. The interaction was chosen to be of the "swap-gate" form, but many interactions can have a similar effect.

A quantity used to visualize the evolution of the whole Bloch sphere is its purity. The purity of a density matrix ρ is given by:

$$P(\rho) = \mathrm{Tr}\left[\rho^2\right]. \tag{4.3}$$

In our example, the purity of the reduced density matrix $\eta^{\mathcal{S}}$ changes with time:

$$P^{\mathcal{S}}(t) = \mathrm{Tr}\left[\eta\left(t\right)^2\right] = \frac{1}{2}\left[1 + a_1\left(t\right)^2 + a_2\left(t\right)^2 + a_3\left(t\right)^2\right]. \tag{4.4}$$

Following a similar procedure we can find the evolution of $\tau^{\mathcal{E}}(t)$ and its purity $P^{\mathcal{E}}$. Figure 5.1 shows how the purity of $\eta^{\mathcal{S}}(t)$ and the purity of $\tau^{\mathcal{E}}(t)$ change with time.

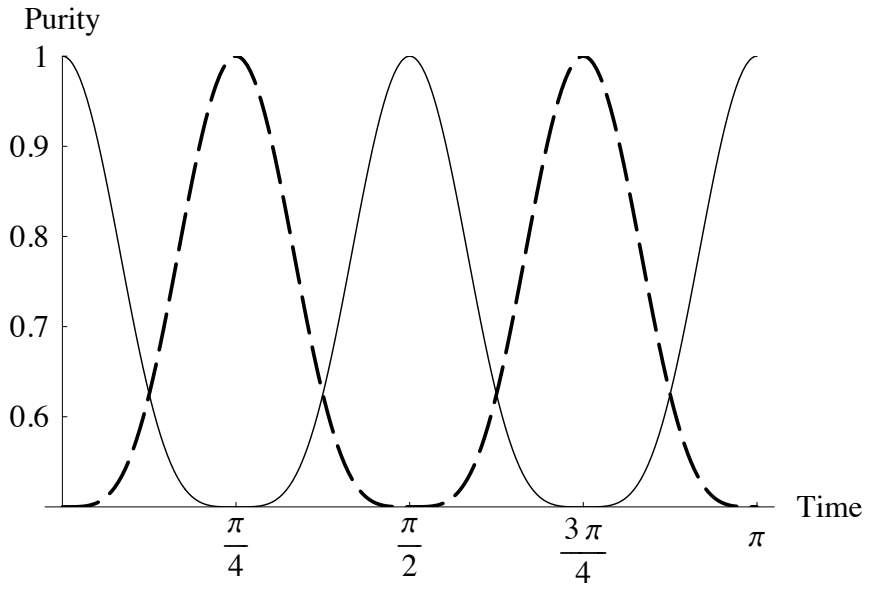

Figure 4.1: Purity as a function of time for $a_1 = 1, a_2 = a_3 = b_1 = b_2 = b_3 = 0$. The solid line represents $P^{\mathcal{S}}(t)$ while the dashed line represents $P^{\mathcal{E}}(t)$. At $t = \pi/4$ purity has been totally swapped.

As time progresses, they start to get entangled and exchange purity through entanglement. $P^{\mathcal{S}}(t)$ and $P^{\mathcal{E}}(t)$ are equal at $t = \pi/8$, where some purity has been lost to correlations among the two. At $t = \pi/4$ they become separable again [32] purifying $\tau^{\mathcal{E}}$ at the expense of $\eta^{\mathcal{S}}$, a dynamical process we call *purity swapping*. If only a certain component of the qubit is measured and no correlations studied, this might look like Rabi oscillations, although the Bloch vector is *not* rotating, but oscillating in length.

We remark that for a weak coupling of this type, at very short times δt, $P^{\mathcal{S}}(\delta t)$ can only decrease (except in trivial cases). This can be considered to be a mechanism of decoherence. We can model a reservoir as a stream of $\left\{\tau_i^{\mathcal{E}}\right\}$, where each of them interact independently for a short average time [31], swapping some purity from $\eta^{\mathcal{S}}$ to each $\tau_i^{\mathcal{E}}$, but stopping the coupling before there is enough time to return the stolen purity. We can think of this as a quantum version of the Boltzmann gas [33]. This corresponds to acting with the dynamical map from Eq. (3.10) in sequence:

$$\eta^{\mathcal{S}} \to \mathfrak{B}^{(t_{n-1},t_n)} \star \mathfrak{B}^{(t_{n-2},t_{n-1})} \star \ldots \star \mathfrak{B}^{(t_0,t_1)} \left(\eta^{\mathcal{S}}\right). \tag{4.5}$$

By controlling the strength, duration and number of these reservoir interactions it is possible to model decoherence processes using only a finite number of degrees of freedom for the reservoir.

If we treat each interaction in our example to take time T, after N interactions, where a total time $t = NT$ has passed, the density matrix is of the form:

$$\eta(t) = \frac{1}{2}\Big(\mathbb{I}^{\mathcal{S}} + \cos\left(2T\right)^{2N} a_j(t_0)\sigma_j^{\mathcal{S}}\Big).$$

Since $N = t/T$, the Bloch vector shrinks as:

$$\overrightarrow{a}(t) = \cos\left(2T\right)^{2t/T} \overrightarrow{a}(0). \tag{4.6}$$

which depends on two different time scales, T for short times and t for long times. The shrinking factor can be rewritten as:

$$\cos\left(2T\right)^{2N} = e^{-t\frac{2}{T}\ln\left(\frac{1}{\cos(2T)}\right)}. \tag{4.7}$$

This result was first derived by Rau in [31].

If we let the interaction time T to be of significant length, the short time behavior tends to dominate. For example, if $a_3(0) = 1$ and the refreshing time is $T = 17\pi/8$, we obtain a behavior for the polarization $a_3(t)$ that is plotted in Fig. 4.2. For a shorter refreshing time, an overall long time envelope

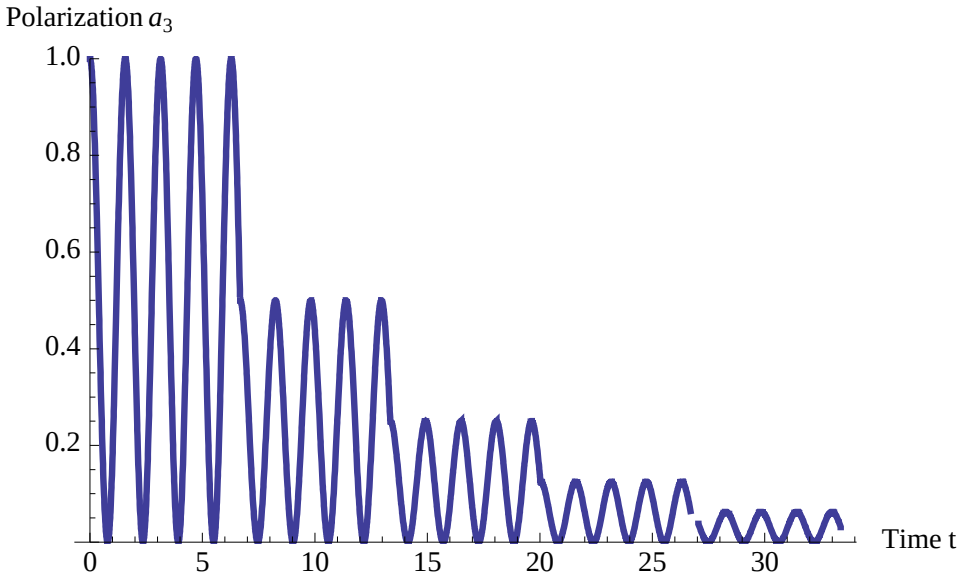

Figure 4.2: Polarization $a_3(t)$ with refreshing time $T = 17\pi/8$

begins to appear. For $T = 5\pi/8$, we obtain $a_3(t)$ as shown in Fig. 4.3. If the refreshing time is even shorter, a long time behavior dominates and the short time behavior is suppressed. If we consider $T = \pi/8$, the polarization $a_3(t)$ behaves now as in Fig. 4.4. This starts to suggest exponential decay, a signature of thermodynamic behavior.

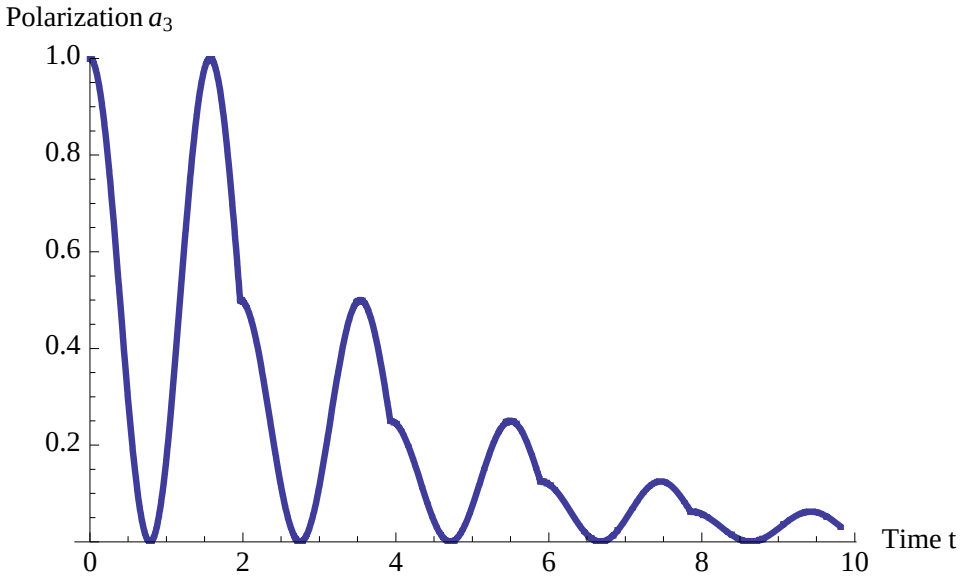

Figure 4.3: Polarization $a_3(t)$ with refreshing time $T = 5\pi/8$

To get a fully thermodynamic decay, we make the approximation:

$$\frac{2}{T}\ln\left(\frac{1}{\cos(2T)}\right) \approx \gamma. \tag{4.8}$$

where γ is a constant. This approximation gives an exponential decay:

$$\eta(t) = \frac{1}{2}\left(\mathbb{I}^{\mathcal{S}} + e^{-\gamma(t-t_0)}a_j(t_0)\sigma_j^{\mathcal{S}}\right).$$

This exponential decay can be written as a first order differential equation,

$$\dot{\eta}(t) = \mathfrak{L}(\eta) = \gamma\left(\frac{1}{2}\mathbb{I} - \eta(t)\right), \tag{4.9}$$

that is of the Kossakowski-Lindblad form:

$$\frac{\partial\eta}{\partial t} = \sum_{\alpha=0}^{3}\frac{1}{2}\left(2\mathrm{L}_\alpha\eta\mathrm{L}_\alpha^\dagger - \mathrm{L}_\alpha^\dagger\mathrm{L}_\alpha\eta - \eta\mathrm{L}_\alpha^\dagger\mathrm{L}_\alpha\right),$$

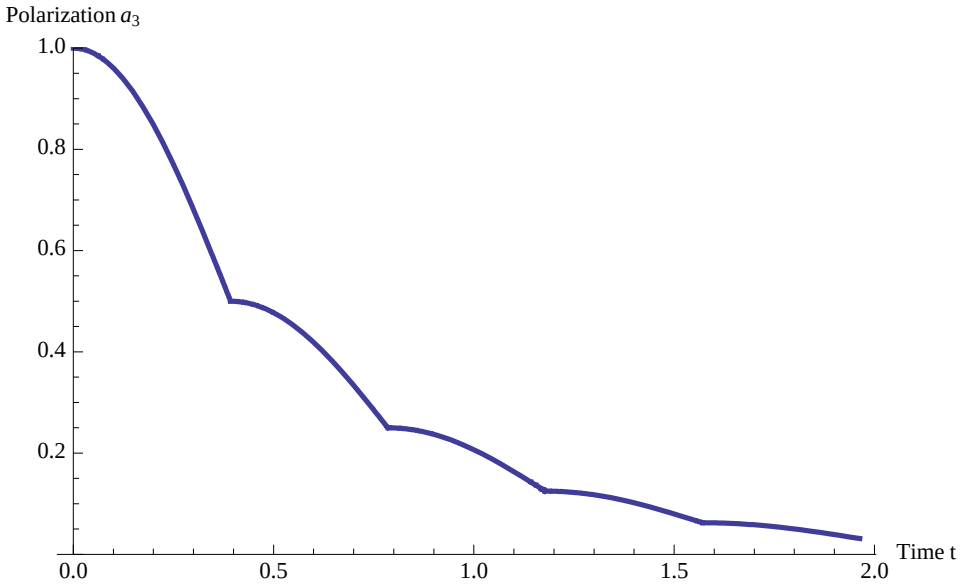

Figure 4.4: Polarization $a_3(t)$ with refreshing time $T = \pi/8$

if we choose:

$$\mathrm{L}_0 = \sqrt{\frac{\gamma}{3!}}\,\mathbb{I}, \quad \mathrm{L}_\alpha = \sqrt{\frac{\gamma}{3!}}\,\sigma_\alpha,$$

since

$$\sigma_\alpha^2 = \mathbb{I},$$

and

$$\mathbb{I}\sigma_j\mathbb{I} + \sigma_1\sigma_j\sigma_1 + \sigma_2\sigma_j\sigma_2 + \sigma_3\sigma_j\sigma_3 = 0,$$

for all $j = \{1, 2, 3\}$.

Irreversibility was obtained by a series of approximations and assumptions. First, the system was assumed to be uncoupled from the environment. The environment is a series of short interactions with environmental particles. After each interaction, the environmental particle is *discarded* and is

never allowed to appear again, a process called "refreshing". This refreshing is irreversible in principle, throwing away all correlations developed with the environment. An additional approximation was made to force only on one time regime and not two. This is the Markov approximation. These approximations are only reasonable for very short times.

All these effectively prevented the environment to act back on the system, in the same manner developed by Boltzmann in his collision model. In general, environmental effects only appear at higher orders of time [34]. This will become important when we discuss non-Markovian effects.

There are many cases where the periodic couplings are a good approximation and their properties can be exploited to prevent decoherence. Bang-bang control, for example, is a technique where the periodicity (on average) of a decoherence coupling can be synchronized with a local control pulse effectively creating a decoherence-free space for the state of interest [35, 36].

Next, we study the case of the Markov approximation of the refreshing model, and its connection to the Kossakowski-Lindblad master equation.

4.2 Kossakowski-Lindblad master equation

If the refreshing from the Rau refreshing model is thought to happen at infinitesimal times, an exponential decay can be found. It corresponds to the case where there is only one timescale, and the environment is not allowed to "kickback" at the system. Information (purity) that goes into the environment

is completely discarded and never comes back. There is no periodicity of purity swapping in that limit.

A general evolution of this kind can be written as the Kossakowski-Lindblad master equation [2, 37, 38]. In this section we review and discuss the connection between the dynamical maps and the Kossakowski-Lindblad master equation.

A dynamical map of states that were uncorrelated at t_0 might have developed correlation through time, its history reducing the allowed set of states at time t_1 such that,

$$\mathfrak{B}_{(t_2|t_0)} \neq \mathfrak{B}_{(t_2|t_1)} \star \mathfrak{B}_{(t_1|t_0)}.$$

In order to develop the Kossakowski-Lindblad master equation, the Markov approximation is invoked for short times [2], making

$$\mathfrak{B}_{(t_2|t_0)} \approx \mathfrak{B}_{(t_2|t_1)} \star \mathfrak{B}_{(t_1|t_0)}.$$

The maps now form a dynamical semigroup. The Markov approximation might lead to unphysical results [39]. To justify this, infinite-dimensional baths are sometimes called upon. Tied to these assumptions, demands for completely positive dynamics have also been imposed [37, 38]. Altogether, these restrictions can describe dissipative processes at the expense of discarding non-Markovian memory effects and correlations with the environment. We now show how the Kossakowksi-Lindblad master equation is related to the dynamical map.

4.2.1 Derivation of the Kossakowski-Lindblad master equation from the dynamical map

A master equations is a first-order differential equation of the time evolution of a probability density and has the form:

$$\frac{\partial \rho}{\partial t} = \mathfrak{L}\rho,$$

where the super operator $\mathfrak{L}$ is the Liouvillian. The Liouvillian is related to the dynamical map by,

$$\mathfrak{B} = e^{t\mathfrak{L}}.$$

If the dynamical map is assumed to depend only on the first orders of t, the Kossakowski-Lindblad master equation can be derived. This was first pointed out by E.C.G. Sudarshan in private communication, and later discussed in [40]. First, we start with the map in the Choi representation:

$$\eta \to \mathfrak{B}_t\, \eta(0) = \sum_{\alpha=1}^{N} \lambda_\alpha \mathrm{C}_\alpha\, \eta(0)\, \mathrm{C}_\alpha^\dagger. \tag{4.10}$$

The Kossakowski-Lindblad master equation originally was derived for completely positive evolutions, such that $0 \leq \lambda_\alpha$. Thus, we assume this condition for the purpose of this derivation. With it, we can write:

$$\begin{aligned} \sqrt{\lambda_1}\mathrm{C}_1 &= \mathbb{I} + \sqrt{t}\, \mathrm{L}_1, \\ \sqrt{\lambda_\alpha}\mathrm{C}_\alpha &= \sqrt{t}\, \mathrm{L}_\alpha \quad \text{for} \quad \alpha > 1, \end{aligned} \tag{4.11}$$

so the action of the map for small t is:

$$\begin{aligned}\eta(t) &= \Big(\mathbb{I}+\sqrt{t}\,\mathrm{L}_1\Big)\,\eta(0)\,\big(\mathbb{I}+\sqrt{t}\,\mathrm{L}_1\big)^\dagger+\sum_{\alpha>1}^{N} t\,\mathrm{L}_\alpha\,\eta(0)\,\mathrm{L}_\alpha^\dagger \\ &= \eta(0)+\sqrt{t}\big(\mathrm{L}_1\,\eta(0)+\eta(0)\,\mathrm{L}_1^\dagger\big)+\sum_{\alpha=1}^{N} t\,\mathrm{L}_\alpha\,\eta(0)\,\mathrm{L}_\alpha^\dagger.\end{aligned}$$

To get the differential form needed for the master equation, we reorganize it as a difference equation:

$$\frac{\eta(t)-\eta(0)}{t}=\frac{1}{\sqrt{t}}\big(\mathrm{L}_1\,\eta(0)+\eta(0)\,\mathrm{L}_1^\dagger\big)+\sum_{\alpha=1}^{N}\mathrm{L}_\alpha\,\eta(0)\,\mathrm{L}_\alpha^\dagger. \tag{4.12}$$

Using the trace preservation condition $\sum_\alpha \lambda_\alpha \mathrm{C}_\alpha^\dagger \mathrm{C}_\alpha$ that in this form reads:

$$\big(\mathbb{I}+\sqrt{t}\,\mathrm{L}_1\big)^\dagger\big(\mathbb{I}+\sqrt{t}\,\mathrm{L}_1\big)+\sum_{\alpha>1}^{N} t\,\mathrm{L}_\alpha^\dagger\mathrm{L}_\alpha=\mathbb{I},$$

we find the property:

$$\frac{1}{\sqrt{t}}\big(\mathrm{L}_1^\dagger+\mathrm{L}_1\big)=-\sum_{\alpha=1}^{N}\mathrm{L}_\alpha^\dagger\mathrm{L}_\alpha,$$

from which we can rewrite the term first term from Eq. (4.12) into a commutator and anticommutator:

$$\frac{1}{\sqrt{t}}\big(\mathrm{L}_1\eta(0)+\eta(0)\mathrm{L}_1^\dagger\big)=\frac{1}{2\sqrt{t}}\Big[\mathrm{L}_1-\mathrm{L}_1^\dagger,\ \eta(0)\Big]-\frac{1}{2}\sum_{\alpha=1}^{N}\Big\{\mathrm{L}_\alpha^\dagger\mathrm{L}_\alpha,\ \eta(0)\Big\}.$$

With this, Eq. (4.12) can be rewritten as:

$$\begin{aligned}\frac{\eta(t)-\eta(0)}{t}&=\frac{1}{2\sqrt{t}}\Big[\mathrm{L}_1-\mathrm{L}_1^\dagger,\ \eta(0)\Big] \\ &+\frac{1}{2}\sum_{\alpha}\Big(\big[\mathrm{L}_\alpha\,\eta(0),\mathrm{L}_\alpha^\dagger\big]+\big[\mathrm{L}_\alpha,\eta(0)\,\mathrm{L}_\alpha^\dagger\big]\Big).\end{aligned} \tag{4.13}$$

Any matrix M can be rewritten in terms of a Hermitian M_H and anti-Hermitian part $i\mathrm{M}_A$ such that $\mathrm{M} = \mathrm{M}_H + i\mathrm{M}_A$. From this, $\mathrm{M} - \mathrm{M}^\dagger = -i2\mathrm{M}_A$, where M_A is Hermitian ($\mathrm{M}_A = \mathrm{M}_A^\dagger$). From this, we conclude that in Eq. (4.13), $\mathrm{L}_1 - \mathrm{L}_1^\dagger$ is anti-Hermitian and could be written as,

$$\mathrm{L}_1 - \mathrm{L}_1^\dagger \equiv -i\sqrt{t}H_o, \qquad H_o = H_o^\dagger.$$

The Hamiltonian part is now rescaled to implicitly carry a time dependence of a higher order in t. With this, and taking the limit of Eq. (4.13) where $t \to 0$, the Kossakowski-Lindblad master equation is obtained:

$$\frac{\partial \eta}{\partial t} \;=\; \mathfrak{L}\eta \equiv -i[H_o, \eta] + \sum_\alpha \frac{1}{2}\left(2\mathrm{L}_\alpha \eta \mathrm{L}_\alpha^\dagger - \mathrm{L}_\alpha^\dagger \mathrm{L}_\alpha \eta - \eta \mathrm{L}_\alpha^\dagger \mathrm{L}_\alpha\right),$$

which corresponds to a Markovian process where H_o, is the effective local evolution, resembling a Hamiltonian, while L_α are the operators that generate the completely positive dynamical semigroup [2, 37, 38]. Dynamical semigroups are not groups as they do not have an inverse. They are irreversible.

In order to define the time derivative of the dynamical map, the Kossakowski approach is to first take the Markov approximation and then reorganize the terms. The Markov approximation throws away information from the environment. For infinitely large environments it is often assumed that this is a reasonable assumption. We will study when this assumption is not applicable.

4.2.2 Limitations of the Kossakowski-Lindblad master equation

To obtain the Kossakowski-Lindblad master equation several assumptions were necessary. First, not only a completely positive map is argued for, but one for a state initially uncorrelated with its environment (tensor-product). This condition is poorly motivated, as there is no physical reason why a map should always be completely positive. Also, preparing states in an uncorrelated form is often not possible in experiments. The consequences of complete positivity for the master equation were studied by Gorini, Kossakowski and Sudarshan in [37]. In Chapter 5 we discuss the connection between correlations and not completely positive maps.

Another important assumption is the Markov approximation, where the final state of a system after a stochastic evolution for a very short time only depends on its initial state. It does not depend on its history or other parameters. A consequence of this is that the interaction is short enough that correlations with the environment are not important, and from this that the rate of change must be constant for all times, giving rise to exponential decays. This is suspicious, as we have argued before that the main mechanism of decoherence is purity swapping, where the purity of the state is reduced as correlations with the environment increased.

Also, although exponential decays are very natural solutions to decay equations, it has been shown that in the quantum mechanical case, for very short times, this is not correct. A simple intuitive motivation for corrections to an exponential decay for short times is that at time $t = 0$ the function will

not be differentiable. The correction to exponential decay for short times is known as the quantum Zeno effect [41].

The consistency of the Markov approximation in this case is questionable. First, it is assumed to be valid for short times with disregards of any connection to the evolution of an open system in interaction with a finite environment and thus has as solutions exponential decays. However, quantum Zeno effects warns that exponential decay are *not* valid for very short times.

The Kossakowski-Lindblad master equation is sometimes praised as the fundamental source of decoherence of a quantum system. In some textbooks, such as Nielsen and Chuang [42], the non-Hamiltonian terms are referred to as the dissipator operator. This language suggests that from this master equation the question of the source of irreversibility leading to decoherence has been resolved. This is not so.

Decoherence is a direct consequence of all the assumptions and approximations made. The discarded higher orders of t introduce irreversibility into the equation [43], giving rise to thermodynamic effects. In the Markov approximation memory effects are destroyed, making the present independent of the past, the state independent of its correlations with the environment [44]. In general, these assumptions are not reasonable and should always be kept in mind. How to relax these assumptions is the main result of this dissertation.

Chapter 5

Initial Correlations

In the mathematical theory of open quantum systems [45] it is often assumed that the system of interest and its environment are initially in a product state. This restrictive assumption precludes the theory from describing a wide variety of experimental situations including the one in which an open system is simply observed for some interval of time without attempting to initialize it in any particular state at the beginning of the observation period. If dynamical maps [1] are used to describe the open evolution, then an initial product state would lead to dynamics of the system described in terms of completely positive maps [5, 20]. There has been significant experimental and theoretical interest in quantum correlations, entanglement and coherence in the context of quantum information theory [42]. It is only recently that interest has picked up in investigating how these properties, when present in the initial state of a system and its environment, affects the open evolution of the system [10, 14–16, 18, 40, 46, 47].

We have suggested before that there is a connection between the Markov approximation and ignoring correlations with the environment. In order to relax this approximation to the non-Markovian regime, we need to understand

the role of initial correlations in the dynamics of an open system.

Imagine that the time evolution of the state of an open system is observed and found to be completely positive. What does this say about the relationship between the system and its environment at the start of the quantum process? From the observed evolution, is it possible to conclude that the two were initially in a product state? In this chapter we investigate the question of how to relax the initial product state assumption and still obtain dynamics for the system that are described by completely positive transformations. We find that the system and its environment can initially be in a more complicated state than a product and certain restricted types of correlations between the two will not destroy the complete positivity of the reduced system dynamics.

Consider a generic finite-dimensional bipartite state $\rho^{\mathcal{SE}}$ of a quantum system $\mathcal{S}$ and its environment $\mathcal{E}$. Unitary evolution of $\rho^{\mathcal{SE}}$ induces a transformation on the system that is described by a trace-preserving Hermitian superoperator called a dynamical map $\mathfrak{B}$. The dynamical map is defined by

$$\eta \to \mathfrak{B}(\eta) \equiv \mathrm{Tr}_{\mathcal{E}} \left[U \, \rho^{\mathcal{SE}} \, U^{\dagger} \right] = \eta', \tag{5.1}$$

where $\eta = \mathrm{Tr}_{\mathcal{E}} \rho^{\mathcal{SE}}$ is the initial state of $\mathcal{S}$ and η' is its final state. The connection between the map of the reduced state and the total state is summarized by the following diagram:

$$\begin{array}{ccc} \rho^{\mathcal{SE}} & \leftrightarrow & U \rho^{\mathcal{SE}} U^{\dagger} \\ \downarrow & & \downarrow \\ \eta & \to & \mathfrak{B}(\eta) = \eta' \end{array} \tag{5.2}$$

where the downarrows $\downarrow$ refer to the partial trace $\mathrm{Tr}_{\mathcal{E}}$, that reduce the space to the system of interest. By assumption, only the state of the system can be directly observed. The dynamical map is linear; consequently none of the parameters that determine the state of the system appear in it. On the other hand, parameters that determine the overall state $\rho^{\mathcal{SE}}$ but do not appear in η can appear in the map and they will effectively be identified as parameters that describe the evolution and not the state of the system of interest.

We use η to represent density matrices of the system $\mathcal{S}$ and τ to represent density matrices of the environment $\mathcal{E}$. The action of the map can be written in terms of its eigenmatrices $\{\mathrm{C}_{(\alpha)}\}$ and eigenvalues $\{\lambda_\alpha\}$,

$$\mathfrak{B}(\eta) = \sum_\alpha \lambda_\alpha \, \mathrm{C}_{(\alpha)} \, \eta \, \mathrm{C}_{(\alpha)}{}^\dagger. \tag{5.3}$$

If the initial states of of the system and its environment are product states, $\rho^{\mathcal{SE}} = \eta \otimes \tau$, then the eigenvalues of the dynamical map are all positive for any choice of unitary evolution [5, 20]. In this case we can redefine $\sqrt{\lambda_\alpha}\mathrm{C}_{(\alpha)} \to \mathrm{C}_{(\alpha)}$ to get

$$\mathfrak{B}(\eta) = \sum_\alpha \mathrm{C}_{(\alpha)} \, \eta \, \mathrm{C}_{(\alpha)}{}^\dagger, \tag{5.4}$$

with $\sum_\alpha \mathrm{C}_{(\alpha)}{}^\dagger \mathrm{C}_{(\alpha)} = \mathbb{I}$. Any map that can be written in this form is completely positive [1, 5, 12, 13].

Can the dynamical maps formalism still be used if the initial system and environment state is not a product state? It can be, but correlations of the system with the environment mean that a few extra considerations apply. For one, the dynamical map is usually not completely positive and very often

not even positive [14]. The not completely positive nature of the map means that only a subset of the set of states of the system gets mapped to other states by the dynamical maps. The dynamical map is well defined if it is positive on a large enough set of states such that it can be extended by linearity to all states of the system. The set of states that get mapped to other states by the map defined for a particular time is called the *positivity domain* corresponding to that time. These are the set of states that get mapped to other states by the map defined at all times. It can be shown that this set of states is precisely those that are *compatible* with the correlations that are assumed to be present in the initial state of the system and the environment [15, 47]. All the states that get mapped to matrices that do not represent states at some time or the other by the map are precisely those states that were excluded by the correlations that were assumed to be present in the initial combined state. This realization gives a physical interpretation to the action of not completely positive maps. We note here that the positivity of the map should not be confused with the property of complete positivity. Complete positivity is a property of the *form* of the map (it has positive eigenvalues), while positivity is a property of the *action* of the map (it maps density matrices to density matrices).

Do all correlations of the initial state of the system and the environment lead to not completely positive maps or are there certain kinds of correlations that preserve the complete positivity of the reduced evolution of states of the system? In this chapter we identify a general class of initial states that under

any unitary transformation induce completely positive reduced dynamics for the system. Simply separable states are of a tensor product form, such as $\rho^{\mathcal{SE}} = \eta \otimes \tau$, are a subset of this general class of states. To characterize this class we will use the notion of quantum discord introduced by Ollivier and Zurek [48]. But first, let us illustrate by means of example how correlations can lead to not completely positive dynamics.

5.1 Correlations and not completely positive maps

Since we know that entanglement in $\rho^{\mathcal{SE}}$ typically leads to not completely positive dynamics for $\mathcal{S}$ [10] we first look to see if separability of the initial state is sufficient to guarantee complete positivity. We find that this is not so and illustrate this with an example that shows how not completely positive dynamics arise in physically realizable situations where the initial state is separable but not a product. Let $\mathcal{S}$ and $\mathcal{E}$ both be qubits in a combined initial state,

$$\rho^{\mathcal{SE}} = \frac{1}{4}(\mathbb{I} \otimes \mathbb{I} + a_j \sigma_j \otimes \mathbb{I} + e_{23} \sigma_2 \otimes \sigma_3), \tag{5.5}$$

where $j = \{1, 2, 3\}$, σ_j are the Pauli matrices, a_j, e_{23} are real, and repeated indices are summed over. The state $\rho^{\mathcal{SE}}$ is separable according to the Peres separability criterion [32]. The initial state of the system is

$$\eta = \mathrm{Tr}_{\mathcal{E}}[\rho^{\mathcal{SE}}] = (\mathbb{I} + a_j \sigma_j)/2.$$

The state η depends on the parameters $\{a_j\}$, which are the components of the Bloch vector such that $||\vec{a}|| \leq 1$. Furthermore, η will also be limited by the

non negativity condition of the *total* state $\rho^{\mathcal{SE}}$, which implies that $\vec{a}$ must be compatible with the value of the parameter e_{23}. All possible values of $\{a_j\}$ that comply with this constraint are said to belong to the compatibility domain [47].

Consider a unitary evolution of $\rho^{\mathcal{SE}}$ given by

$$U = \cos(\omega t)\mathbb{I}\otimes\mathbb{I} - i\sin(\omega t)\sigma_j\otimes\sigma_j. \tag{5.6}$$

The state of the system at time t is given by [17, 22],

$$\eta(t) = \frac{1}{2}\big[\mathbb{I} + \cos^2(2\omega t)a_j\sigma_j + e_{23}\cos(2\omega t)\sin(2\omega t)\sigma_1\big].$$

The dynamical map $\mathfrak{B}$ that describes the open evolution of the system qubit $\mathcal{S}$ is an affine transformation [21] that squeezes the Bloch sphere of the qubit into a sphere of radius $\cos^2(2\omega t)$ and shifts its center by $e_{23}\cos(2\omega t)\sin(2\omega t)$ in the σ_1 direction. By writing $\mathfrak{B}$ in the form Eq. (5.3), we obtain:

$$\mathfrak{B} = \frac{1}{2}\begin{pmatrix} 1+c^2 & 0 & e_{23}cs & 2c^2 \\ 0 & 1-c^2 & 0 & e_{23}cs \\ e_{23}cs & 0 & 1-c^2 & 0 \\ 2c^2 & e_{23}cs & 0 & 1+c^2 \end{pmatrix}, \tag{5.7}$$

where $c \equiv \cos(2\omega t)$ and $s \equiv \sin(2\omega t)$. The eigenvalues of $\mathfrak{B}$ are

$$\begin{aligned} \lambda_{1,2} &= \frac{1}{2}\big[1 - \cos^2(2\omega t) \pm e_{23}\cos(2\omega t)\sin(2\omega t)\big], \\ \lambda_{3,4} &= \frac{1}{2}\big[1 + \cos^2(2\omega t) \pm \cos(2\omega t)\sqrt{4\cos^2(2\omega t) + e_{23}^2\sin^2(2\omega t)}\big]. \end{aligned}$$

Note that λ_3 and λ_4 are always positive. For λ_1 and λ_2 to be positive we need

$$\sin^2(2\omega t) \geq \pm e_{23}\cos(2\omega t)\sin(2\omega t).$$

We can choose e_{23} such that this condition will be violated for some values of ωt making the map $\mathfrak{B}$ not completely positive and it cannot be written in the form given in Eq. (5.4). This example shows that even separable states can lead to not completely positive maps. A similar example has been worked out in [16]. The map $\mathfrak{B}$ has a physical interpretation as long as it is applied to initial states η that are *compatible* with the total state $\rho^{S\mathcal{E}}$ [40]. However, the positivity domain can depend on the particular evolution. In this example, if we take $\omega = 0$ such that the evolution is trivial, the eigenvalues of the map are always positive even though there were initial correlations.

5.2 General Initially Correlated Two Qubit State

The previous example illustrates how initial correlations might lead to not completely positive dynamics. A more general two-qubit example can be calculated. Eqs. (3.2,3.7,3.8) may be extended in a straightforward fashion to the case where the initial state, ρ^{AB}, is not simply separable, i.e.:

$$\rho^{S\mathcal{E}} = \frac{1}{4}\sum_{i,j}\left[\mathbb{I}\otimes\mathbb{I} + e_{i0}\sigma_i\otimes\mathbb{I} + e_{0i}\mathbb{I}\otimes\sigma_i + e_{ij}\sigma_i\otimes\sigma_j\right], \tag{5.8}$$

where it is *not* necessary that $e_{ij} = e_{i0}\times e_{0j}$. This would include initially entangled states. The evolution for the state ρ^{AB} under the unitary given by Eq. (3.5) can be computed using the result from Eq. (3.6):

$$
\begin{aligned}
\rho^{AB}(t) = \frac{1}{4}\sum_{i=1}^{3} \big[& \mathbb{I}^A \otimes \mathbb{I}^B + e_{ii}\sigma_i^A \otimes \sigma_i^B \\
& + e_{i0}\left(c_j c_k \sigma_i^A \otimes \mathbb{I}^B + s_j s_k \mathbb{I}^A \otimes \sigma_i^B + c_k s_j \sigma_k^A \otimes \sigma_j^B - c_j s_k \sigma_j^A \otimes \sigma_k^B\right) \\
& + e_{0i}\left(c_j c_k \mathbb{I}^A \otimes \sigma_i^B + s_j s_k \sigma_i^A \otimes \mathbb{I}^B + c_k s_j \sigma_j^A \otimes \sigma_k^B - c_j s_k \sigma_k^A \otimes \sigma_j^B\right) \\
& + e_{ij}\left(c_i c_j \sigma_i^A \otimes \sigma_j^B + s_i s_j \sigma_j^A \otimes \sigma_i^B + c_i s_j \sigma_k^A \otimes \mathbb{I}^B - c_j s_i \mathbb{I}^A \otimes \sigma_k^B\right) \\
& + e_{ji}(c_i c_j \sigma_j^A \otimes \sigma_i^B + s_i s_j \sigma_i^A \otimes \sigma_j^B + c_i s_j \mathbb{I}^A \otimes \sigma_k^B - c_j s_i \sigma_k^A \otimes \mathbb{I}^B)\big] . \quad (5.9)
\end{aligned}
$$

Again, to find the reduced dynamics of the system we just need to carry out the partial trace, and the evolution of each of the components become:

$$
e_{i0}(t) \;=\; e_{i0}c_j c_k + e_{0i}s_j s_k + e_{jk}c_j s_k - e_{kj}c_k s_j .
$$

As before, we would like to construct the dynamical map for this evolution. This time, the map has to carry the parameters of the traced out qubit *as well as the cross-terms*. Some of the terms that could be factored before into parameters in the reduced state and parameters in the map cannot be. This leads to the following map:

$$
\mathfrak{B} = \frac{1}{2}\begin{pmatrix}
\begin{matrix}1 + c_1c_2 \\ +e_{03}s_1s_2 \\ +e_{12}c_1s_2 - e_{21}c_2s_1\end{matrix} & 0 & \begin{matrix}e_{01}s_2s_3 - ie_{02}s_3s_1 \\ +e_{23}c_2s_3 - e_{32}c_3s_2 \\ -ie_{31}c_3s_1 + ie_{13}c_1s_3\end{matrix} & (c_1 + c_2)\,c_3 \\
0 & \begin{matrix}1 - c_1c_2 \\ +e_{03}s_1s_2 \\ +e_{12}c_1s_2 - e_{21}c_2s_1\end{matrix} & (c_2 - c_1)\,c_3 & \begin{matrix}e_{01}s_2s_3 - ie_{02}s_3s_1 \\ +e_{23}c_2s_3 - e_{32}c_3s_2 \\ -ie_{31}c_3s_1 + ie_{13}c_1s_3\end{matrix} \\
\begin{matrix}e_{01}s_2s_3 + ie_{02}s_3s_1 \\ +e_{23}c_2s_3 - e_{32}c_3s_2 \\ +ie_{31}c_3s_1 - ie_{13}c_1s_3\end{matrix} & (c_2 - c_1)\,c_3 & \begin{matrix}1 - c_1c_2 \\ -e_{03}s_1s_2 \\ -e_{12}c_1s_2 + e_{21}c_2s_1\end{matrix} & 0 \\
(c_1 + c_2)\,c_3 & \begin{matrix}e_{01}s_2s_3 + ie_{02}s_3s_1 \\ +e_{23}c_2s_3 - e_{32}c_3s_2 \\ +ie_{31}c_3s_1 - ie_{13}c_1s_3\end{matrix} & 0 & \begin{matrix}1 + c_1c_2 \\ -e_{03}s_1s_2 \\ -e_{12}c_1s_2 + e_{21}c_2s_1\end{matrix}
\end{pmatrix}.
$$

The first thing to note about this map is that there are some elements that are 0. This is due to the fact that not all terms can be decomposed as a

product that divide parameters between the state and the action of the map. In other words, the map $\mathfrak{B}$ carries all the information in the cross terms of the initial two qubit state. To guarantee that this map correspond to something physical, we need to observe that due to the initial correlations of the bipartite state, only certain values are permitted for the reduced intimal state. The map has some information of its allowed domain, and as long as it acts on it the evolution can still be given physical interpretation [49] and its eigenvalues in general can be negative. There are some experimental examples of these not completely positive maps [50].

In general, do all correlations lead to not completely positive maps? Is there a way of characterizing these correlations that let us easily see if a given initial state will lead to completely positive dynamics under *any* unitary?

5.3 Classical and Quantum Correlations

The traditional division of bipartite density matrices ρ^{XY} into separable and entangled is often taken to be synonymous with classical correlations and quantum correlations respectively, as introduced by Werner in [51]. In this prescription, separable states of the form:

$$\rho^{\mathsf{XY}} = \sum_j p_j \rho_j^{\mathsf{X}} \otimes \rho_j^{\mathsf{Y}},$$

where $0 \leq p_j$ and $\sum_j p_j = 1$ are said to be classically correlated as they represent a classical ensemple of uncorrelated particles $\rho_j^{\mathsf{X}} \otimes \rho_j^{\mathsf{Y}}$. States that are not of this form, Werner will say, are entangled and quantum correlated.

Ollivier and Zurek [48] and independently Henderson and Vedral [52] have proposed a different definition for classical and quantum correlations in density matrices based on information theoretic considerations. Suggestions for characterizing the correlations along similar lines were also made by Bennett et al. in [53, 54].

Correlations in classical information theory between random variables X and Y that describe a probability distribution can be measured by the mutual information

$$\mathbf{J}(\mathsf{Y} : \mathsf{X}) = \mathbf{H}(\mathsf{Y}) - \mathbf{H}(\mathsf{Y}|\mathsf{X}),$$

where $\mathbf{H}$ is Shannon's entropy, $\mathbf{H}(\mathsf{Y}|\mathsf{X})$ is the conditional entropy of Y given X. As a consequence of Bayes' rule the conditional entropy can be written as

$$\mathbf{H}(\mathsf{Y}|\mathsf{X}) = \mathbf{H}(\mathsf{Y}, \mathsf{X}) - \mathbf{H}(\mathsf{X}).$$

This leads to a different but equivalent formula for the classical mutual information

$$\mathbf{I}(\mathsf{Y} : \mathsf{X}) = \mathbf{H}(\mathsf{X}) + \mathbf{H}(\mathsf{Y}) - \mathbf{H}(\mathsf{X}, \mathsf{Y}).$$

These definitions have to be reexamined for quantum correlations. Since the information that can be obtained from a quantum system depends on the choice of measurements that are performed on it, the quantum version of the conditional entropy differs from the conditional entropy for classical information. If X and Y are quantum systems with their state described by the density matrix ρ^{XY}, then the conditional entropy of the system Y depends on the outcomes of system X due to a set of measurements made on it. These measure-

ment can be written in terms of a particular set of one-dimensional orthogonal projectors $\{\Pi_j^{\mathsf{X}}\}$ acting on the space of X. Hence to compute $\mathbf{J}(\mathsf{Y} : \mathsf{X})$, we change the definition of $\mathbf{H}(\mathsf{Y}|\mathsf{X})$ to

$$\mathbf{H}(\mathsf{Y}|\mathsf{X}) = \mathbf{H}\big(\mathsf{Y}\big|\{\Pi_j^{\mathsf{X}}\}\big)$$

where

$$\mathbf{H}\big(\mathsf{Y}\big|\{\Pi_j^{\mathsf{X}}\}\big) = \sum_j p_j \mathbf{H}(\rho_{\mathsf{Y}|\Pi_j^{\mathsf{X}}}),$$

with

$$p_j = \mathrm{Tr}_{\mathsf{X},\mathsf{Y}} \Pi_j^{\mathsf{X}} \rho^{\mathsf{XY}}$$

and

$$\rho_{\mathsf{Y}|\Pi_j^{\mathsf{Y}}} = \Pi_j^{\mathsf{X}} \rho^{\mathsf{XY}} \Pi_j^{\mathsf{X}} / p_j,$$

and the Shannon's entropy is replaced by the von Neumann entropy [9]. The difference between $\mathbf{I}$ and $\mathbf{J}$ is called *quantum discord* and it is taken as a measure of non-classical correlations in a quantum state [48].

A quantum state with only classical correlations satisfies the condition

$$\rho^{\mathsf{XY}} = \sum_j \Pi_j^{\mathsf{X}} \rho^{\mathsf{XY}} \Pi_j^{\mathsf{X}}.$$

States of this form are a subset of the set of all separable states and the subset includes all simply separable (tensor product) states. On the other hand, not all separable states have only classical correlations implying that quantum correlations must be taken to mean more than just entanglement. The information theoretic characterization of quantum states based on the

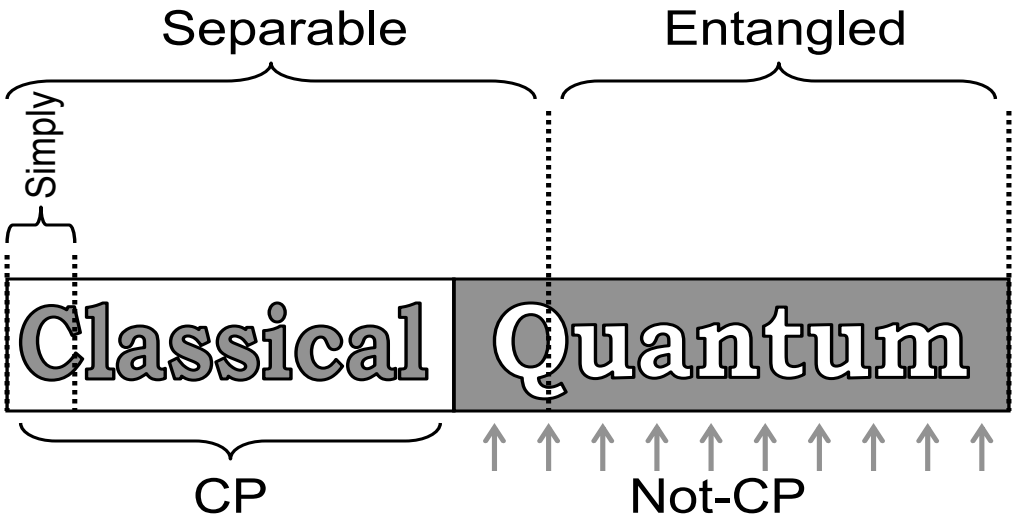

Figure 5.1: Quantum states of bipartite systems can be divided into having classical and quantum correlations. Separable states can have quantum correlations while simply separable states have only classical correlations. Not all quantum correlations are equivalent to entanglement. Also shown is the nature of the dynamical maps induced by any unitary evolution of the state of a system and its environment when the initial state belongs to each class. Classically correlated states are a sufficient condition for completely positive maps while there are examples, indicated by the arrows, showing that states with quantum correlations can lead to not completely positive maps.

nature of the correlations present is compared with the traditional division into separable and entangled states in Fig. 5.1.

Since measurements can be used to initialize quantum states, classically correlated states are of experimental interest. This is done by performing a complete set of (non-selective) orthogonal projective measurements $\{\Pi_j\}$ on the system. After the measurements, the initial state of the system and its

environment are *not* uncorrelated, having the form

$$\rho^{\mathcal{SE}} = \sum_j \Pi_j \rho^{\mathcal{SE}} \Pi_j = \sum_j p_j \Pi_j \otimes \tau_j, \tag{5.10}$$

where τ_j are density matrices for $\mathcal{E}$, $\left\{\Pi_j\right\}$ are a complete set of orthogonal projectors on $\mathcal{S}$, $p_j \geq 0$ and $\sum_j p_j = 1$. Sending a beam of photons through a polarizer or an electron beam through a Stern-Gerlach apparatus are examples of this type of preparations. Thus, classically correlated states appear often as the initial state for many quantum processes.

5.4 Classical Correlations and Complete Positivity

We would like to show that systems that are classically correlated with their environment lead to completely positive dynamics. In this section we give a short proof of this theorem, but a more detailed proof can be found in Appendix B.

We start with the reduced evolution of a system η as given by a dynamical map of the form from Eq. (2.6). The connection between the total dynamics and the reduced dynamics is:

$$\begin{array}{ccc} \rho(t_i) & \longleftrightarrow & \rho(t_f) = U_{(t_f|t_i)} \rho(t_i) U^\dagger_{(t_f|t_i)} \\ \downarrow & & \downarrow \\ \eta(t_i) & \dashrightarrow & \eta(t_f) = \mathrm{Tr}_{\mathcal{E}} \left[\rho(t_f)\right]. \end{array} \tag{5.11}$$

To reduce the space space, we defined a trace map

$$\mathfrak{T} \rho^{\mathcal{SE}} \equiv \mathrm{Tr}_{\mathcal{E}} \rho^{\mathcal{SE}} = \eta.$$

It is of interest to define a map $\mathfrak{E}$ that can establish the initial correlations with the environment, such that the entire process is the composition of three maps

$$\mathfrak{B}_{(t_f|t_i)} \equiv \mathfrak{T} \star \mathfrak{U}_{(t_f|t_i)} \star \mathfrak{E}. \tag{5.12}$$

We focus on a map that establishes the initial correlations for states that are classically correlated with their environment. This *embedding map* is defined as:

$$\mathfrak{E}\left(\eta^{\mathcal{S}}\right) = \sum_j \Pi_j^{\mathcal{S}} \, \eta^{\mathcal{S}} \, \Pi_j^{\mathcal{S}} \, \otimes \tau_j^{\mathcal{E}} = \rho^{\mathcal{S}\mathcal{E}}. \tag{5.13}$$

The total state given by the map has only classical correlations as can be verified by:

$$\mathfrak{E}\left(\eta^{\mathcal{S}}\right) = \sum_j \Pi_j^{\mathcal{S}} \otimes \mathbb{I}^{\mathcal{E}} \, \mathfrak{E}\left(\eta^{\mathcal{S}}\right) \, \Pi_j^{\mathcal{S}} \otimes \mathbb{I}^{\mathcal{E}}. \tag{5.14}$$

Now we have everything necessary for the theorem.

Theorem: Initially classically correlated states of the form

$$\rho^{\mathcal{S}\mathcal{E}} = \sum_j \Pi_j^{\mathcal{S}} \otimes \mathbb{I}^{\mathcal{E}} \, \rho^{\mathcal{S}\mathcal{E}} \, \Pi_j^{\mathcal{S}} \otimes \mathbb{I}^{\mathcal{E}},$$

will lead to completely positive dynamics.

Proof: We define the dynamical map as the composition of three maps, as given by Eq. (5.12). The first part of the map, the trace $\mathfrak{T}$, is completely positive as it can always be written as:

$$\mathfrak{T}\rho^{\mathcal{S}\mathcal{E}} = \sum_e \langle e^{\mathcal{E}}|\rho^{\mathcal{S}\mathcal{E}}|e^{\mathcal{E}}\rangle,$$

where $|e^{\mathcal{E}}\rangle$ defines a basis on the environment state. This is of the completely positive form. The second part of the map, the unitary, is also of the completely positive form

$$\mathfrak{U}\,\rho^{\mathcal{SE}} = U\;\rho^{\mathcal{SE}}\;U^{\dagger}.$$

The third part of the map, the embedding $\mathfrak{E}$ is also completely positive as it is written as

$$\mathfrak{E}\left(\eta^{\mathcal{S}}\right) = \sum_{j} \Pi_j^{\mathcal{S}} \otimes \sqrt{\tau_j^{\mathcal{E}}}\;\eta^{\mathcal{S}}\;\Pi_j^{\mathcal{S}} \otimes \sqrt{\tau_j^{\mathcal{E}}}.$$

The composition of all three completely positive map lead to a completely positive dynamical map. Thus, classical correlations with the environment guarantee that the dynamics will be completely positive.

Remark: The map $\mathfrak{B}$ comes from the contraction of the unitary evolution of the combined state. Note that by specifying the initial state $\rho^{\mathcal{SE}}$ in Eq. (5.10) we have restricted ourselves to the subset of all possible initial system states that is spanned by the projectors $\left\{\Pi_j\right\}$. We have shown that the reduced dynamics on these states coming from arbitrary unitary transformations on the extended, classically correlated, state is completely positive. Once the superoperator describing these dynamics has been identified, its action can be extended to all states of the system and the complete positivity of the map guarantees that it will transform states to other states. For all the states inside the subset spanned by $\left\{\Pi_j\right\}$ we have the additional benefit of seeing how the map could arise in real physical systems. For states outside

this subset we do not have the advantage of an obvious mechanism that would explain the action of the map, but all the same the map takes density matrices to density matrices. Our result shows that *any* reduced unitary evolution of an open system that is initially *classically correlated* will be completely positive[1].

The evolution of an open system that has initial quantum correlations with the environment might lead to not completely positive maps as shown in Fig. 5.1. We propose that if a not completely positive map is found in an experiment, this should be considered as a signature that the system had quantum correlations with the environment [2].

5.4.1 Example of Completely Positive Map from Classical Correlations

We can compute an example of completely positive maps coming from a classically correlated state by preparing the state given by Eq. (5.5) with a set of projective measurements $\left\{\Pi_j\right\}$ along the σ_2 direction on the system space. This gives the initial state,

$$\sum_j \Pi_j \rho^{\mathcal{SE}} \Pi_j = \frac{1}{4}(\mathbb{I}\otimes\mathbb{I} + a_2\sigma_2\otimes\mathbb{I} + e_{23}\sigma_2\otimes\sigma_3),$$

[1] This result is different from Tong et al. [55]. They showed that a *particular* initial state can be connected to a particular final state by matrices that have a form similar to Eq. (5.4). However, since their matrices depend both on the initial and final state, their result had to be interpreted as a point to point connection that might not be map.

[2] Our definition of quantum correlations is different from the ones considered in previous studies by other authors [16, 18].

which is only classically correlated. By evolving this state using the unitaries given by Eq. (5.6), the following dynamical map is obtained:

$$\mathfrak{B} = \frac{1}{2}\begin{pmatrix} 1 & 0 & e_{23}cs & c^2 \\ 0 & 1 & -c^2 & e_{23}cs \\ e_{23}cs & -c^2 & 1 & 0 \\ c^2 & e_{23}cs & 0 & 1 \end{pmatrix}, \tag{5.15}$$

where $c \equiv \cos(2\omega t)$ and $S \equiv \sin(2\omega t)$. Its eigenvalues are

$$\begin{aligned} \lambda_{1,2} &= \frac{1}{2}\Big[1 + \sqrt{\cos^4(2\omega t) + \big(e_{23}\cos(2\omega t)\sin(2\omega t)\big)^2}\Big], \\ \lambda_{3,4} &= \frac{1}{2}\Big[1 - \sqrt{\cos^4(2\omega t) + \big(e_{23}\cos(2\omega t)\sin(2\omega t)\big)^2}\Big], \end{aligned}$$

which are always positive as expected.

5.5 Importance of not completely positive maps

We have shown how for generalized initial correlations the condition of complete positivity (and even of positivity) must be relaxed for the dynamical maps. This is necessary for a proper physical interpretation of open quantum systems correlated with their environments. With this insight, we can go beyond the Markov approximation and directly study non-Markovian open quantum systems. We feel that a complete theory of non-Markovian open quantum system dynamics has eluded many authors as they have tried to confine it only within completely positive dynamics. In the next chapter we derive the non-Markovian dynamical map by allowing it to be not completely positive.

Chapter 6

Non-Markovian Dynamical Maps

In the previous chapter we studied the impact that initial correlations can have on the eigenvalues of a dynamical map. In this chapter we study the relationship between initial correlations and the composition property of the dynamical map. With it, we can consistently define a dynamical map that accounts for correlations at all times. This map is fully non-Markovian.

First, let us consider the case of a closed system that undergoes a unitary evolution. Since unitary evolutions form a group, the unitary maps have the composition property

$$\mathfrak{U}_{(t_2|t_0)} = \mathfrak{U}_{(t_2|t_1)} \star \mathfrak{U}_{(t_1|t_0)}.$$

However, this property is not true for all dynamical maps that correspond to open systems. A dynamical map of states that were uncorrelated at t_0 might have developed correlation through time, its history reducing the allowed set of states at time t_1 such that:

$$\mathfrak{B}_{(t_2|t_0)} \neq \mathfrak{B}_{(t_2|t_1)} \star \mathfrak{B}_{(t_1|t_0)}.$$

In order to derive the Kossakowski-Lindblad master equation, the Markov

approximation was invoked for short times [2], making

$$\mathfrak{B}_{(t_2|t_0)} \approx \mathfrak{B}_{(t_2|t_1)} \star \mathfrak{B}_{(t_1|t_0)}.$$

The maps now form a dynamical semigroup. This approximation might lead to unphysical results [39]. It also discards correlations at all times. Tied to these assumptions, demands for completely positive dynamics have also been imposed [37, 38]. Altogether, these restrictions can describe dissipative processes at the expense of discarding all non-Markovian memory effects and correlations with the environment, as described in Chapter 4. We will study how to relax these assumptions to account for physically meaningful initial correlations by allowing not completely positive dynamical maps.

6.1 Correlations and History

System-environment states in a tensor product can be evolved to develop correlations with their dynamical maps computed as before,

$$\begin{array}{ccc} \rho(t_0) = \eta(t_0) \otimes \tau & \leftrightarrow & \rho(t_2) = \mathfrak{U}_{(t_2|t_0)}\Big(\rho(t_0)\Big) \\ \downarrow & & \downarrow \\ \eta(t_0) & \rightarrow & \mathfrak{B}_{(t_2|t_0)}\Big(\eta(t_0)\Big) = \eta(t_2). \end{array} \tag{6.1}$$

$\mathfrak{B}_{(t_2|t_0)}$, since it comes from initially uncorrelated states, is completely positive. If we introduce an intermediate time t_1 the situation becomes,

$$\begin{array}{ccccc} \rho(t_0) & \leftrightarrow & \rho(t_1) = \mathfrak{U}_{(t_1|t_0)}\Big(\rho(t_0)\Big) & \leftrightarrow & \rho(t_2) = \mathfrak{U}_{(t_2|t_1)}\Big(\rho(t_1)\Big) \\ \downarrow & & \downarrow & & \downarrow \\ \eta(t_0) & \rightarrow & \mathfrak{B}_{(t_1|t_0)}\Big(\eta(t_0)\Big) = \eta(t_1) & \dashrightarrow & \mathfrak{B}_{(t_2|t_1)}\Big(\eta(t_1)\Big) = \eta(t_2). \end{array} \tag{6.2}$$

$\mathfrak{B}_{(t_2|t_0)}$ as well as $\mathfrak{B}_{(t_1|t_0)}$ are completely positive, but $\mathfrak{B}_{(t_2|t_1)}$ might come from a total state,

$$\rho(t_1) \neq \eta(t_1) \otimes \tau.$$

Maps with initial correlations, such as entanglement [14] and more generalized quantum correlations [17] have been studied, and in general are not even positive. To develop a prescription to consistently describe maps for initially correlated states, we need to find the inverse of the trace at time t_1, $\mathfrak{T}\rho(t_1) = \eta(t_1)$, such that $\eta(t_1) \rightarrow \rho(t_1)$, and using this write a dynamical map. This was accomplished in Section 2.2.5 by introducing a completely positive embedding map, Eq. (2.9). For initially correlated states it is necessary to relax the positivity condition. Since complete positivity is a stronger condition than positivity, this will need to be relaxed as well, as was proposed by Pechukas [14]. We will study when these not completely positive maps have a physical interpretation when we account for non-Markovian quantum dynamics.

6.2 Inverse Maps

We need a consistent way to define $\mathfrak{B}_{(t_2|t_1)}$ that follows the property

$$\mathfrak{B}_{(t_2|t_0)} = \mathfrak{B}_{(t_2|t_1)} \star \mathfrak{B}_{(t_1|t_0)}.$$

This can be achieved by exploiting the group property of the unitary maps $\mathfrak{U}$ in the total system-environment space. The correlations that exists at time t_1 can possibly be mapped back to a time t_0 where they were uncorrelated. Correlations at t_1, by definition, limit the valid domain of states at that time.

Identically, the history from $[t_0, t_1]$ can limit the domain at time t_1. Correlations are treated as a consequence of the memory effects from $[t_0, t_1]$. Non-Markovian dynamics are obtained from system variables that are correlated with outside variables.

A consistent way to define maps after they have developed correlations is by the use of inverse maps. Inverse maps have been studied before [56], but here we will consider the general form described in Section 2.2: find a matrix inverse $\widetilde{\mathfrak{A}_{(t_f|t_i)}}$ of the map $\mathfrak{A}_{(t_f|t_i)}$ that evolves the state backwards in time. Inverse maps require that the original map be one-to-one. Since we are considering the maps that come from an evolution in time, if for the particular final time t_f the map behaves as a pin map, that is, shrinks the whole space into a point, the map will not be one-to-one will not be invertible. But, for some other time close enough to t_f the map would be one-to-one. By exploring the neighborhood in time of the map, its inverse can be found.

The map is not unique [5], as additional information is necessary to select among all the possible ones. This additional information is the history as given by the unitary evolution. From this, the inverse dynamical map $\widetilde{\mathfrak{B}}_{(t_i|t_f)} \equiv \widetilde{\mathfrak{B}_{(t_f|t_i)}}$ can be found, which is in general not a positive map. $\widetilde{\mathfrak{B}}_{(t_i|t_f)}$ can only be meaningfully applied on the set $\mathfrak{B}_{(t_f|t_i)}\eta(t_i)$ for all density matrices $\{\eta(t_i)\}$. The compatibility domain is identical to the set of states compatible with the history from $[t_0, t_1]$. It should be applied only where it is meant to be [10]. States outside the compatibility domain will be inconsistent with its history, and when its evolution is reversed it might not be mapped to a valid

physical state. There is no reason for these maps to be positive in all cases, much less completely positive. On the contrary, history effects should create correlations that might limit the domain of validity.

Experimentally, inverse maps can be found from their forward counterparts. Since we are considering finite-dimensional environments, the evolution will have Poincaré recurrences in it. The Poincaré recurrences imply that the system will have quasi periodicity and repeatedly it will get very close to the original state. The recurrence time gets longer as the environment is of larger dimensions, but the effective environment might not need be very large. It has been shown in [5] that the evolution of a system state of N dimensions can be modeled with at most an environment with N^2 dimensions. This makes the number of parameters needed to be found tractable; their complication brought by the specifics of the Hamiltonian dynamics.

For example, if we consider only time-independent Hamiltonians which creates a periodic evolution of the system, we only need to know the evolution forward in time for one period to find the inverse map. If the evolution is quasi periodic, approximations to the inverse evolution can be obtained by knowing a successive higher order derivatives. For time-dependent Hamiltonians, the situation is more complicated. This can be done for a qubit system coupled to a qubit environment, and was developed in [57], where only a finite number of derivatives was shown to be needed to (almost) fully characterize the evolution of the total state. Another procedure for determining the total Hamiltonian of qubit systems is given in [58]. Full knowledge might not be accomplished prac-

tically and we will need to study the limitations that partial knowledge impose in the reconstructed dynamics. We will show how incomplete knowledge of the evolution leads to irreversibility in Chapter 8.

6.3 Canonical Dynamical Maps

With the inverse map $\widetilde{\mathfrak{B}}$, we can now define a *canonical dynamical map* $\mathfrak{B}^{\mathbb{C}}_{(t_f|t_i)}$ for initially correlated states at time t_1. This represents the additional variables needed to extend a system space to make a non-Markovian evolution into a Markovian one in the total space. The difficulty is that in order to describe them, full knowledge of the history is needed: the canonical dynamical map is non-Markovian.

To define the canonical map, we compose the maps to find the evolution from $t_1 \to t_2$ as in Fig. (6.1). First, we map the state from t_1 to t_0 using the inverse map, and from there evolve the state forward to t_2:

$$\mathfrak{B}^{\mathbb{C}}_{(t_2|t_1)} \equiv \mathfrak{B}_{(t_2|t_0)} \star \widetilde{\mathfrak{B}}_{(t_0|t_1)}. \tag{6.3}$$

That is easily computed in the $\mathfrak{A}$ form of the map; composition in it is just matrix multiplication. From Eq. (6.3), since the map depends on a time interval, the canonical dynamical maps follow the composition property:

$$\mathfrak{B}^{\mathbb{C}}_{(t_f|t_i)} = \mathfrak{B}^{\mathbb{C}}_{(t_f|t)} \star \mathfrak{B}^{\mathbb{C}}_{(t|t_i)}, \tag{6.4}$$

without need of any approximations.

It has been implied that $t_0 < t_1 < t_2$, but this needs not be. If $t_1 = t_0$, the original completely positive map is obtained. If $t_0 \leq t_1$ but $t_2 = t_0$, we

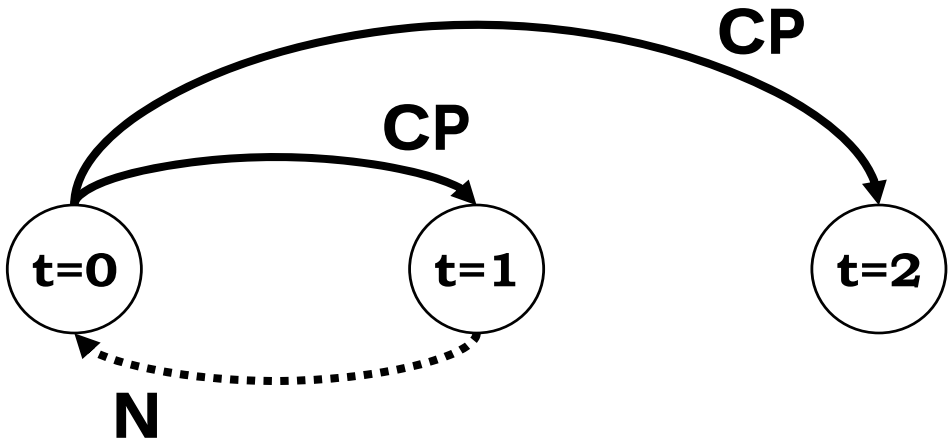

Figure 6.1: This diagram represents the evolution described by Eq. (6.2). **CP** is Completely Positive evolution, **N** is Not Positive Evolution. A not positive dynamical map from $t_1 \to t_2$ can be defined going to t_0, and from there forward to t_2, as in Eq. (6.3).

obtain

$$\mathfrak{B}^{\mathbb{C}}_{(t_0|t_1)} = \mathfrak{B}_{(t_0|t_0)} \star \widetilde{\mathfrak{B}}_{(t_0|t_1)} = \widetilde{\mathfrak{B}}_{(t_0|t_1)}, \tag{6.5}$$

using the identity $\mathfrak{B}_{(t_0|t_0)} = \mathbb{I}$. Since

$$\mathfrak{B}^{\mathbb{C}}_{(t_i|t_f)} \star \mathfrak{B}^{\mathbb{C}}_{(t_f|t_i)} = \mathfrak{B}^{\mathbb{C}}_{(t_f|t_i)} \star \mathfrak{B}^{\mathbb{C}}_{(t_i|t_f)} = \mathbb{I},$$

we conclude that inverse maps are also canonical maps. Canonical maps have the composition property given in Eq. (6.4), and have an inverse from Eq. (6.5), forming a one parameter group in time. They preserve the trace and hermiticity, but they are in general not positive and are only valid within their compatibility domain. This is what we wanted: a map that allows for correlations with the environment such that any incompatible state with the correlations

will be an unphysical total state. Only some canonical maps $\mathfrak{B}^{\mathbb{C}}_{(t'|t)}$ (such as the unitary map) might be completely positive for any choice of t and t'. With the aid of the canonical dynamical map, we can now define an embedding map for initially correlated systems.

6.4 Canonical Embedding Map

We had mentioned the need for the embedding map $\mathfrak{E}_{t_i}$ that could consistently invert the trace map $\mathfrak{T}$ for states uncorrelated at time t_i. In this section we will focus only on the embedding from Eq. (2.9) for initially uncorrelated states, but the procedure can be generalized to any other valid embedding (completely positive or not completely positive) such as the ones proposed by Pechukas [14] and Alicki [46]. With the use of the canonical dynamical map, we can generalize these embedding maps to all times, even when the initial correlations have evolved, such that:

$$\eta(t) \to \mathfrak{E}^{\mathbb{C}}_t \eta(t) = \rho(t) \text{ for all } t.$$

Such an embedding map will use the knowledge of the history of the evolution of the reduced state to "close" the open system evolution into the one given by the total state. The procedure is to evolve the state backwards to the time where we had defined a valid embedding map, undo the trace then, and then unitarily go forward. From Eq. (2.7), this would be pictorically represented

by:

$$\begin{array}{ccccc} & & \mathfrak{U}_{(t|t_0)} & & \\ \rho(t_0) & & \Rightarrow & & \rho(t) = \mathfrak{E}_t^{\mathbb{C}}\eta(t) \\ \mathfrak{E}_{t_0} \quad \Uparrow & & & & \uparrow \\ \eta(t_0) & & \Leftarrow & & \eta(t). \\ & & \mathfrak{B}^{\mathbb{C}}_{(t_0|t)} & & \end{array}$$

This *canonical embedding map* from $\eta(t) \to \rho(t)$ is defined as:

$$\mathfrak{E}_t^{\mathbb{C}} \equiv \mathfrak{U}_{(t|t_0)} \star \mathfrak{E}_{t_0} \star \mathfrak{B}^{\mathbb{C}}_{(t_0|t)}. \tag{6.6}$$

Since it is defined using $\mathfrak{B}^{\mathbb{C}}$, the canonical embedding map preserves hermiticity and trace, but might not be positive, its compatibility domain corresponding to the system space compatible with the correlations existing at time t. The rest is the set of states that will give unphysical evolutions since they are incompatible with the memory effects of the environment.

We do not even need an embedding map for an uncorrelated total state for t_0, any valid embedding for any other time t will do:

$$\begin{aligned} \mathfrak{E}_t^{\mathbb{C}} &= \mathfrak{U}_{(t|t_0)} \star \mathfrak{E}_{t_0} \star \mathfrak{B}^{\mathbb{C}}_{(t_0|t)}, \\ &= \mathfrak{U}_{(t|t')} \star \left(\mathfrak{U}_{(t'|t_0)} \star \mathfrak{E}_{t_0} \star \mathfrak{B}^{\mathbb{C}}_{(t_0|t')} \right) \star \mathfrak{B}^{\mathbb{C}}_{(t'|t)}, \\ &= \mathfrak{U}_{(t|t')} \star \mathfrak{E}_{t'} \star \mathfrak{B}^{\mathbb{C}}_{(t'|t)}. \end{aligned} \tag{6.7}$$

By knowing one embedding map for a time t', any other embedding for another t can be found, as long as the unitary operator is known in the interval $[t, t']$. Although in this discussion it has been implied that $t' < t$, since we are using a canonical dynamical map, this needs not be. The valid defined embedding

at time t' might be at any time, even after t. Thus for one embedding at any t' the embedding for all times t can be found.

The unitary operator can be found from monitoring the system's evolution with sufficient precision. Again, if it yields a periodic evolution, it needs to be known only within a finite time interval. If it is pseudo-periodic or time dependent, it can be approximated by determining the process to a sufficient number of derivatives. We refer again to the procedure of how this can be implemented for a qubit system and environment that was presented in [57, 58].

This approach explicitly shows the connection between the correlations of the state and its history. Correlations at one time can be changed to correlations at another as long as the history is known. The necessity of additional knowledge to establish an embedding map makes it non-Markovian. The possible negativity of the map shows how the history limits some of the states in the system space to be compatible with the total system-environment state [10, 11, 21, 56].

6.5 Example

We return to the example from the evolution of a qubit coupled to a fully mixed qubit environment as given by Eq. (2.12) to illustrate how to compute an inverse map, from it the canonical dynamical map and the canonical embedding map. We want to map the Bloch vector $\overrightarrow{a}$ from the final time t_f

to the initial time t_i. In its affine form this is:

$$\overrightarrow{a}(t_i) = \overline{R}^{-1}_{(t_f|t_i)} \cdot (\overrightarrow{a}(t_f) - \overrightarrow{r}) .$$

For the particular example from Eq. (2.12),

$$\overrightarrow{a}(0) = \frac{1}{c^2}\overrightarrow{a}(t).$$

The inverse $\widetilde{\mathfrak{A}}_{(t_0|t)} \equiv \widetilde{\mathfrak{A}_{(t|t_0)}}$ can be consistently found from the dynamics,

$$\widetilde{\mathfrak{A}}_{(t_0|t)} = \frac{1}{2}\begin{pmatrix} 1+c^{-2} & 0 & 0 & 1-c^{-2} \\ 0 & 2c^{-2} & 0 & 0 \\ 0 & 0 & 2c^{-2} & 0 \\ 1-c^{-2} & 0 & 0 & 1+c^{-2} \end{pmatrix}.$$

By index exchange, we get the map in its Hermitian $\mathfrak{B}$ form to obtain $\widetilde{\mathfrak{B}}_{(t_0|t)}$, which in the Choi form has as eigenvalues and eigenmatrices:

$$\begin{aligned} \lambda_0(t-t_0) &= \frac{1}{2}\left(1+3c^{-2}\right), \qquad \mathrm{C}_0 = \tfrac{1}{\sqrt{2}}\mathbb{I}, \\ \lambda_{1,2,3}(t-t_0) &= \frac{1}{2}\left(1-c^{-2}\right), \quad \mathrm{C}_{1,2,3} = \tfrac{1}{\sqrt{2}}\sigma_{1,2,3}, \end{aligned} \tag{6.8}$$

that for certain values of t are not completely positive. This represents the periodic behavior of the original map: as the state is squeezed, the compatibility domain of its inverse maps also shrinks. For the times where $c = 0$, the only compatible state is the center of the Bloch sphere. States outside the compatibility domain are not relevant to the physical dynamics of the open system as they are inconsistent with the developed correlations and history.

We can define the canonical dynamical map by means of Eq. (6.3). The composition property is easier to apply on the $\mathfrak{A}$ form of the map, since it is

just matrix multiplication. By computing $\mathfrak{A}_{(t'|t_0)} \cdot \widetilde{\mathfrak{A}}_{(t_0|t)} = \mathfrak{A}_{(t'|t)}$, we exchange the indices to obtain the $\mathfrak{B}^{\mathbb{C}}$ form of the canonical dynamical map, that has as its eigensystem:

$$\lambda_0(t'-t) = \frac{1}{2}\left(1 + 3\frac{c^2}{\widetilde{c}^2}\right), \qquad \mathrm{C}_0 = \frac{1}{\sqrt{2}}\mathbb{I},$$
$$\lambda_{1,2,3}(t'-t) = \frac{1}{2}\left(1 - \frac{c^2}{\widetilde{c}^2}\right), \qquad \mathrm{C}_{1,2,3} = \frac{1}{\sqrt{2}}\sigma_{1,2,3},$$

where $c \equiv \cos(t'-t_0)$ and $\widetilde{c} \equiv \cos(t-t_0)$. With $t = t_0$ the map is completely positive, while $t' = t$ makes it the inverse map.

Finally, a canonical embedding map can be computed from Eqs. (2.9), (6.6) and (6.8):

$$\mathfrak{E}_t^{\mathbb{C}}\Big(\eta(t)\Big) = U_{(t|t_0)}\left(\left[\mathfrak{B}^{\mathbb{C}}_{(t_0|t)}\Big(\eta(t)\Big)\right] \otimes \tau\right) U^{\dagger}_{(t|t_0)}.$$

From Eq. (2.11), with $\eta(t) = \frac{1}{2}\left(\mathbb{I} + a_j(t)\sigma_j\right)$ and $\tau = \frac{1}{2}\mathbb{I}$, we carry out the calculation to reach the final result:

$$\mathfrak{E}_t^{\mathbb{C}}\Big(\eta(t)\Big) = \frac{1}{4}\Big[\mathbb{I}\otimes\mathbb{I} + a_j(t)\Big(\sigma_j \otimes \mathbb{I}$$
$$+ \tan(t)^2\mathbb{I}\otimes\sigma_j + \tan(t)\left(\sigma_k\otimes\sigma_l - \sigma_l\otimes\sigma_k\right)\Big)\Big], \tag{6.9}$$

summing over index j, with $\{j,k,l\}$ being cyclic. The canonical embedding map connects the system space to the total space:

$$\mathfrak{E}_t^{\mathbb{C}}\Big(\eta(t)\Big) = \rho(t), \quad \mathrm{Tr}_{\mathcal{E}}\,\rho(t) = \eta(t).$$

The compatibility domain is represented here by the unbounded character of $\tan(t)$. Periodically the compatible set of vectors $\overrightarrow{a}(t)$ tend to the point at center of the Bloch sphere. In other words, as the correlations change periodically, so must do their compatible system parameters.

6.6 Discussion

In this chapter we have defined two new concepts. First, the canonical dynamical map that allows us to treat dynamical maps and their inverses in the same manner and has the desired composition property. With it, a canonical embedding map was defined to "close" the evolution of an open quantum system. Although the embedding map might seem as putting the horse before the carriage as it would allow us to forget the open dynamics of the system by understanding the total evolution of the total state, it should be thought of as a useful mathematical device. This will be exploited in Chapter 7 in order to derive a non-Markovian master equation. In Chapter 8 we will consider the realistic case where full knowledge of the embedding map is not possible, and how this leads to decoherence.

Chapter 7

Non-Markovian Master Equation

In Chapter 6 we defined a canonical dynamical map that has a composition property which the regular dynamical map was missing. To derive the Kossakowski-Lindblad master equation, this property was approximated by assuming a Markovian limit. Thanks to the canonical dynamical map, we have no need for this approximation. Also, with it, we can now define an embedding map that consistently relates the evolution of the system state with the total evolution of the state, properly accounting for correlations. We now proceed to derive the main result of this dissertation.

7.1 Derivation of the Non-Markovian Master Equation

The non-Markovian master equation can be derived from the canonical dynamical map from Eq. (6.6). The time derivative of the unitary operator is

$$\frac{\partial}{\partial t}U = \dot{U} = -iHU,$$

and it follows that the time derivative of the canonical dynamical map is:

$$\begin{aligned}\dot{\mathfrak{B}}^{\mathbb{C}}_{(t|t_i)}\Big(\eta(t_i)\Big) = \frac{\partial \eta(t)}{\partial t} = &-i\mathrm{Tr}_{\mathcal{E}}\left[HU_{(t|t_i)}\rho(t_i)U^{\dagger}_{(t|t_i)}\right] \\ &+i\mathrm{Tr}_{\mathcal{E}}\left[U_{(t|t_i)}\rho(t_i)U^{\dagger}_{(t|t_i)}H\right],\end{aligned}$$

and is equivalent to a von Neumann equation reduced to the system space,

$$\mathrm{Tr}_{\mathcal{E}}\left[\dot{\rho}(t)\right] = -i\mathrm{Tr}_{\mathcal{E}}\left[H, \rho(t)\right].$$

To make the differential equation to depend explicitly only on the system space, we use the canonical embedding map $\mathfrak{E}_t^{\mathbb{C}}$ from Eq. (6.7). The non-Markovian master equation is:

$$\frac{\partial}{\partial t}\eta(t) = -i\mathrm{Tr}_{\mathcal{E}}\left[H, \mathfrak{E}_t^{\mathbb{C}}\Big(\eta(t)\Big)\right].$$

Now, we write the total Hamiltonian as $H = H_O + H_I$, where H_O is the local (system) part of the Hamiltonian. This local part acts through the embedding map without changing it. With this, we have the standard form of the non-Markovian master equation:

$$\frac{\partial}{\partial t}\eta(t) = -i\Big[H_O, \eta(t)\Big] + \mathfrak{K}_t\Big(\eta(t)\Big), \tag{7.1}$$

with $\mathfrak{K}_t(\cdot) \equiv \mathfrak{F}_t(\cdot) + \mathfrak{F}_t^{\dagger}(\cdot)$, where:

$$\begin{aligned} \mathfrak{F}_t(\cdot) &= -i\mathrm{Tr}_{\mathcal{E}}\left[H_I\mathfrak{E}_t^{\mathbb{C}}(\cdot)\right], \\ \mathfrak{F}_t^{\dagger}(\cdot) &= +i\mathrm{Tr}_{\mathcal{E}}\left[\mathfrak{E}_t^{\mathbb{C}}(\cdot)H_I\right]. \end{aligned} \tag{7.2}$$

The Hermitian superoperator $\mathfrak{K}_t$ is related to the time derivative of the canonical dynamical map by:

$$\frac{\partial}{\partial t}\mathfrak{B}^{\mathbb{C}}(\cdot) = -i\left[H_O, \cdot\right] + \mathfrak{K}_t(\cdot). \tag{7.3}$$

The H_O term is the Hamiltonian evolution of the system and $\mathfrak{K}_t$ carries all the effects of the environment, including decoherence and memory. This is a generalization of the von Neumann equation to open quantum systems.

If the canonical embedding map is completely positive for all t, the master equation is completely positive, but even for not completely positive canonical maps this equation will be physically consistent for the set of states that are compatible with the history and correlations of the non-Markovian process.

Since the environment is finite-dimensional, there will be some periodicity [1] to this evolution as information goes from the system to the environment, and back. At certain times the space is being contracted, while at others it is expanded. These Poincaré recurrences are a consequence of the canonical maps forming a group. This should be contrasted to the Kossakowski-Lindblad master equation, that uses the Markov approximation to obtain a dynamical semigroup. The Markovian master equation can be obtained by forcing $\mathfrak{K}_t$ to be time independent.

7.2 Example

We will continue the example from Eq. (6.9) to illustrate how a master equation of the form Eq. (7.1) can be calculated. In this case, $H_O = 0$, $H_I = \frac{1}{2}\sum_j \sigma_j \otimes \sigma_j$ and $\mathfrak{E}_t^{\mathbb{C}}(\eta(t))$ was calculated in Eq. (6.9). We can calculate

[1] In general it is quasi periodic.

$\mathfrak{F}_t$ from Eq. (7.2) to be:

$$\mathfrak{F}_t\Big(\eta(t)\Big) = \sum_j \frac{1}{4}\Big(- i\tan(t)^2 - 2\tan(t)\Big)a_j(t)\sigma_j.$$

The non-Markovian master equation is then:

$$\dot{\eta}(t) = \mathfrak{K}_t\Big(\eta(t)\Big) = -\sum_j \tan(t)a_j(t)\sigma_j = 2\tan(t)\Big(\mathbb{I} - 2\eta(t)\Big). \tag{7.4}$$

If we only look at the σ_j component, the evolution of its expectation value

$$a_j(t) = \mathrm{Tr}\left[\eta(t)\ \sigma_j\right]$$

is:

$$\dot{a_j}(t) = -2\tan(t)a_j(t),$$

and has as solution

$$a_j(t) = \cos(t - t_0)^2 a_j(t_0),$$

which agrees with the starting point from Eq. (2.12). This is an example of how to find the canonical dynamical map from the non-Markovian master equation. There is no dissipation in this equation, as expected from the Poincaré recurrences for the finite system.

7.3 Relationship to other master equations

We have developed a generalized non-Markovian master equation for open quantum systems by accounting for correlations with the environment. Previous work on completely positive non-Markovian master equations can be

treated as special classes of the non-Markovian master equation in this dissertation. For example, Shabani and Lidar proposed a class of master equations whose memory comes from total states with correlations derived from measurement approach [59]. This is equivalent to having an embedding map from Eq. (6.7) for the particular time t' given by a measurement on the environment. From this, a canonical embedding equation can be developed for all times, and their master equation obtained. This class of embedding is completely positive, at the expense of limiting to only classical correlations of the environment with the system at time t' [17, 60]. Breuer proposes another class of embedding maps for a different restricted kind of correlations [61]. Our approach permits any kind of correlations, classical or quantum.

Chapter 8

Non-Equilibrium Quantum Thermodynamics

The Kossakowski-Lindblad master equation may be obtained by taking the Markov approximation and neglecting higher order terms of the dynamical map for the process. From this approximation, irreversibility is introduced and relaxation into thermodynamic equilibrium can be obtained. Exponential decays are natural solutions to many instances of this equation.

However, the non-Markovian master equation from Eq. (7.1) allows us to know the full evolution of the system without irreversibility. Thermodynamic effects can be introduced by expanding $\mathfrak{K}_t$ for short times without the need of the Markov approximation. As larger orders in time are computed in the approximation, longer memory effects are introduced and higher order correlations with the environment appear as well. Higher orders in time allow us to go beyond the thermodynamic regime; non-equilibrium quantum thermodynamical effects can be studied. We illustrate this with an example.

8.1 Example

The master equation from the example in Eq. (7.4) is not only non-Markovian, it is also periodic. To introduce some dissipation and decay, and

connect it to (non-equilibrium) thermodynamics, we must make an approximation for short times in the master equation, only the memory effects of that order in time will be kept. This approximation discards some knowledge of the evolution; irreversibility comes from the limited information. Experimentally, this could come from monitoring the system for only a short time, and trying to find the master equation from this incomplete information.

We approximate

$$\tan(t) \approx t,$$

and Eq. (7.4) becomes:

$$\dot{\eta}(t) = 2t\Big(\mathbb{I} - 2\eta(t)\Big),$$

and the evolution of just one component is,

$$\dot{a_j}(t) = -2t\ a_j(t).$$

The solution to this differential equation is

$$a_j(t - t_0) = e^{-(t-t_0)^2} a_j(t_0).$$

As time goes to infinity, the polarization of the vector shrinks to zero through a non-exponential decay due to the short-time memory effects retained from the bath. In other words, the bath is not an ideal (passive) thermodynamic bath as it is dynamically allowed to "kick back" slightly. This is an example of a non-equilibrium quantum thermodynamical effect. Its decay of the form e^{-t^2} should be contrasted to the thermodynamic (Markovian) decay $e^{-\gamma t}$ from

Eq. (4.9). The non-equilibrium thermodynamic decay can be faster than exponential for very small values of γ, while it can be slower for large values of γ. At intermediate values, $\gamma \approx 1$, the non-Markovian decay is slower than exponential at first, and then much faster, as shown in Figure (8.1). Accounting

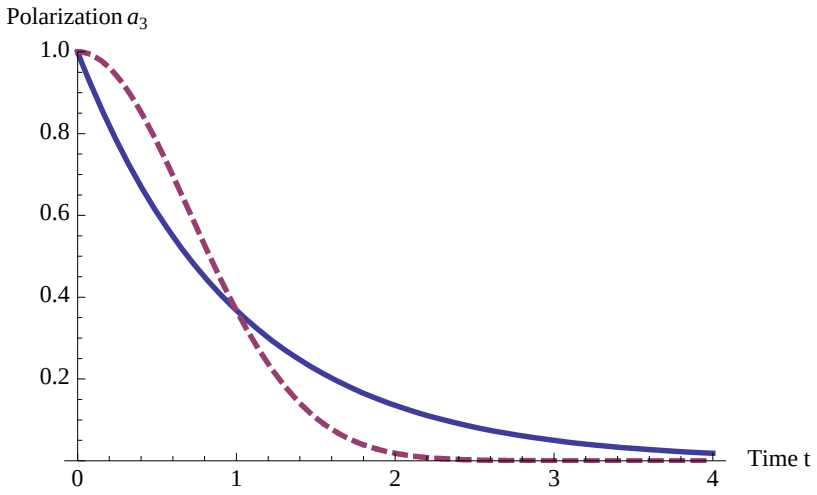

Figure 8.1: The solid line represents an exponential decay e^{-t} as found from the Kossakowski-Lindblad master equation. The dashed line represents a gaussian decay of the form e^{-t^2} from the non-Markovian master equation.

for memory effects can make the decays faster or slower.

The non-Markovian decay also differs from exponential decay close to the initial time. In this non-equilibrium thermodynamic solution, the initial time derivative of the polarization is zero, which is crucial to obtaining the quantum Zeno effect [41]. Before, quantum Zeno could be obtained only from the Hamiltonian part of the Kossakowski-Lindblad master equation. Now,

even the interaction with the environment can give rise to a Zeno region.

8.2 Discussion

The main difference of the non-Markovian approach to the Kossakowski-Lindblad approach to get irreversibility can be summarized as follows. In the Kossakowski-Lindblad case, the Markov approximation is made in order to be able to find the time derivative of the dynamical map. In contrast, with the use of the canonical dynamical map we can define the derivative of the dynamical map without need for approximations. If desired, approximations can be taken afterwards in order to get decoherence while still accounting for some memory effects. This leads to a deviation from the exponential decay.

Chapter 9

Conclusion

In conclusion, we have discussed how not completely positive dynamical maps in open quantum systems represent the limited domain due to correlations with the environment. We computed the dynamical map of the most general evolution for two qubits. We showed the differences in the maps when the initial states are simply-separable or not. Through examples, we illustrated how purity and entanglement are interchangeable quantities. We studied dynamical purity swapping, and its connection to decoherence phenomena. Our simple two qubit interaction is flexible enough to study the fundamentals of decoherence that are usually studied as an interaction with an infinite degrees of freedom reservoir.

We have studied the effect of initial correlations with the environment on the complete positivity of dynamical maps that describe the open systems evolution. We proved that classical correlations of the state of the system and its environment, as indicated by zero discord, are a sufficient condition the maps induced by any unitary evolution of the combined state to be completely positive. This result is more general than the previously known result for simply separable initial states, and it is important towards clarifying the

boundary between completely positive and not completely positive maps.

With the understanding of the role of correlations in connection with not completely positive maps, a canonical dynamical map was developed that can be applied for any initially correlated systems. The canonical dynamical maps form a dynamical group, different from the dynamical semigroup from the Kossakowski-Lindblad equation. A canonical embedding map can be constructed to express the correlations with the environment at any time, effectively closing the evolution of the open system. For this to be accomplished, full knowledge of the system's history is required. A generalized non-Markovian master equation was constructed that was local in time and corresponds to the reduced space von Neumann equation. Approximations to this equation, such as the ones given by a limited knowledge of the history, can lead to irreversible behavior beyond the purely thermodynamic regime. This theory permits the study of non-equilibrium quantum thermodynamic effects.

9.1 Experimental Implications

We have studied the role that correlations and history play on the mathematical properties of dynamical maps. These have experimental implications. The eigenvalues of the dynamical map can be exploited to study the correlations of the system with the environment. The non-Markovian master equation could be used to prevent decoherence by means of quantum control. Also, the non-Markovian master equation should be used to study experiments were non-Markovian effects have been identified.

9.1.1 Identifying Correlations using Quantum Process Tomography

It is often assumed that quantum process tomography corresponds to the experimental reconstruction of dynamical maps [42]. A number of known initial states, sufficient to span the space of density matrices of the system, are allowed to evolve as a result of an unknown process. We look at a quantum process tomography experiment on a solid-state qubit performed by Howard et al. in [50] in the light of the results presented above. In this experiment, the system of interest is a qubit formed in a nitrogen vacancy defect in a diamond lattice. The qubit was initialized to the state η_0 with

$$p_0 = \mathrm{Tr}\left[|\phi\rangle\langle\phi|\eta_0\right] = 0.7.$$

The state is not pure; it cannot be ruled out that the system could be correlated to the environment. The map corresponding to the decoherence process was found to have negative eigenvalues. The not completely positive map found in this experiment could be interpreted as an indication that the initial state of the system is not just classically correlated with the environment. Given that the qubit is in a large crystal lattice, it is perhaps not very surprising that it had quantum correlations with its surroundings. A detailed study of the connection of the evolution of open quantum systems and quantum process tomography can be found in [19].

9.1.2 Non-Markovian effects in Quantum Control

Non-Markovian open quantum system have been found and exploited experimentally for more than 50 years, but a complete theory was missing

until now. This made them difficult to classify, understand and to model.

An early attempt to exploit the memory effects of the environment was developed by Hahn [62], and is known as *spin echoes*. This was applied to a nuclear magnetic resonance experiment, where the decoherence of a spin state could be partially recovered by a local pulse. This is a purely non-Markovian effect that cannot be modeled by the Kossakowski-Lindblad master equation. Similar approaches have been developed that focus on the preservation of quantum information [35]. All of them have the following in common: there is irreversibility due to decoherence, but there are some memory effects in the bath and these can be exploited by means of local operations. To find the series of local operations that must be made in order to preserve the information is very difficult.

With the non-Markovian master equation this problem could be attacked. If the decohering process is described in the form from Eq. (7.3), and the local operations that can be controlled by the experimentalist with a Hamiltonian H_L, we obtain:

$$\frac{\partial}{\partial t}\mathfrak{B}^{\mathbb{C}}(\cdot) = -i\left[H_O, \cdot\right] - i\left[H_L, \cdot\right] + \mathfrak{K}_t(\cdot),$$

where it is implied that both H_O and H_L could be time dependent. Since we are interested in preventing the decoherence, we want to make the derivative of the dynamical map to be zero. This in turn means that the density matrix will not change in time. The control sequence H_L that the experimentalist will have to perform is simply given by solving the equation given by the

superoperators:

$$[H_L, \cdot] = [H_O, \cdot] + i\mathfrak{K}_t(\cdot).$$

This relationship should be explored and applied to specific experiments.

9.1.3 Non-Markovian effects in photosynthesis

Non-Markovian quantum effects have proven to be important in biology. Photosynthesis is the conversion of light energy into chemical energy by living organisms. The energy source is sunlight, and the end-products include glucose and oxygen. It is the most important biochemical pathway. The light energy is converted to chemical energy using the light-dependent reactions. This chemical energy production is more than 90% efficient with only 5-8% of the energy transferred thermally. How is the energy transferred so efficiently?

The Fenna-Matthews-Olson (FMO) complex is a protein complex appears in green sulfur bacteria and mediates the excitation energy transfer from the light-harvesting chlorosomes (the antenna) to the membrane embedded bacterial reaction center (the center that transforms light into chemical energy). This complex is often used in photosynthesis experiments. The structure of the FMO complex contains seven bacteriochlorophyll molecules. A very important property is the local transition energy (site energy) of the bacteriochlorophyll molecules which is different for each of them, due to their individual local protein environment. The site energies of the bacteriochlorophyll molecules determine the direction of the energy flow. It has been experimentally shown that the energy transfer in photosyntesis happens through

the seven bacteriochlorophyll molecules. In a resent experiment it was shown that this transfer is a quantum mechanical effect, the site energies of the FMO complex change from one to the other through quantum coherent effects [63].

The most surprising aspect of this discovery is that in nature this must happen at room temperature. Understanding how plants can maintain quantum coherence at such high temperatures would lead to significant advancements in solar cells and also in quantum information. The experiment [63] suggests that this could be a result of non-Markovian open quantum systems, but a full model of has not be done as a complete theory was missing. The non-Markovian master equation should be applied to study this experiment.

9.2 Future Directions

In Chapter 6 we described the connection between embedding maps and memory effects. We feel that although embedding maps are not new, they have not been studied in detail. A general form for embedding maps needs to be found in order to determine all possible canonical dynamical embedding maps.

Experimentally it is assumed that quantum process tomography can be used to find dynamical maps. We have pointed out here that if the system has correlations with the environment the picture is not as simple. How can canonical dynamical maps, that depend on correlations, be measured? How can the non-Markovian master equation's parameter be defined in an operational way? These open questions are crucial in order to determine the applicability of the theory developed in this dissertation.

Also, we have suggested that with enough knowledge of the local evolution, the total evolution might be inferred. What is sufficient knowledge is not clearly understood in a manner that can be readily applied to experiments.

The connection between non-equilibrium quantum thermodynamics was suggested in Chapter 8. This observation should be explored in depth as it is of fundamental importance. Also, the deviation from exponential decay could be defined in operational scheme. Such a definition would allow for experimental protocols to study non-Markovian open quantum systems.

9.3 Final Remarks

A lesson learned from the Kossakowski-Lindblad master equation is to always be honest about the approximations made and the limitations they impose. After understanding the physical implications of not completely positive maps, it is natural to develop a theory for non-Markovian open quantum systems. The work presented here should contribute to the foundations of the study of non-Markovian open quantum systems and its role in decoherence.

Appendices

Appendix A

Optimal entanglement generation

Entanglement is a resource for a quantum information processor [42, 64], while entanglement of elements of the information processor with its environment leads to undesirable loss of purity and decoherence. Naturally, there has been a lot of interest[1] in understanding [65], quantifying [66–70], and controlling [71–73] entanglement and also preventing decoherence. We show that both the loss of purity of qubits and the generation of entanglement between two qubits in an optimal way can be understood in terms of the dynamics generated by the same general two qubit interaction under different conditions.

In this appendix we continue the discussion from Chapter 3, where the full dynamics of two initially uncorrelated qubits was computed. With that machinery at hand, an interesting regime to study is related to the creation of maximally entangled Bell states. Assume that we have initially two pure states, $\{a_1 = 1,\ a_2 = a_3 = 0\}, \{b_2 = 1,\ b_1 = b_3 = 0\}$. At a specific time t_{bell}, each of the qubits' purity goes to a minimum. For $\gamma_3 = 1$, the minimum is at

[1] "As the strong man exults in his physical ability, delighting in such exercises as call his muscles into action, so glories the analyst in that moral activity which *disentangles*." [sic] Poe, E.A. "The Murders in the Rue Morgue" *Complete Stories and Poems of Edgar Allan Poe*. Ed. Doubleday & Company, Inc. Garden City, NY (1966)

$t_{bell} = \pi/4$, and we get that

$$\rho^{AB}(t_{bell}) = \frac{1}{4}\left[\mathbb{I}^A \otimes \mathbb{I}^B + \sigma_1^A \otimes \sigma_2^B - \sigma_2^A \otimes \sigma_3^B + \sigma_3^A \otimes \sigma_1^B\right], \tag{A.1}$$

that, given some freedom to choose the basis for ρ^B, would be equivalent to the Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. A similar, experimentally feasible time-reversed procedure would be responsible for extracting purity out of entanglement [74].

How much can an entanglement creation experiment be improved? From Eq. (3.7) an entanglement optimization protocol can be determined, given certain reasonable constraints. In particular, we would like to show how given a certain two qubit state and certain experimental limitations in the Hamiltonian that can be applied, the evolution can be optimized to maximize the entanglement between them.

Let us illustrate this with a simple example for the case of the creation of entanglement from initially pure qubits. Limitations on the allowed interaction and their duration would come from particular experimental requirements. This example, although very simple, contains all the elements to illustrate how a procedure like this can be implemented. The more general protocol is discussed afterwards.

Imagine some experimental setup that prepares two qubits with the Bloch vectors **a** and **b** representing their states oriented at some angle with respect to each other. The aim is to entangle these two. Assume that only two kinds of couplings between them are allowed and we can only act first with one kind followed by the other, due to some experimental constraints.

The only thing that can be controlled is the duration for which each coupling is used. The total time available is restricted by decoherence. This type of interaction can be similar to the "strongly modulating" pulses in nuclear magnetic resonance implementation of quantum algorithms, but is not limited to it. How long should we act with each of them to maximize the entanglement rate?

Let the two qubits ρ^A and ρ^B, initially be in the states given by $a_1 = 1$, $a_2 = a_3 = 0$ and $b_1 = b_2 = 1/\sqrt{2}$, $b_3 = 0$. The allowed interactions are $\gamma_2 = 1,\ \gamma_1 = \gamma_3 = 0$ for some time $[0, t']$ and followed by $\gamma_3 = 1,\ \gamma_1 = \gamma_2 = 0$ at t' for an interval $(t', \pi]$. Using Eq. (3.7) we can calculate the state $\rho^{AB}(t)$ of the system at t'. Using $\rho^{AB}(t')$ as the new initial condition in Eq. (5.8) and the new coupling, $\gamma_3 = 1$ we can compute the state of the two qubits during $(t', \pi]$. Eq. (3.9) gives us the reduced density matrix of one of the qubits as a function of time from which we can compute its purity at every time.

What is the time t' that gives us the maximum entanglement? This protocol is not dependent on a particular measure of entanglement, but we will choose for simplicity the entropy of entanglement [66], which is a good measure as long as $\rho^{AB}(t)$ remains pure. Since it is monotonically related to the linear entropy [28], the entanglement measure $\mathcal{E}$ can also be chosen:

$$\mathcal{E} \sim 1 - \mathrm{Tr}\left[(\rho^A)^2\right] = 1 - \mathrm{Tr}\left[(\rho^B)^2\right] = 1 - P. \tag{A.2}$$

Using Eqs. (3.10) and (4.4), we find that for our choices of the parameters:

$$\mathcal{E} \sim 1 - \frac{3\cos(8t') + 29}{32}. \tag{A.3}$$

which is maximized at $t' = \pi/8,\ 3\pi/8,\ 5\pi/8$ or $7\pi/8$. We admit that this example is rather simple, and was chosen because it can be easily solved algebraically. More complicated and realistic couplings and limitations can be solved numerically with somewhat similar results.

This method can be applied to any interaction of the form Eq. (3.4), allowing us to optimize a very general class of entanglement creation procedures. It is significantly different from the procedure proposed in [75], in that we do not need to assume full control over the local transformations on each qubit at all times.

The general scheme of this entanglement optimization protocol can be summarized as follows:

1. Choose the initial conditions for the system, and express them in the form of either Eq. (3.2) or Eq. (5.8).

2. Identify the coupling parameters and constraints for Eq. (3.4). Compute the evolution due to the unitary operator from Eq. (3.5) by using the transformations in Eqs. (3.7,3.8).

3. Choose the measure of entanglement of your preference [66–70].

4. Considering the experimental constraints, optimize with respect to the desired parameters.

Appendix B

Proof of Classical Correlations Lead to Completely Positive Dynamics

Theorem: Initially classically correlated state of the form

$$\rho = \sum_j p_j \Pi_j \otimes \tau_j,$$

always lead to completely positive dynamics.

Proof: We start from the classically correlated state from Eq. (5.10) for the system and its environment. The initial state of the system is

$$\eta = \sum_j p_j \Pi_j.$$

From Eq. (5.1) we have

$$\begin{aligned} \eta'_{rs} &= \big[\mathfrak{B}\big]_{rr';ss'}\eta_{r's'} \\ &= \mathrm{Tr}_{\mathcal{E}}\Big\{ \big[U\big]_{ra;r'a'}\Big(\sum_j p_j \left[\Pi_j\right]_{r's'} \left[\tau_j\right]_{a'b'}\Big)\big[U\big]^*_{sb;s'b'}\Big\}. \end{aligned}$$

Taking the trace with respect to the environment by contracting indices a and b we get,

$$\eta'_{rs} = \sum_j p_j \big[D_j^{kl}\big]_{rr'}[\Pi_j]_{r's}\big[D_j^{kl}\big]^*_{ss'},$$

where $[D_j^{kl}]_{rr'} \equiv [U]_{rl;r'a'}[\sqrt{\tau_j}]_{a'k}$. We have used the fact that $\{\tau_j\}$ are positive to take their square root. After combining indices k and l into a single index α we obtain,

$$\eta' = \sum_{j,\alpha} p_j D_j^{(\alpha)} \Pi_j D_j^{(\alpha)\dagger}.$$

Expanding $D_j^{(\alpha)}$ as $\sum_m D_m^{(\alpha)} \delta_{jm}$ and using $\Pi_j^2 = \Pi_j$,

$$\eta' = \sum_{j,\alpha} p_j \Big(\sum_m D_m^{(\alpha)} \delta_{jm} \Pi_j \Big) \Pi_j \Big(\sum_n \Pi_j \delta_{jn} D_n^{(\alpha)\dagger} \Big).$$

Now we can use the orthogonality of projectors, $\Pi_m \Pi_j = \delta_{mj} \Pi_j$ to drop the dependency of $D_j^{(\alpha)}$ on index j and write

$$\eta' = \sum_{j,\alpha} p_j \Big(\sum_m D_m^{(\alpha)} \Pi_m \Big) \Pi_j \Pi_j \Pi_j \Big(\sum_n D_n^{(\alpha)} \Pi_n \Big)^\dagger.$$

We can redefine $C^{(\alpha)} \equiv \sum_m D_m^{(\alpha)} \Pi_m$ to obtain

$$\eta' = \sum_\alpha C^{(\alpha)} \Big(\sum_j p_j \Pi_j \Big) C^{(\alpha)\dagger} = \sum_\alpha C^{(\alpha)} \eta C^{(\alpha)\dagger},$$

which is identical to Eq. (5.4) showing that it is a completely positive map.

This completes the proof.

Appendix C

Recreation of a photograph of young Boltzmann

I have been interested in the history of irreversibility in physics, in particular, the fierce debate around Boltzmann's H-Theorem. This debate has shaped my perspective on the role of irreversibility in quantum mechanics, one of the main topics of this dissertation.

It was pointed out by Carlos Rodríguez and independently by Camil Aponte that I slightly resemble the young Ludwig Boltzmann. On January 2008, I recruited the assistance of Mr. Kavan Modi in order to reconstruct this picture. We decided against the use of image editing software, and instead proceeded to dress myself in clothes that looked like they were from the era. Due to copyright restrictions it is not possible for me to include for comparison the original picture of young Boltzmann. However, a most motivated reader that performs an internet search for such an image and compares it to Fig. (C.1) will be rewarded with a moment of jocular amusement.

Figure C.1: A picture of the author impersonating Ludwig Boltzmann. Picture was taken on January 2008.

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Vita

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