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Characterization of optimal quantum states with maximal memory effects

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Zusammenfassung

In dieser Arbeit beschäftige ich mich mit einem kürzlich eingeführten Maß zur Quantifizierung von nicht-Markov'schem Verhalten in der Zeitentwicklung offener Quantensysteme, das auf dem Austausch von Information zwischen dem offenen System und seiner Umgebung beruht [5]. In diesem von *Breuer, Laine und Piilo* entwickelten Ansatz, wird die Stärke der Gedächtniseffekte in der Systemdynamik mit gewissen optimalen Paaren von Anfangszuständen verknüpft. Das Ziel dieser Arbeit ist eine mathematische Charakterisierung dieser speziellen Anfangszustände zu erarbeiten.

In dieser Arbeit charakterisiere ich einen Rand des Zustandsraums, der einzig auf der konvexen Struktur der Menge der Quantenzustände basiert. Dieses Konzept eines Randes, das wohlbekannt in der konvexen Analysis ist, stellt die Grundlage für die Beweise der mathematischen Eigenschaften optimaler Zustandspaare dar. Ich beweise, dass optimale Zustandspaare auf diesem Rand des Zustandsraums und überdies orthogonal sein müssen. Dies bedeutet, dass für Zustände, die zu Beginn durch eine Messung eindeutig unterscheidbar sind und damit einen maximalen Informationsgehalt haben, mögliche Quantengedächtniseffekte am stärksten sind. Ich zeige zwei Varianten für den Beweis dieser Aussage. Der zweite Beweis basiert dabei auf der anschaulichen Idee der gemeinsamen Verschiebbarkeit von Zustandspaaren, die tiefe Einblicke in die Struktur des Zustandsraums erlaubt.

Auf der Orthogonalität optimaler Zustände aufbauend, zeige ich, dass es möglich ist, einen Eingangszustand in der Definition des Maßes fest zu wählen und schließlich nur über Zustände auf dem Rand einer speziellen Menge die Größe zu maximieren. Hieraus ergibt sich eine neue Darstellung des Maßes für nicht-Markov'sches Verhalten quantenmechanischer Systeme, die die Nutzung von Gradientenmethoden bei der numerischen Maximierung erleichtert.

Die Beweise all dieser Aussagen basieren einzig auf der Konvexität des Zustandsraums und der Linearität der dynamischen Abbildungen. Dies bedeutet, dass keine zusätzlichen Annahmen über die Eigenschaften der Dynamik des offenen Quantensystems vonnöten sind, um diese Aussagen abzuleiten. Meine Ergebnisse können daher für beliebige Hilberträume und jeden dynamischen Prozess, der durch eine einparametrische Familie von linearen dynamischen Abbildungen beschrieben wird, angewandt werden.

Neben diesen Ergebnissen konstruiere ich ein explizites Beispiel für eine Systemdynamik, das offenlegt, dass optimale Quantenzustände nicht notwendigerweise reine Zustände sind. Dies zeigt, dass die Orthogonalität optimaler Zustände tatsächlich die allgemeinstmögliche Aussage ist, die getroffen werden kann.

Abstract

The purpose of this thesis is to study a recently proposed measure for the quantification of quantum non-Markovianity in the dynamics of open systems [5] which is based on the exchange of information between the open system and its environment. This measure, introduced by *Breuer, Laine and Piilo*, relates the degree of memory effects to certain optimal initial state pairs featuring a maximal flow of information from the environment back to the open system. The main goal of the present work is to provide a mathematical characterization of these special initial state pairs.

Within this thesis, I characterize a boundary of the state space based solely on the convex structure of the state space. This concept, which is well-known in convex analysis, is important for the proofs of the mathematical properties of optimal state pairs: I rigorously prove that the states of these pairs must lie on this boundary of the space of physical states and that they must be orthogonal. This implies that quantum memory effects are maximal for states which are initially distinguishable with certainty, having a maximal information content. I present two proofs for this statement. The second one is based on the new concept of joint translatability of a pair of states. This geometric idea elucidates the special structure of the state space.

Employing the orthogonality of states of optimal pairs, I show that it is possible to fix one input state and to maximize the quantity merely over the states of the boundary of a particular set. This yields a new and more convenient representation of the measure for quantum non-Markovianity, which enables to apply gradient methods more easily when the maximization is performed numerically.

The proof of all these statements relies solely on the convexity of the state space and on the linearity of the dynamical maps. That is, no additional requirements on the properties of the dynamics are needed to derive these statements. My results can thus be applied to any quantum process describable by a family of linear dynamical maps in any Hilbert space.

In addition, I construct an explicit example which demonstrates that optimal quantum states need not be pure states implying that orthogonality of optimal states is indeed the most general statement which can be made.

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Chapter 1

Introduction

Perfect isolation of any quantum system is almost impossible to realize since it is usually influenced by the coupling to an environment. Typically, the interaction of the system with its environment cannot be neglected so that a modelling of a quantum physical systems as a closed system fails to give a correct description of the system's dynamics. The theory of open quantum systems [6] takes the effects of exchanging energy and information between system and its environment into account. As a complete microscopic description of the environmental degrees of freedom is too complicated in general, the main concern of this theory is to develop effective models for the reduced, open system. The information about the environmental state is neglected by averaging over its degrees of freedom.

In the past, the most prominent approach resorts to an approximation of the open system dynamics in terms of a so-called Markovian master equation which includes several rather drastic assumptions on the properties of the system and environment. In this case, the time evolution of an open system is described by a quantum dynamical semigroup, which is most generally represented in the Lindblad form¹ [13, 30]. It is not surprising that there exist complex systems for which this relatively simple description fails to give a faithful picture of the dynamics (see e.g. [6]).

There has been a significant progress in developing a general theory allowing a realistic description of a large class of physical problems [4, 14, 39, 41, 58]. At the same time the differentiation of quantum processes in Markovian and non-Markovian dynamics came up. These terms have been widely used in physics literature referring, loosely speaking, to the absence or presence of memory effects in the dynamics which follows the interpretation of Markovian and non-Markovian stochastic processes in classical probability theory [6, 22]. However, there has been no proper definition of (non-)Markovianity in the quantum regime as the classical definition can not be implemented [51]. Recently, several proposals to detect and quantify memory effects in open system dynamics were made, e.g. [5, 29, 34, 42, 56] to name just a few. The proposed measures are based on different mathematical and physical concepts so that the very definition of non-Markovianity and quantification of quantum memory effects in the dynamics of open systems is still under discussion.

In the thesis at hand I investigate the non-Markovianity measure proposed

¹Sometimes this form is also referred to as Lindblad-Gorini-Kossakowski-Sudarshan form. I will use Lindblad form short hand for this lengthy expression.

in [5] which determines the degree of memory effects in terms of the amount of information exchanged between the open system and its environment. The central part of this quantity is the trace distance which represents a measure for the distinguishability of two quantum states [18–20]. This feature allows the interpretation that the measure determines the backflow of information from the environment to the open system. Within this approach the degree of non-Markovianity is connected to certain optimal initial pairs of quantum states, which lead to a maximal flow of information to the open system.

Up to now, the measure has only been studied regarding the requirements to detect non-Markovianity [29], compared to other measures [11, 15, 51] and applied to physical models (see, e.g. [12, 35]). Moreover, several experiments have been performed including the maximization over all initial state pairs [28, 32, 33, 50]. Here, I will now focus on the definition of this quantity. I study the mathematical and physical properties of optimal state pairs which finally yield a simplification of the maximization procedure involved in the definition of the investigated measure.

The thesis is organized as follows:

In *Chapter 2* I recapitulate the description of a physical state of a quantum system. After having clarified the notation, I will focus on the specific structure of the set of states. Within this discussion I present some first results on boundaries of the state space which yield the basic concept for further statements on the mathematical properties of optimal pairs. I will show that a boundary based solely on the convex structure of the state space is completely characterized in terms of eigenvalues. To conclude the discussion of this boundary, its relation to boundaries derived from norms on the state space is elucidated.

In the subsequent part, *Chapter 3*, I briefly review the basic concepts of the theory of open quantum systems. The notion of a quantum dynamical map is introduced and different representations of such maps are discussed. From this, the general mathematical properties of a one-parameter family of dynamical maps describing the evolution of an open system are developed. On the basis of these properties, several signatures for non-Markovian effects are discussed and, finally, the concept of quantum non-Markovianity, based on the information flow, is presented.

Chapter 4 contains the main results of my work concerning the mathematical and physical properties of optimal state pairs. First, I show in *Section 4.1* that optimal pairs of states must lie on the previously defined boundary of the state space. In *Section 4.2* I then proceed to demonstrate that the states of any optimal pair must even be orthogonal which is physically very plausible since it implies that the maximal flow of information from the environment back to the open system emerges if the initial state pair is distinguishable with certainty, i.e. has a maximal information content. The comparison between finite and infinite systems, which has already been initiated for the boundary, is continued. Moreover, an alternative proof for the orthogonality of optimal state pairs of finite systems which employs the joint translatability of non-orthogonal states is given in *Section 4.4*. A more convenient maximization procedure, applying the orthogonality of optimal states, is developed in *Section 4.3*. It yields technical improvements for numerical and experimental realizations of the maximization procedure. Moreover, this result allows further insight into the nature of the measure and strengthens its fundamental character.

In *Chapter 5* the purity of optimal states is investigated. In the simple case of a qubit, the orthogonality of the optimal pair implies that the states of the pair must be pure and antipodal. In this chapter it is shown that this statement does not hold true in general for higher dimensional systems. To this end, an example of a dynamics of a three-level system (Λ -system) – for which the optimal pair is not a pure state pair – is given.

Finally, in *Chapter 6*, I review my studies, summarize the results and draw some conclusions. In addition, I provide an outlook on the further perspective of the studies of quantum non-Markovianity and its applications.

Chapter 2

The state space

In this section I briefly review the concept of physical states of a quantum mechanical system in order to clarify and fix the notation, and to discuss the structure of this set of states, usually called the state space. For the present work, it is of great relevance to define and characterize a boundary of the state space. Apart from boundaries based on norms, the very fundamental property of convexity of the set of physical states gives rise to a definition of a boundary. It is shown that the boundary arising solely from the convex structure – and referred to as the intrinsic boundary – is directly linked to zero eigenvalues of the states of arbitrary systems and, therefore, features the ideal framework for the studies of the optimal state pairs considered in chapter 4. Moreover, I prove that a boundary obtained from a norm on the state space is identical to the intrinsic one. This emphasizes the significance of the intrinsic boundary regarding its definition.

The basic elements for the description of a quantum system are quantum states. Physical states of a quantum system are characterized by density operators ρ . They represent positive trace class operators with unit trace on a Hilbert space \mathcal{H} over the field of complex numbers \mathbb{C} . Thus, density operators are bounded linear operators on \mathcal{H} satisfying the additional constraints

$$\rho = \rho^\dagger, \quad \rho \geq 0, \quad \text{Tr}(\rho) = 1 . \quad (2.1)$$

The second requirement is the acronym for a state ρ being positive. This implies that all eigenvalues are non-negative while the last condition in (2.1) enforces the sum of eigenvalues to converge to unity. More precisely, the eigenvalues must constitute an ℓ^1 -convergent series for infinite-dimensional systems. In the case of a finite-dimensional Hilbert space, the notion of physical states reduces to positive matrices whose diagonal elements sum to one. Due to this feature, the eigenvalues can be interpreted as probabilities. A state has also to be Hermitian (the first requirement in (2.1)) which already follows from the positivity of a state as the underlying Hilbert space \mathcal{H} is over the field of complex numbers [1]. Throughout the present work, the set of physical states of a quantum system is denoted by $\mathcal{S}(\mathcal{H})$, i.e.

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{B}(\mathcal{H}) \mid \rho \geq 0, \text{Tr}(\rho) = 1\} , \quad (2.2)$$

where $\mathcal{B}(\mathcal{H})$ refers to the set of bounded linear operators on \mathcal{H} .

A fundamental property of the state space is convexity, which means that for any $\rho, \sigma \in \mathcal{S}(\mathcal{H})$ and $\lambda \in [0, 1]$ one has

$$\rho_\lambda = (1 - \lambda)\sigma + \lambda\rho \in \mathcal{S}(\mathcal{H}) . \quad (2.3)$$

This signifies that the straight line connecting ρ and σ is entirely contained in $\mathcal{S}(\mathcal{H})$. Later on, I define a boundary of the state space on the basis of the convex structure.

Because Hermitian operators are in particular normal operators, that is, the operator commutes with its Hermitian conjugate, the spectral theorem [44] applies yielding the spectral decomposition of a state

$$\rho = \sum_{i=1}^{\dim \mathcal{H}} p_i |\psi_i\rangle\langle\psi_i| , \quad (2.4)$$

in terms of its eigenvalues p_i and eigenvectors $|\psi_i\rangle$. These vectors constitute an orthonormal basis of the Hilbert space.

2.1 The intrinsic boundary

The convex structure of the state space gives rise to the definition of a boundary $\partial\mathcal{S}(\mathcal{H})$ of the state space as follows:

Definition 2.1. *A point $\rho \in \mathcal{S}(\mathcal{H})$ is called an interior point of $\mathcal{S}(\mathcal{H})$ if and only if for all $\sigma \in \mathcal{S}(\mathcal{H})$ there is a real number $\lambda > 1$ such that*

$$\rho_\lambda = (1 - \lambda)\sigma + \lambda\rho \in \mathcal{S}(\mathcal{H}) . \quad (2.5)$$

Denoting the set of interior points by $\mathring{\mathcal{S}}(\mathcal{H})$, this set is thus given by

$$\mathring{\mathcal{S}}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid \text{for any } \sigma \in \mathcal{S}(\mathcal{H}), \exists \lambda > 1, \text{ s.t. } \rho_\lambda \in \mathcal{S}(\mathcal{H})\} . \quad (2.6)$$

Having in mind the figurative description of convexity in terms of lines connecting points, a point in the interior has the property that any line, which terminates in this point, can be extended. In other words, an inner point is surrounded by states. Note that $\rho_\mu = (1 - \mu)\sigma + \mu\rho$ belongs to $\mathcal{S}(\mathcal{H})$ for all $0 \leq \mu \leq \lambda$ by the convexity of the state space.

The corresponding boundary $\partial\mathcal{S}(\mathcal{H})$ is the set difference, i.e. $\partial\mathcal{S}(\mathcal{H}) = \mathcal{S}(\mathcal{H}) \setminus \mathring{\mathcal{S}}(\mathcal{H})$, which yields

$$\partial\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid \exists \sigma \in \mathcal{S}(\mathcal{H}), \text{ s.t. } \forall \lambda > 1, \rho_\lambda \notin \mathcal{S}(\mathcal{H})\} . \quad (2.7)$$

Thus, $\rho \in \partial\mathcal{S}(\mathcal{H})$ if and only if there exists $\sigma \in \mathcal{S}(\mathcal{H})$ such that for all $\lambda > 1$ the operator $\rho_\lambda = (1 - \lambda)\rho + \lambda\sigma$ does not belong to the state space $\mathcal{S}(\mathcal{H})$. Because of its natural definition based solely on the convex structure, and not on a certain topology, I call this boundary the *intrinsic boundary*. It is indeed an intrinsic feature of the set. Note that the intrinsic boundary is a subset of the state space, i.e. $\partial\mathcal{S}(\mathcal{H}) \subset \mathcal{S}(\mathcal{H})$, by definition.

This concept for a boundary is well-known in convex analysis [43], where the interior (boundary) of a convex set C in \mathbb{R}^n defined as above is referred to as the relative interior (boundary). This term is motivated by the fact that these sets

are defined relatively to the affine hull of the convex set which is the smallest affine set that contains C . The relative interior (boundary) is thus the interior (boundary) of C with respect to the Euclidean structure of \mathbb{R}^n constrained to C 's affine hull. If the affine hull of the convex set C is contained in a hyperplane, this definition leads to significantly different interiors (boundaries) compared to the ordinary, Euclidean ones. If one considers, for example, a (two-dimensional) square embedded in \mathbb{R}^3 , the relative boundary is only given by the edges while the boundary with respect to any metric on \mathbb{R}^3 is the entire square.

I proceed to study the intrinsic boundary in order to develop a characterization of this set. It reveals a direct connection to the distribution of the eigenvalues of the states. As a first result, I show that a density operator belongs to the boundary if it has a zero eigenvalue.

Lemma 2.1. *Let $\rho \in \mathcal{S}(\mathcal{H})$. Then, $\rho \in \partial\mathcal{S}(\mathcal{H})$ if $0 \in \text{spec}(\rho)$.*

Proof. Let $\rho \in \mathcal{S}(\mathcal{H})$ be an arbitrary state such that $0 \in \text{spec}(\rho)$, i.e. it has a zero eigenvalue. Denote by $|\varphi\rangle$ the normalized eigenvector of ρ with zero eigenvalue and let $P = |\varphi\rangle\langle\varphi|$ refer to the corresponding projection. Then, for all $\lambda > 1$ the operator $(1 - \lambda)P + \lambda\rho$ has the negative eigenvalue $1 - \lambda < 0$ with associated eigenvector $|\varphi\rangle$ showing that it does not belong to the set of physical states. Hence, $\rho \in \partial\mathcal{S}(\mathcal{H})$ due to the definition of the boundary (2.7). \square

This characterization emphasizes the intrinsic nature of the boundary, as zero is the intermediate value between positive and negative real numbers. Thus, it separates positive eigenvalues, which determine elements of $\mathcal{S}(\mathcal{H})$, from negative ones corresponding to nonphysical operators.

For finite-dimensional systems the converse holds as well. One way to show this is to determine the states in the interior. The restriction to finite systems is not due to technicalities as one might think. This will become clear later on.

Theorem 2.1. *Let $\dim \mathcal{H} < \infty$ and $\rho \in \mathcal{S}(\mathcal{H})$. Then, $\rho \in \partial\mathcal{S}(\mathcal{H})$ if and only if $0 \in \text{spec}(\rho)$.*

Proof. For the converse of lemma 2.1, suppose that $\rho \in \mathcal{S}(\mathcal{H})$ is a state whose spectrum does not contain zero. I want to show that $\rho \in \mathring{\mathcal{S}}(\mathcal{H})$. Consider the operator $(1 - \lambda)\sigma + \lambda\rho$ for $\lambda > 1$ and an arbitrary state σ . It can be rewritten by setting $\lambda = 1 + \epsilon$ with $\epsilon > 0$ which yields $\rho' = (1 + \epsilon)(\rho - \epsilon(1 + \epsilon)^{-1}\sigma)$. This shows that the contribution of σ can be seen as a small perturbation for an appropriate choice of ϵ . It follows from the positivity of ρ 's eigenvalues and the continuity of the roots of the characteristic polynomial (with respect to its coefficients) that all eigenvalues of ρ' are also positive for sufficiently small ϵ . This shows that ρ' is positive and, thus, ρ is in the interior $\mathring{\mathcal{S}}(\mathcal{H})$. \square

Hence, for finite-dimensional systems the intrinsic boundary is completely described by states with zero eigenvalues,

$$\partial\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid 0 \in \text{spec}(\rho)\} . \quad (2.8)$$

It is clear that the reasoning using the characteristic polynomial only works in finite dimensions. However, the following, surprising theorem shows that this is indeed all one can get.

Theorem 2.2. *For $\dim \mathcal{H} = \infty$ all points $\rho \in \mathcal{S}(\mathcal{H})$ are on the boundary, i.e. $\partial\mathcal{S}(\mathcal{H}) = \mathcal{S}(\mathcal{H})$.*

Proof. Let ρ be an arbitrary state. Since I have already shown that $\rho \in \partial\mathcal{S}(\mathcal{H})$ if $0 \in \text{spec}(\rho)$ for arbitrary dimensions, I assume $0 \notin \text{spec}(\rho)$. I then construct a state $\sigma \in \mathcal{S}(\mathcal{H})$ such that for all $\lambda = 1 + \epsilon > 1$ one has $(1 - \lambda)\sigma + \lambda\rho = -\epsilon\sigma + (1 + \epsilon)\rho \notin \mathcal{S}(\mathcal{H})$. From this, it follows that $\rho \in \partial\mathcal{S}(\mathcal{H})$.

Let ρ be written in terms of its spectral decomposition by

$$\rho = \sum_{i=1}^{\infty} p_i |\psi_i\rangle\langle\psi_i|, \quad (2.9)$$

where $p_i > 0 \ \forall i \in \{1, 2, \dots\}$ due to the assumption $0 \notin \text{spec}(\rho)$. According to the constraint on the trace of the state, which implies $\sum_{i=1}^{\infty} p_i = 1$, the sequence

$$r_n \equiv \sum_{i=n+1}^{\infty} p_i, \quad n = 0, 1, 2, \dots \quad (2.10)$$

is strictly monotonically decreasing and converges to zero, i.e. $r_n \searrow 0 \ (n \rightarrow \infty)$. Note that $r_0 = \sum_{i=1}^{\infty} p_i = 1$. The coefficients

$$q_m \equiv \sqrt{r_{m-1}} - \sqrt{r_m}, \quad \forall m = 1, 2, \dots \quad (2.11)$$

are thus strictly positive and add up to one as the sum is a telescoping series:

$$q_m > 0 \quad \forall m \in \{1, 2, \dots\}, \quad \sum_{m=1}^{\infty} q_m = \sqrt{r_0} = 1. \quad (2.12)$$

Moreover, the m 'th coefficient is bounded from below according to

$$q_m = \frac{r_{m-1} - r_m}{\sqrt{r_{m-1}} + \sqrt{r_m}} \geq \frac{p_m}{2 \cdot \sqrt{r_{m-1}}} \Leftrightarrow \frac{q_m}{p_m} \geq \frac{1}{2 \cdot \sqrt{r_{m-1}}}, \quad (2.13)$$

which shows that $q_m/p_m \rightarrow \infty \ (m \rightarrow \infty)$ as the sequence r_m converges monotonically to zero. Due to (2.12), the operator

$$\sigma = \sum_{i=1}^{\infty} q_i |\psi_i\rangle\langle\psi_i| \quad (2.14)$$

defines a state that has the same spectral decomposition as ρ so that one obtains

$$-\epsilon\sigma + (1 + \epsilon)\rho = \sum_{i=1}^{\infty} ((1 + \epsilon)p_i - \epsilon q_i) |\psi_i\rangle\langle\psi_i|. \quad (2.15)$$

However, for any $\epsilon > 0$ there exists $i_0 \in \mathbb{N}$, so that for all $j \geq i_0$

$$\frac{q_j}{p_j} > \frac{1 + \epsilon}{\epsilon}, \quad (2.16)$$

since the ratio q_m/p_m diverges. This inequality shows that $-\epsilon\sigma + (1 + \epsilon)\rho$ has the negative eigenvalue $(1 + \epsilon)p_j - \epsilon q_j < 0$ for some j and any possible choice of ϵ . Thus, it does not belong to the state space. This proves the claim, i.e. $\rho \in \partial\mathcal{S}(\mathcal{H})$. \square

Hence, there exists indeed no extension of the preceding theorem, as it has been mentioned before, since all states are already on the boundary. This peculiar result might lead to the conjecture that either the feature defining the boundary (cf. (2.7)) is too coarse or the state space of infinite systems is special. In the next section I show that there is strong evidence that it is the latter which holds true.

2.2 A boundary based on a norm

This section is devoted to an alternative boundary of the state space based on a norm on the state space. By a fundamental result in functional analysis, one knows that all norms on a finite-dimensional vector space are equivalent [44]. As the state space is a subset of the real vector space of Hermitian matrices, it therefore does not make any difference which norm I choose for the definition of the boundary for finite systems. For convenience, I consider the p -norm which is given by

$$\|\cdot\|_p = \left(\text{Tr}(|\cdot|^p) \right)^{1/p}, \quad (2.17)$$

for¹ $1 \leq p < \infty$. The modulus of an operator A is defined as $|A| \equiv \sqrt{A^\dagger A}$ specifying a positive element associated to a given operator. For a self-adjoint operator A , which is determined by its eigenvectors $|\psi_i\rangle$ and eigenvalues a_i , the spectral decomposition (2.4) of $|A|$ obeys

$$|A| = \sum_i |a_i| |\psi_i\rangle\langle\psi_i|. \quad (2.18)$$

Hence, for a self-adjoint operator the p -norm (2.17) reads

$$\|A\| = \left(\sum_i |a_i|^p \right)^{1/p}. \quad (2.19)$$

Up to a factor of $1/2$, the 1-norm is equivalent to the trace norm whose induced metric will be introduced in section 3.3, and the 2-norm is typically referred to as the Hilbert-Schmidt norm and denoted by $\|\cdot\|_{HS}$.

The purpose of this section is to elucidate the previously studied intrinsic boundary regarding its relation to boundaries based on a norm. I establish the same characterization for the boundary induced by a p -norm as the one obtained for the intrinsic boundary. By this, $\partial\mathcal{S}(\mathcal{H})$ defines the same set as any norm based boundary for finite-dimensional systems. The intrinsic boundary thus provides merely a more practical definition of the same set in terms of the extensibility of lines. This feature will be needed in the next chapter.

Definition 2.2. *The boundary based on the p -norm for some $1 \leq p < \infty$ is defined by*

$$\partial_p \mathcal{S}(\mathcal{H}) = \{ \rho \in \mathcal{S}(\mathcal{H}) \mid \forall \epsilon > 0 : \hat{B}_\epsilon^{(p)}(\rho) \cap \mathcal{S}(\mathcal{H})^c \neq \emptyset \}, \quad (2.20)$$

where $\mathcal{S}(\mathcal{H})^c$ refers to the complement of $\mathcal{S}(\mathcal{H})$ with respect to the set of Hermitian operators of unit trace $\mathcal{E}_1(\mathcal{H}) = \{ A \in \mathcal{B}(\mathcal{H}) \mid A = A^\dagger, \text{Tr} A = 1 \}$, i.e.

¹It is also possible to choose $p = \infty$ in the definition (2.17). In this case, the norm is given by the supremum of the modulus of the eigenvalues.

$\mathcal{S}(\mathcal{H})^c \equiv \mathcal{E}_1(\mathcal{H}) \setminus \mathcal{S}(\mathcal{H})$, and $\hat{B}_\epsilon^{(p)}(\rho) = \{\sigma \in \mathcal{S}(\mathcal{H}) \mid \|\rho - \sigma\|_p \leq \epsilon\}$ denotes the closed ball surrounding ρ in terms of the considered p -norm.

I call $\partial_p \mathcal{S}(\mathcal{H})$ the p -boundary. Hence, a state ρ is on the p -boundary if and only if there exists a non-positive operator in any ball with respect to the p -norm centered at ρ . It is worth noting that the p -boundary is always contained in $\mathcal{S}(\mathcal{H})$ by definition in contrast to the general definition of a topological boundary where this only holds if and only if the set is closed.

One readily obtains that for arbitrary systems, states with a zero eigenvalue are also on the p -boundary. This result is established using a similar construction as in lemma 2.1.

Lemma 2.2. *Let $\rho \in \mathcal{S}(\mathcal{H})$. Then, $\rho \in \partial_p \mathcal{S}(\mathcal{H})$ if $0 \in \text{spec}(\rho)$.*

Proof. Let $\rho \in \mathcal{S}(\mathcal{H})$ be a state with a zero eigenvalue and $|\varphi\rangle \in \mathcal{H}$ is the corresponding normalized eigenvector. Denote by $|\psi\rangle \in \mathcal{H}$ another normalized eigenvector orthogonal to $|\varphi\rangle$. Then, for all $\epsilon > 0$ the operator

$$\tilde{\rho} = \rho + \frac{\epsilon}{2}|\psi\rangle\langle\psi| - \frac{\epsilon}{2}|\varphi\rangle\langle\varphi| \in \mathcal{E}_1(\mathcal{H}) \setminus \mathcal{S}(\mathcal{H}) \quad (2.21)$$

defines a Hermitian operator with unit trace that has a negative eigenvalue. However, it is contained in the ϵ -ball centered at ρ since

$$\|\tilde{\rho} - \rho\|_p = \left(\text{Tr} \left(\left| \frac{1}{2}\epsilon|\psi\rangle\langle\psi| - \frac{1}{2}\epsilon|\varphi\rangle\langle\varphi| \right|^p \right) \right)^{1/p} = \frac{2^{1/p}}{2}\epsilon \leq \epsilon. \quad (2.22)$$

Hence, $\rho \in \partial_p \mathcal{S}(\mathcal{H})$ as there exists a Hermitian, non-positive operator with unit trace contained in the ϵ -ball of ρ for any $\epsilon > 0$. \square

By a similar reasoning as in theorem 2.1 one obtains even equivalence for finite-dimensional systems: A state is on the p -boundary if and only if it has a zero eigenvalue. Thus, one arrives at the same characterization for the two boundaries in terms of the eigenvalues. Again, the restriction to finite-dimensional systems is not based on the chosen proof as it will be shown.

Theorem 2.3. *Let $\dim \mathcal{H} = N < \infty$ and $\rho \in \mathcal{S}(\mathcal{H})$. Then, $\rho \in \partial_p \mathcal{S}(\mathcal{H})$ if and only if $0 \in \text{spec}(\rho)$.*

Proof. For the converse of the preceding lemma, suppose $\rho_0 \in \mathcal{S}(\mathcal{H})$ such that $0 \notin \text{spec}(\rho_0)$. For any $\epsilon > 0$, every operator $\rho \in \hat{B}_\epsilon^{(p)}(\rho_0)$ can be written as the sum of ρ_0 and a traceless Hermitian operator A , i.e. $\rho = \rho_0 + A$. The eigenvalues $p_A^{(i)}$ of A have to obey

$$(\|A\|_p)^p = \sum_{i=1}^N (p_A^{(i)})^p \leq \epsilon^p, \quad (2.23)$$

showing that A is only a small perturbation of ρ_0 for $\epsilon \ll 1$. Thus, if ϵ is chosen sufficiently small, it follows again from the continuity of the roots of the characteristic polynomial that all eigenvalues of ρ are positive, too. One obtains $\hat{B}_\epsilon(\rho_0) \subset \mathcal{S}(\mathcal{H})$ for sufficiently small ϵ so that $\rho_0 \in \mathring{\mathcal{S}}(\mathcal{H})$ and, therefore, $\mathring{\mathcal{S}}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid 0 \notin \text{spec}(\rho)\}$ which finally proves the theorem. \square

Theorem 2.4. *For $\dim \mathcal{H} = \infty$ and any $1 \leq p < \infty$, all points $\rho \in \mathcal{S}(\mathcal{H})$ are on the p -boundary, i.e. $\partial_p \mathcal{S}(\mathcal{H}) = \mathcal{S}(\mathcal{H})$.*

Proof. Suppose $\rho \in \mathcal{S}(\mathcal{H})$ such that $\rho > 0$. Its spectral decomposition is given by $\rho = \sum_{i=1}^{\infty} p_i |\psi_i\rangle\langle\psi_i|$. As the eigenvalues are an ℓ^1 -series, there exists for any $\epsilon > 0$ an index $m \in \mathbb{N}$ such that the m -th eigenvalue of ρ satisfies $p_m < \epsilon/2$. For any $k \neq m$, the operator

$$A = \sum_{i=1}^{\infty} q_i |\psi_i\rangle\langle\psi_i|, \quad (2.24)$$

where

$$q_i = \begin{cases} p_k + \frac{\epsilon}{2} & , \text{ if } i = k \\ p_i & , \text{ if } i \neq m, k \\ p_m - \frac{\epsilon}{2} & , \text{ if } i = m \end{cases}, \quad (2.25)$$

defines a non-positive, Hermitian operator with trace one. Since one has

$$\rho - A = \frac{\epsilon}{2} |\psi_m\rangle\langle\psi_m| - \frac{\epsilon}{2} |\psi_k\rangle\langle\psi_k|, \quad (2.26)$$

this operator is in the ϵ -ball centered at ρ for any p -norm. Thus, $\rho \in \partial_p \mathcal{S}(\mathcal{H})$ which proves the claim. \square

One concludes that the boundaries based on the p -norm and the intrinsic one coincide for all kind of systems. The intrinsic boundary is indeed only a more convenient representation which reveals the underlying structure of the state space. Therefore, I will henceforth simply talk about *the boundary* and denote it by $\partial \mathcal{S}(\mathcal{H})$. Summing up the previous results, the boundary of state space is completely determined by the set of states with zero eigenvalues,

$$\partial \mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid 0 \in \text{spec}(\rho)\} \quad (2.27)$$

for finite systems, while the intrinsic boundary and the one based on any p -norm is equal to the entire state space for $\dim \mathcal{H} = \infty$. These results endorse the statement that the state space for infinite systems is special as it is different for at least two major classes of boundaries.

2.3 Generalized Bloch representation

I now return to finite-dimensional systems in order to introduce the famous representation of states in terms of vectors in a real vector space which is typically referred to as the generalized Bloch representation [1]. Moreover, some properties of the corresponding convex set of states are discussed.

For a quantum system described by a Hilbert space \mathcal{H} with dimension N , there is a unique representation of states in terms of vectors in \mathbb{R}^{N^2-1} . Using traceless, Hermitian and orthogonal representatives of the generators of the $(N^2 - 1)$ -dimensional special unitary group $\text{SU}(N)$, one obtains

$$\rho = \frac{1}{N} \left\{ \mathbb{1}_N + \sum_{i=1}^{N^2-1} \sqrt{\frac{N(N-1)}{\text{Tr}(\sigma_i^\dagger \sigma_i)}} v_i^{(\rho)} \sigma_i \right\}, \quad (2.28)$$

where the vector $\vec{v}^{(\rho)} = (v_1^{(\rho)}, \dots, v_{N^2-1}^{(\rho)}) \in \mathbb{R}^{N^2-1}$ is called the generalized Bloch vector associated to the state ρ . The $SU(N)$ -generators are usually chosen to obey

$$\sigma_i \sigma_j = \frac{2}{N} \delta_{ij} + i f_{ijk} \sigma_k + d_{ijk} \sigma_k , \quad (2.29)$$

where f_{ijk} are the so-called structure constants (completely antisymmetric) and d_{ijk} refers to the symmetric d -tensor [7]. This yields

$$\rho = \frac{1}{N} \{ \mathbb{1}_N + c(N) \vec{v}^{(\rho)} \vec{\sigma} \} , \quad c(N) = \sqrt{\frac{N(N-1)}{2}} , \quad (2.30)$$

where the coefficients are determined by $v_i^{(\rho)} = \text{Tr}(\rho \sigma_i)$. It is well known that there exist a smallest and a largest ball with respect to the Euclidean norm in \mathbb{R}^{N^2-1} centered at zero which define the smallest isotropic superset and largest isotropic subset of $\mathcal{S}(\mathcal{H})$, respectively [16, 24]. Due to the choice of $c(N)$, the radius R_{out} of the smallest ball enclosing the convex set of generalized Bloch vectors is one, i.e. $R_{out} = 1$. It can be readily shown that the Bloch vector of a state is on the sphere determined by R_{out} if and only if the state is pure [16, 24]. The radius of the largest ball entirely contained in the set of generalized Bloch vectors is denoted by r_{in} and one has $r_{in} = \frac{2}{N}$. The former ball is typically called the *outsphere* while the latter one is referred to as the *insphere*. Thus, to any vector in \mathbb{R}^{N^2-1} with norm less than or equal to r_{in} , there corresponds a quantum state according to equation (2.28), i.e. for any $r \leq r_{in}$

$$B_r(0) = \{ \vec{v} \in \mathbb{R}^{N^2-1} \mid \|\vec{v}\| \leq r \} , \quad (2.31)$$

determines an isotropic subset of the state space. Since $\|\rho - \frac{1}{N} \mathbb{1}_N\|_{HS}^2 = \text{Tr}((\rho - \frac{1}{N} \mathbb{1}_N)^2) = \|\vec{v}^{(\rho)}\|^2$, one can define this set also directly in terms of positive operators with trace one,

$$\hat{B}_r(\frac{1}{N} \mathbb{1}_N) \equiv \{ \rho \in \mathcal{E}_1(\mathcal{H}) \mid \|\rho - \frac{1}{N} \mathbb{1}_N\|_{HS} \leq r \} \subset \mathcal{S}(\mathcal{H}) . \quad (2.32)$$

Although this representation looks simple, the precise shape of the set of permissible vectors is extremely complicated. The constraint of positivity induces a lattice of N nested inequalities which are given by the coefficients of the characteristic polynomial. More precisely, the roots of a polynomial are positive if and only if all coefficients are positive semi-definite [23]. In terms of the vector $\vec{v} \in \mathbb{R}^{N^2-1}$, the first three coefficients of the characteristic polynomial $\det(\rho - \lambda \mathbb{1}_N)$ are given by

$$a_1 = 1 , \quad (2.33)$$

$$a_2 = \frac{N-1}{2N} (1 - \vec{v} \cdot \vec{v}) , \quad (2.34)$$

$$a_3 = \frac{(N-1)(N-2)}{6N^2} (1 - 3\vec{v} \cdot \vec{v} + 2(\vec{v} \star \vec{v}) \cdot \vec{v}) , \quad (2.35)$$

where the \star -product is defined as

$$(\vec{v} \star \vec{w})_k = \sqrt{\frac{N(N-1)}{2}} \frac{1}{N-2} d_{ijk} v_i w_j . \quad (2.36)$$

At this point, the algebra structure of $SU(N)$ enters. As the first coefficient a_1 is trivially positive, there is only one constraint given by $a_2 \geq 0$ for two-level systems. One immediately recognizes that this yields the famous Bloch ball: all vectors in \mathbb{R}^3 with norm smaller than or equal to one correspond to quantum states. In this case, the state space is represented by an isotropic subset in \mathbb{R}^3 which is convenient, for example, for simulations applying Monte Carlo methods. Moreover, the in- and outsphere coincide for two-dimensional systems. However, already for a three-level system, the positivity of a_3 causes that $r_{in} < R_{out}$ and, therefore, that the set of permissible vectors is a proper subset of the outsphere. Even though there is only one further constraint for a three-level system, it is very tedious to check whether a vector in \mathbb{R}^8 belongs to a state or not. Of course, all this gets even worse for higher-dimensional systems. Although some progress has been made [7, 23, 24], a complete understanding of the set of generalized Bloch vectors is still missing. The set apparently lacks a simple symmetry. Due to these difficulties, the representation is mostly used only for two-level systems.

2.3.1 Antipodal and antiparallel states

On the basis of the convex combination of two states (2.3), one can define particular pairs of states for finite-dimensional systems. Two states ρ_1 and ρ_2 on the boundary $\partial\mathcal{S}(\mathcal{H})$ are said to be *antipodal* if and only if there exists a real number $0 < \lambda < 1$ such that

$$\lambda\rho_1 + (1 - \lambda)\rho_2 = \frac{1}{N}\mathbb{1}_N . \quad (2.37)$$

That is, a pair of states is antipodal if the line connecting them passes through the maximally mixed state. Using the Bloch representation (2.30), it follows that the convex combination of ρ_1 and ρ_2 also defines a line in the set of generalized Bloch vectors and that for antipodal states this line crosses the origin $\vec{v} = 0$. Hence, applying a point reflection with respect to the origin and a scaling, the Bloch vectors of antipodal states are mapped onto each other. That is, the Bloch vectors corresponding to antipodal states have opposite directions but different lengths with respect to the Euclidean norm. If two Bloch vectors mapped onto each other by a point reflection but without any scaling, the associated states are referred to as *antiparallel*. I emphasize that the sets of antipodal and antiparallel states do not coincide unless the Hilbert space is two-dimensional [16].

Chapter 3

Open quantum systems

After having studied different features of the state space in the preceding chapter, I proceed to study open systems and their dynamics. The fundamental concepts of the theory of open quantum systems, such as completely positive dynamical maps, master equations and divisibility of dynamical maps are briefly summarized. Finally, I turn my attention to the definition of non-Markovianity in the quantum regime and quote a recently developed measure [5] for non-Markovian behaviour of open quantum systems which I study throughout the thesis.

3.1 Microscopic approach to open systems

The term *open system* refers to a quantum physical system S that interacts with another system E which one calls the environment. Almost every quantum physical system of practical relevance constitutes an open system as the interaction with an environment is ubiquitous. The open system S can be seen as a subsystem of the total system $S + E$ consisting of the open system and its environment. The Hilbert space \mathcal{H} of the total system is thus given by the tensor product of the open system's Hilbert space \mathcal{H}_S and of the environmental Hilbert space \mathcal{H}_E , i.e. $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. The total system is typically assumed to be closed so that the time evolution of any of its states $\rho \in \mathcal{S}(\mathcal{H})$ is governed by the *Liouville-von Neumann equation*

$$\frac{d}{dt}\rho(t) = -i[H, \rho(t)] , \quad (3.1)$$

where Planck's constant is set to $\hbar = 1$, and H refers to the Hamiltonian of the total system. The Hamiltonian is time independent as the total system is assumed to be closed. Denoting the self-Hamiltonians of the open system and environment by H_S and H_E , respectively, and defining H_I to be any interaction Hamiltonian mediating between system and environment, H can be split into three parts so that it reads¹

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_I . \quad (3.2)$$

¹Here, $\mathbb{1}_{S,E}$ refers to the identity operator on the open system and the environment, respectively.

The Liouville-von Neumann equation (3.1) defines a one-parameter family of unitary operators given by $U(t) = \exp(-iHt)$ which determines the time evolution of states of the total system according to

$$\rho(t) = U(t)\rho(0)U^\dagger(t) . \quad (3.3)$$

The actual state of the system S at time t is then obtained by taking the partial trace over the environmental Hilbert space \mathcal{H}_E of $\rho(t)$, which is denoted by Tr_E , i.e.

$$\rho_S(t) = \text{Tr}_E(U(t)\rho(0)U^\dagger(t)) . \quad (3.4)$$

That is, one takes the average over all environmental degrees of freedom so that solely the quantities of the open system remain in which one is interested in. The major difficulty of this formalism is to determine the full solution of the equations of motion. Hence, one of the objectives of the theory of open quantum systems [6] is to provide an analytically or numerically feasible formulation of the dynamical evolution of the open system. Employing this theory, an effective description of actual systems present in various experiments is possible. In the following, several concepts are introduced and discussed.

3.2 Quantum dynamical maps

The key concept of the theory of open quantum systems is the notion of dynamical maps. It summarizes the fundamental mathematical properties of the dynamical evolution defined by equation (3.4) for initially uncorrelated total system states given by the tensor product $\rho(0) = \rho_S(0) \otimes \rho_E(0)$. Here, the density operators $\rho_S(0)$ and $\rho_E(0)$ refer to the open system's initial degrees of freedom and those of the environment, respectively. The assumption of factorizing initial conditions means that the open system and the environment are statistically independent at the initial time. Applying this, equation (3.4) reads

$$\rho_S(t) = \text{Tr}_E(U(t)\rho_S(0) \otimes \rho_E(0)U^\dagger(t)) . \quad (3.5)$$

For a fixed initial environmental state $\rho_E(0)$ this equation defines a linear map on the state space $\mathcal{S}(\mathcal{H}_S)$ at any time $t \geq 0$,

$$\Phi_{t,0} : \mathcal{S}(\mathcal{H}_S) \rightarrow \mathcal{S}(\mathcal{H}_S) , \quad (3.6)$$

where $\Phi_{0,0}$ is the identity operator. It is readily shown that this map preserves the trace and Hermiticity, and is positive, i.e. one has

$$\text{Tr}_S(\Phi_{t,0}(A)) = \text{Tr}_S(A) \quad (3.7)$$

$$\Phi_{t,0}(A)^\dagger = \Phi_{t,0}(A^\dagger) \quad \forall A \in \mathcal{B}(\mathcal{H}_S) \quad (3.8)$$

and

$$\Phi_{t,0}(A) \geq 0 \quad \forall 0 \leq A \in \mathcal{B}(\mathcal{H}_S) , \quad (3.9)$$

respectively. Positivity of a map thus means that it maps positive operators to positive operators. The map $\Phi_{t,0}$ therefore defines an endomorphism on the state space $\mathcal{S}(\mathcal{H}_S)$ and determines for any initial state $\rho_S(0)$ of the open system

the corresponding open system state $\rho_S(t)$ at time t according to the action of the dynamics:

$$\rho_S(0) \in \mathcal{S}(\mathcal{H}_S) \mapsto \rho_S(t) \equiv \Phi_{t,0}(\rho_S(0)) . \quad (3.10)$$

This map is called the quantum dynamical map corresponding to time t with initial time $t = 0$. The attentive reader might ask why one requires to have a linear map since the state space is merely a convex set. However, any affine map has a unique linear extension to the underlying linear vector space so that I always refer to the linear extension of the dynamical map on the set of bounded operators $\mathcal{B}(\mathcal{H}_S)$ if necessary [18].

Apart from the above listed properties, a dynamical map has another important feature: it is not only positive but also completely positive. That is, it is n -positive for all $n \in \mathbb{N}$ which is defined as:

Definition 3.1. *A map $\Phi_{t,0}$ is said to be n -positive if and only if the linear tensor extension of the map defined by $(\Phi_{t,0} \otimes \mathbb{1}_n)(A \otimes B) = \Phi_{t,0}(A) \otimes B$ for $B \in \mathcal{B}(\mathbb{C}^n)$ and $A \in \mathcal{B}(\mathcal{H}_S)$ is positive.*

The combined map $\Phi_{t,0} \otimes \mathbb{1}_n$ can be interpreted as an operation which acts only non-trivially on the open systems Hilbert space \mathcal{H}_S . The second factor of the tensor product Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathbb{C}^n$, describing an ancillary n -level system, is left unchanged. Due to the fundamental property of entanglement in quantum theory, the requirement of complete positivity is essential for a dynamical map in order to represent a physical operation.

1-positivity is obviously equivalent to positivity of a dynamical map and the notion of n -positivity is hierarchical which means that $\Phi_{t,0}$ n -positive implies $\Phi_{t,0}$ k -positive for all $1 \leq k \leq n$ [2]. The converse, however, does not hold in general [10, 48]. For an open system of finite dimension N_S , one has a relatively simple criterion for complete positivity [9]: a linear map is completely positive if and only if it is N_S -positive.

An alternative characterization of completely positive maps is obtained by the Kraus representation [26]: a linear map $\Lambda : \mathcal{B}(\mathcal{H}_S) \rightarrow \mathcal{B}(\mathcal{H}_S)$ is completely positive if and only if there exist operators Ω_i , acting on the underlying Hilbert space \mathcal{H}_S , such that Λ can be written as

$$\Lambda(A) = \sum_i \Omega_i A \Omega_i^\dagger , \quad (3.11)$$

for any $A \in \mathcal{B}(\mathcal{H}_S)$. By cyclicity of the trace, one easily determines that such a map is trace preserving if and only if the Kraus operators satisfy the normalization² $\sum_i \Omega_i^\dagger \Omega_i = \mathbb{1}_S$. One easily determines the Kraus operators for any dynamical map of the kind of equation (3.5) using the spectral decomposition of the environmental state. Therefore, any dynamical map based on a microscopic approach is indeed completely positive.

This representation of a completely positive (**CP**) and trace preserving (**T**) map can be derived from Stinespring's dilation theorem [48]. The theorem states that any such map between states of finite-dimensional Hilbert spaces are of the

²Operations which at least do not increase the trace are considered frequently in quantum information theory. These maps obey the following modified normalization: $\sum_i \Omega_i^\dagger \Omega_i \leq \mathbb{1}_S$.

kind of equation (3.5): for a CPT-map Λ on $\mathcal{S}(\mathcal{H}_S)$ there exists an auxiliary system \mathcal{H}_κ and a unitary U on $\mathcal{H}_S \otimes \mathcal{H}_\kappa$ such that

$$\Lambda(\rho) = \text{Tr}_\kappa(U\rho \otimes \rho_\kappa U^\dagger), \quad (3.12)$$

for all $\rho \in \mathcal{S}(\mathcal{H}_S)$ whereas ρ_κ refers to some state on \mathcal{H}_κ . The auxiliary system's Hilbert space can be chosen such that $\dim \mathcal{H}_\kappa \leq (\dim \mathcal{H}_S)^2$.

It is important to notice that the representation (3.12) is only unique up to unitary equivalence. One thus infers from this theorem that any completely positive and trace preserving linear mapping can be related to a certain microscopic approach. The sets of CPT-maps and dynamical maps arising from microscopic approaches with factorizing initial conditions are actually identical.

The set

$$\Phi = \{\Phi_{t,0} \mid t \geq 0, \Phi_{0,0} = \mathbb{1}_S\} \quad (3.13)$$

defines a one-parameter family of dynamical (CPT-)maps and characterizes totally the quantum dynamical process as it contains all information about the time evolution of any state. Any quantum dynamical process of an open quantum system is formally given by a one-parameter family of CPT-maps.

Recall that an initial environmental state $\rho_E(0)$ was chosen for the definition of the dynamical map $\Phi_{t,0}$. Any other state $\tilde{\rho}_E(0)$ defines another dynamical process $\tilde{\Phi}$ whereas the total system evolves due to the same unitary dynamics. Thus, by changing the environmental contribution to the factorizing initial state one obtains a whole bunch of quantum dynamical processes.

If one considers the derivation of the dynamics based on a microscopic treatment (3.6), one recognizes that the map can be split up into three parts: the map consists of the so-called assignment map $\phi : \mathcal{S}(\mathcal{H}_S) \rightarrow \mathcal{S}(\mathcal{H})$ which assigns a state of the total system $\rho_{SE}(0) \equiv \phi(\rho_S(0))$ to an open system state ρ_S , a subsequently applied unitary evolution and the partial trace over the environment, i.e. $\Phi_{t,0} : \rho_S(0) \mapsto \text{Tr}_E(U_t \phi(\rho_S(0)) U_t^\dagger)$. Factorizing initial conditions are one possibility for an assignment map corresponding to $\phi : \rho_S(0) \mapsto \rho_S(0) \otimes \rho_E(0)$ for a certain environmental state which even reveals the input state, i.e. $\rho_S(0) = \text{Tr}_E(\rho_{SE}(0))$. If the assignment ϕ has exactly this property, the dynamics based on a microscopic approach is clearly equal to the identity for $t = 0$. Hence the question occurs whether there is another type of assignment map revealing this feature which yields a dynamics governed by linear CPT-maps? The answer is “no”: it has been shown [31, 49] that there is only the map associated to factorizing initial conditions which satisfies all the requirements. Thus, the rather drastic assumption of factorizing initial conditions is indeed the only possibility to obtain a microscopically motivated dynamical map unless either the trivial action for $t = 0$ or linearity is abandoned. However, these two properties are two intrinsic features of a mapping which describes the evolution of a quantum state.

3.2.1 General master equation

As the determination of the dynamical maps is typically as difficult as solving the Liouville-von Neumann equation (3.1), several other methods for the treatment of the dynamics of open systems were developed. There are several theoretical and numerical approaches, like projection operator techniques [39, 58], influence

functional and path integral techniques [14], quantum Monte Carlo methods and stochastic wave function techniques [4, 41]. Here, I concentrate on a commonly used description for the dynamical evolution of an open quantum state in terms of a so-called quantum master equation. More precisely, time-local quantum master equations, which refer to a first-order linear differential equation, are considered in the following part of the thesis.

According to this approach, the infinitesimal evolution of an open quantum system's state $\rho_S \in \mathcal{S}(\mathcal{H}_S)$ at time t obeys

$$\frac{d}{dt}\rho_S(t) = \mathcal{K}(t)\rho_S(t) . \quad (3.14)$$

The generator $\mathcal{K}(t)$ must then preserve Hermiticity and the trace of the states which implies that

$$[\mathcal{K}(t)A]^\dagger = \mathcal{K}(t)A , \quad \text{Tr}_S(\mathcal{K}(t)A) = 0 , \quad (3.15)$$

holds for all t and Hermitian operators A on \mathcal{H}_S . Based on these requirements, one deduces that the most general form of the generator is given by [3, 13]

$$\begin{aligned} \mathcal{K}(t)\rho_S(t) = & -i[H_S(t), \rho_S(t)] \\ & + \sum_i \gamma_i(t) \left[A_i(t)\rho_S(t)A_i^\dagger(t) - \frac{1}{2}\{A_i^\dagger(t)A_i(t), \rho_S(t)\} \right] . \end{aligned} \quad (3.16)$$

Here, $H_S(t)$ is a system Hamiltonian, which may not coincide with the Hamiltonian of the microscopic approach (3.2), and $A_i(t)$ are arbitrary operators in $\mathcal{B}(\mathcal{H}_S)$. These are the so-called (generalized) Lindblad operators describing the various decay channels of the system. Moreover, $\gamma_i(t)$ refers to the corresponding decay rate. The term $-i[H_S(t), \rho_S(t)]$ represents the reversible, Hamiltonian evolution of the open system whereas the second term on the right-hand side of equation (3.16) takes irreversible effects like dissipation into account for which reason it is called the dissipator.

Complete positivity is not guaranteed by the very structure of the generator and the most general conditions on the components of (3.16) leading to a CPT-map are unfortunately still not known yet. A sufficient condition is given by positive decay rates: if $\gamma_i(t) \geq 0$ for all $t \geq 0$ the arising dynamical map is indeed completely positive. In this special case the generator $\mathcal{K}(t)$ can be brought into Lindblad form (see (3.19)) for any time t . Such a process is usually referred to as a time-dependent Markovian process. Moreover, for a time-independent generator \mathcal{K} with positive rates the induced dynamics is governed by a semigroup. I will return to this in the subsequent section.

It is widely believed that a non-memoryless dynamics necessarily requires a master equation which is non-local in time. This is based on the idea that memory effects can only be described by a non-trivial memory kernel as the term already suggests. However, the existence of a time-local master equation for the description of the system evolution even in the presence of memory effects can be easily motivated: Let the subdynamics of the open system be given by a one-parameter family of CPT-maps, i.e one has $\rho_S(t) = \Phi_{t,0}\rho_S(0)$ for any state $\rho_S(0)$. Assuming a smooth time dependence, one might differentiate this relation with respect to time t which yields

$$\frac{d}{dt}\rho_S(t) = \dot{\Phi}_{t,0}\rho_S(0) . \quad (3.17)$$

Obviously, one obtains a time-local equation from (3.17) if the dynamical evolution is invertible so that the initial state $\rho_S(0)$ can be written in terms of $\rho_S(t)$,

$$\frac{d}{dt}\rho_S(t) = \dot{\Phi}_{t,0}\Phi_{t,0}^{-1}\rho_S(t) . \quad (3.18)$$

Here, $\Phi_{t,0}^{-1}$ denotes the inverse of $\Phi_{t,0}$ in the algebra of superoperators acting on $\mathcal{B}(\mathcal{H}_S)$. However, the reversibility of the dynamics is not guaranteed generally: for very strong couplings of system and environment the inverse $\Phi_{t,0}^{-1}$ might not exist [3, 4]. Nevertheless, one can show [52, 53] that the inverse and, therefore, the generator $\mathcal{K}(t) = \dot{\Phi}_{t,0}\Phi_{t,0}^{-1}$ is mostly well defined if the time dependence is analytic. More precisely, the generator exists apart from isolated singularities. The state evolution can thus be described by a time-local master equation for the intermediate time intervals (see e.g. [29]). I want to stress that the inverse $\Phi_{t,0}^{-1}$ must not be completely positive. In general, it is neither completely positive nor even positive.

Due to this derivation, time-local master equations can indeed provide a valid description for dynamical systems even if they are facing strong memory effects. Time-local master equations of the form (3.14) are efficiently derived from an microscopic approach employing the technique of time-convolutionless projection operators [8, 17, 47] (see also [6]).

3.2.2 Completely positive semigroups

A time-local master equation with a time-independent generator and positive rates deserves special attention as the arising dynamics has particular features. In this case, the generator is in the famous *Lindblad form* [13, 30]

$$\mathcal{L}\rho_S(t) = -i[H_S, \rho_S] + \sum_i \gamma_i \left[A_i \rho_S(t) A_i^\dagger - \frac{1}{2} \{ A_i^\dagger A_i, \rho_S(t) \} \right] , \quad (3.19)$$

where the rates obey $\gamma_i \geq 0$. The solution of the associated time-local master equation

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t) , \quad (3.20)$$

is simply given by $\Phi_{t,0} = \exp\{\mathcal{L}t\}$ which yields a one-parameter family of CPT-maps as already mentioned in the previous section. Moreover, a dynamical process obtained from a Lindblad master equation has the additional feature that it constitutes a semigroup:

Definition 3.2. *A one-parameter family of dynamical maps $\{\Phi_{t,0} \mid t \geq 0, \Phi_{0,0} = \mathbb{1}\}$ defines a semigroup³ if and only if for all $t, s \geq 0$ the map $\Phi_{t+s,0}$ can be represented by*

$$\Phi_{t+s,0} = \Phi_{t,0}\Phi_{s,0} . \quad (3.21)$$

The semigroup property implies that a dynamical map has a universal action on the state evolution which means that its effect on a state is independent of the point in time when it is applied. This property directly reflects the negligence of any memory effects. Dynamical evolutions which are governed by

³More precisely, it is called a *one-parameter semigroup* in this case (see [44]).

a completely positive semigroup are therefore called Markovian. It is clear that not all dynamical processes define a semigroup.

One might ask whether it is possible to derive a time-local master equation for a dynamical process which defines a semigroup. Under very general mathematical conditions⁴, any semigroup has an infinitesimal generator so that any element of the group can be written as exponential of the generator as above. Moreover, the popular Gorini-Kossakowski-Sudarshan-Lindblad theorem [13, 30] establishes a one-to-one connection between the Lindblad form for a generator and the existence of semigroups of completely positive and trace preserving maps: \mathcal{L} is the generator of a semigroup of dynamical maps if and only if it is in Lindblad form (3.19). Hence, any evolution, which is based on a time-local master equation whose generator is in Lindblad form, describes a dynamical process. This theorem thus allows phenomenological approaches for the description of open system dynamics, that is why Lindblad generators have been studied and used intensively in the theory of open quantum systems.

However, it is also possible to derive a master equation with a generator in Lindblad form directly from the underlying microscopic theory for the total system. As the semigroup property (3.21) is a strong requirement on the dynamical evolution, several drastic approximations must be made in order to arrive at such a master equation. Besides the Born and rotating wave approximation, the so-called Markov approximation, which presupposes a separation of the intrinsic time scales of the system and environment, is the most important. More precisely, the system's relaxation time τ_S and the correlation time of the environment τ_E is assumed to obey $\tau_E \ll \tau_S$ which means that the degrees of freedom of the open system are slow compared to those of the environment. There are many examples of physical interest for which the Markov approximation is justified, but its validity is not generally ensured as the title of this thesis might already suggest. For example the presence of a large system-environment coupling or an environment at low temperatures violates the assumption on the time scales yielding a failure of the Markov approximation. For a more detailed description of this and the subsequent approximations and their mathematical implementations, I refer to [6].

The Born approximation is based on the assumption of a weak coupling between system and environment which is also a fundamental requirement for the Markov approximation. Due to the weak interaction of system and environment, the states of the composite system are supposed to be solely weakly correlated for all times and, in addition, a perturbation expansion up to second order in the interaction Hamiltonian of the Liouville-von Neumann equation is done. This yields a closed second order integro-differential equation for the system density matrix to which the Markov approximation can then be applied. Finally, the so-called rotating wave approximation presumes that the time scale of the intrinsic evolution of the open system τ_I is much smaller than the system's relaxation, i.e. $\tau_I \ll \tau_S$. By virtue of this, some terms in the second order differential equation oscillate rapidly and can therefore be neglected.

By the very names of these approximations and the stated features concerning memory effects of a semigroup evolution, it becomes clear that such a dynamics provides the prototype of a memoryless, that is Markovian dynamics.

⁴The semigroup must be continuous with respect to some topology. For example one can require $\lim_{t \rightarrow 0} \|\Phi_{t,0}A - A\| = 0$ for every $A \in \mathcal{B}(\mathcal{H}_S)$, where $\|\cdot\|$ refers to the operator norm (see e.g. [44]).

3.2.3 Divisibility of dynamical processes

The assumption of a dynamical semigroup is very strong so that an arbitrary family of CPT-maps $\{\Phi_{t,0} \mid t \geq 0, \Phi_{0,0} = \mathbb{1}_S\}$, defining the dynamical process, does usually not possess this property. The notion of divisibility of dynamical maps represents a generalization of the composition law (3.21) of a semigroup. It has received some attention in the classification of dynamical evolutions in terms of Markovian or non-Markovian dynamics.

Definition 3.3. *A dynamical process Φ is called divisible if and only if for all $t \geq s \geq 0$ there exists a CPT-map $\Phi_{t,s}$ such that the relation*

$$\Phi_{t,0} = \Phi_{t,s} \Phi_{s,0} , \quad (3.22)$$

holds.

For a dynamics arising from a time-local master equation with generator $\mathcal{K}(t)$ (cf. (3.14)) the connecting map $\Phi_{t,s}$ is given by

$$\Phi_{t,s} = \text{T exp} \left\{ \int_s^t dt' \mathcal{K}(t') \right\} , \quad (3.23)$$

where T denotes the chronological time-ordering operator. This map is CPT if and only if the decay rates are always non-negative, i.e. $\gamma_i(t) \geq 0$ (see e.g. [29]). Thus, the occurrence of a negative rate $\gamma_i(t)$ for some channel at $t \geq 0$ is necessary and sufficient for the breakdown of divisibility of the dynamical map.

A semigroup with generator \mathcal{L} in Lindblad form is always divisible. In this special case, equation (3.23) reduces to

$$\Phi_{t,s} = \exp\{\mathcal{L}(t-s)\} . \quad (3.24)$$

It is clear that the definition of divisibility is trivially satisfied if $t = s$ or $s = 0$ as the identity and the dynamical map $\Phi_{t,0}$ are CPT by assumption. I emphasize that the above given definition of divisibility is a strengthening of the usual notion of divisibility. Typically, a CPT-map Λ is called divisible if and only if there exist CPT-maps Λ_1 and Λ_2 such that $\Lambda = \Lambda_1 \Lambda_2$ where neither Λ_1 nor Λ_2 is a unitary – otherwise the required decomposition is trivial [55]. On the contrary, definition 3.3 demands the existence of a linear CPT-map $\Phi_{t,s}$ for a given second CPT-map $\Phi_{s,0}$, which is determined by the dynamical process, for all $t, s \geq 0$. The mapping $\Phi_{t,s}$ thus maps the time-evolved states at time s to those states at $t \geq s$ and it defines even a dynamical map on its own as it is CPT. Hence, it can actually be applied to any state⁵. Of course, there are many quantum dynamical processes which are not divisible (see e.g. [29]): either there exists no linear map $\Phi_{t,s}$ at all, or it is not CP, or even not positive. If the maps mediating between the dynamical maps are not completely positive but still positive one calls such a dynamical process *P-divisible*.

⁵This is special because there are certainly dynamical maps whose range is not the entire state space (this is actually the generic case). Thus, one might think that it is sufficient for $\Phi_{t,s}$ to be defined on the time-evolved state space in order to link the different stages of the dynamical evolution.

3.3 The trace distance

In this section, I define the trace distance, which is a particular measure on the state space, and summarize some of its important properties including the physical interpretation. Other features of the trace distance and most of the proofs of the stated mathematical properties can be found in [18, 40].

As already remarked in section (2.2), the trace distance of two quantum states ρ_1 and ρ_2 is defined as

$$\mathcal{D}(\rho_1, \rho_2) = \frac{1}{2} \text{Tr}(|\rho_1 - \rho_2|) . \quad (3.25)$$

The range of this functional on $\mathcal{S}(\mathcal{H}) \times \mathcal{S}(\mathcal{H})$ is the interval $[0, 1]$, where the upper and lower bound are saturated,

$$\mathcal{D}(\rho_1, \rho_2) = 0 \quad \Leftrightarrow \quad \rho_1 = \rho_2 , \quad (3.26)$$

$$\mathcal{D}(\rho_1, \rho_2) = 1 \quad \Leftrightarrow \quad \rho_1 \perp \rho_2 . \quad (3.27)$$

Here, $\rho_1 \perp \rho_2$ means that the two states have orthogonal supports. This implies that they have a common spectral decomposition with complementary eigenvalues. That is, the respective sets of eigenvalues regarded as vectors are orthogonal with respect to the usual scalar product. As a state has solely positive eigenvalues, one concludes that orthogonal states must have some zero eigenvalues and, therefore, are located on the boundary (2.7) for any system.

Furthermore, the trace distance is even a metric on the state space, i.e. $\mathcal{D}(\cdot, \cdot)$ is not only positive semi-definite and symmetric, but satisfies also the triangle inequality:

$$\mathcal{D}(\rho_1, \rho_2) \leq \mathcal{D}(\rho_1, \rho_3) + \mathcal{D}(\rho_3, \rho_2) . \quad (3.28)$$

A third, important property of the trace distance, making it a very useful measure for the distance between quantum states, is its invariance under unitary transformations. More generally, all CPT-maps Λ are contractions for the trace distance, i.e.

$$\mathcal{D}(\Lambda\rho_1, \Lambda\rho_2) \leq \mathcal{D}(\rho_1, \rho_2) . \quad (3.29)$$

It is important here that the maps are trace preserving. Moreover, even the larger class of positive trace-preserving maps satisfies this inequality [45]. Hence, a non-positive trace preserving map might yield an increase of the trace distance whereas any dynamical map is contractive.

The trace distance can also be represented in terms of the maximum of a certain functional over all positive operators that are smaller than the identity:

$$\mathcal{D}(\rho_1, \rho_2) = \max_{0 \leq A \leq \mathbb{1}} \text{Tr}\{A(\rho_1 - \rho_2)\} . \quad (3.30)$$

It actually suffices to perform the maximization over the set of all projections. As the trace distance is symmetric, the right hand side must be invariant under interchanging ρ_1 and ρ_2 . However, the maximum will then be attained by a different operator A .

3.3.1 Physical interpretation of the trace distance

On the basis of the representation (3.30), the trace distance of two states ρ_1 and ρ_2 features a nice operational meaning in quantum information.

Suppose there is a sender (Alice) and a receiver (Bob). Alice has two preparation procedures at hand, which yield two unequal states ρ_1 and ρ_2 . She randomly applies (with probability $\frac{1}{2}$) one of these procedures and sends the prepared state, ρ_1 or ρ_2 , to Bob whose task is to determine by a single measurement the state Alice has given to him. Bob knows the two states which can be prepared and that the probability distribution is unbiased. This setup is often called a one-shot, two-state discrimination problem. Because Bob has only a single measurement to gain information about the state, there are cases in which it is impossible to distinguish the quantum states with certainty. Hence, how well can Bob identify the state sent to him in general? In fact, there is an optimal measurement strategy for each pair of states that allows him to discriminate the two states most successful. The corresponding maximal success probability for correct state discrimination of ρ_1 and ρ_2 by a single measurement is given by

$$\mathcal{P}_{discr} = \frac{1}{2}\{1 + \mathcal{D}(\rho_1, \rho_2)\} . \quad (3.31)$$

Thus, the trace distance is the bias in favor of a correct state identification which can be achieved using the optimal strategy. Due to this, \mathcal{D} can be interpreted as a measure for the distinguishability of two quantum states [18–20]. See [18] for a derivation of the relation (3.31).

A perfect state discrimination, $\mathcal{P}_{discr} = 1$, can thus be obtained if and only if $\mathcal{D}(\rho_1, \rho_2) = 1$ which means that the states are orthogonal (cf. Eq. (3.26)). Here, the optimal strategy consists in measuring the projection onto the support of ρ_1 (or ρ_2). More generally, applying the projection P which maximizes equation (3.30), and associating the measurement outcome "1" with ρ_1 and the outcome "0" with ρ_2 defines the optimal strategy. Given this measurement setup and the assignment⁶, the probability of correct state discrimination is given by

$$\mathcal{P}_{discr} = \frac{1}{2}\text{Tr}\{P\rho_1\} + \frac{1}{2}\text{Tr}\{(\mathbb{1} - P)\rho_2\} , \quad (3.32)$$

as $\text{Tr}(P\rho_1)$ and $\text{Tr}((\mathbb{1} - P)\rho_2)$ describe the probability for the outcome "1" given the state is ρ_1 and "0" if the state is ρ_2 , respectively. Moreover, the coefficient $\frac{1}{2}$ refers to the fact that ρ_1 and ρ_2 are equal likely. Rearranging terms on the right-hand side of equation (3.32) directly yields the maximal success probability (3.31) for a one-shot discrimination of ρ_1 and ρ_2 .

3.4 Concepts of non-Markovianity

The term (non-)Markovianity has been widely used in the theory of open quantum systems although its meaning in the quantum realm is not clear. All the difficulties arise because it is impossible to transfer the classical notion of a Markovian stochastic process to quantum theory. The classical definition of a stochastic process is based on the n -point probability distribution functions and a process is called Markovian if and only if for all $n \in \mathbb{N}$ the conditional probabilities depend solely on the preceding value, and not on the remaining past.

⁶On the basis of such an assignment for the measurement outcomes of a POVM (positive operator valued measure) describing a general measurement, one can derive relation (3.31).

Given the present state of a stochastic process, the past and the future are thus independent which motivates the interchangeably used notion of a *Markovian* and a *memoryless* stochastic process.

However, such a hierarchy of n -point probability distribution functions does not exist for quantum systems as there is no possibility to gain information about a quantum system without disturbing it, affecting fundamentally its subsequent evolution. Moreover, the determination of all n -point functions is impossible for practical issues even in the classical setting wherefore the definition of a Markov process must be considered as an abstract, mathematical tool. Due to these difficulties, the fundamental question emerges: How do quantum memory effects manifest themselves in the dynamics of an open quantum systems, and how to quantify them? Moreover, the basic model of a memoryless dynamics given by a master equation in Lindblad form (cf. Sec. 3.2.2) should be still the prototype of a Markovian dynamics. Clearly, the property of a quantum process being Markov cannot depend on the mathematical representation of the dynamics, i.e. for example in terms of a master equation. It must be a fundamental feature of the dynamics and, therefore, the family of dynamical maps $\Phi_{t,0}$ should provide all information to determine the character of a quantum process. Quite recently, several proposals for a definition of quantum (non-)Markovianity have been published [5, 34, 42, 56].

In [42], the notion of quantum Markovianity is connected to the property of divisibility of a dynamical process. According to this definition, a quantum process is called non-Markovian if and only if it is non-divisible. The corresponding measure for quantum non-Markovianity quantifies the amount to which the dynamical process is not divisible. This definition is based on the idea that a quantum process arising from a Lindblad master equation describes a Markovian dynamics. Since the notion of divisibility can be seen as the generalization of the semigroup property (3.21), the term *Markovian* is related to this feature. In addition, the similarity of divisibility and the *Chapman-Kolmogorov equation* for a classical Markovian stochastic process [25] motivates the assignment of Markovianity and divisibility, too. Several other approaches based on this property were suggested.

A second proposal [5, 29] defines and quantifies non-Markovianity solely in terms of the information exchange between the open system and its environment. The basic idea underlying this approach is that memory effects in the dynamics manifest themselves in a backflow of information into the open system. Since the total information is preserved by construction, the past states of an evolution are seen to effect the future states in this way. A backflow thus describes a non-memoryless dynamics which is therefore termed non-Markovian. This idea is made more precise in the following section.

3.4.1 A measure for non-Markovianity

As shown in section 3.3.1, the trace distance defines a measure for the distinguishability of two quantum states. This interpretation and the contractivity under CPT-maps (3.29) directly yield that a dynamical change of $\mathcal{D}(\rho_1, \rho_2)$ for any two states $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H}_S)$ of the open system – indicating a change of distinguishability of these states – points to a flow of information between the open system and its environment. In this connection, the contractivity implies that there is no dynamical process described by a one-parameter family of dynami-

cal maps which increases the distinguishability of a state pair above its initial value. The open system can thus only recover at most as much information from the environment as previously flowed out of the system. This manifests a preservation of the total amount of information. Moreover, the invariance of the trace distance under unitary transformations indicates that information is preserved in closed quantum systems, supporting the suggested interpretation in terms of an information flow.

An increase of the trace distance then signifies a backflow of information into the system while a decreasing value of the trace distance is identified with a loss of information into the environment. More precisely, when speaking about loss or gain of information, one means the change of the relative information on the pair of states which allows a distinction of these states and is solely obtained by measurements on the open system's degrees of freedom. This implies that the information is not only swapped between the open system and the environment, but can also be carried by and taken from system-environment correlations.

In view of these considerations, the quantity of interest is the rate of change of the trace distance for two states evolving according to the studied dynamical process. One thus defines a dynamical process described in terms of a one-parameter family of dynamical maps $\Phi_{t,0}$ to be non-Markovian if and only if there exists a pair of initial states $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H}_S)$ and a time $t > 0$ such that

$$\sigma(t, \rho_1, \rho_2) \equiv \frac{d}{dt} \mathcal{D}(\rho_1(t), \rho_2(t)) > 0, \quad (3.33)$$

where $\rho_{1,2}(t) = \Phi_{t,0}\rho_{1,2}$ such that $\rho_{1,2}(0) = \rho_{1,2}$. The total increase of distinguishability of two states, i.e. the total amount of information flowing from the environment back to the system, is then obtained by integrating over all times for which the trace distance increases, that is, for which one has $\sigma > 0$. Moreover, one maximizes over all pairs of input states as the measure should be independent of the choice of initial states.

Definition 3.4. A measure $\mathcal{N}(\Phi)$ for the non-Markovianity of a quantum process Φ given in [5, 29] is defined by

$$\mathcal{N}(\Phi) \equiv \max_{\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H}_S)} \int_{\sigma > 0} dt \, \sigma(t, \rho_1, \rho_2) \in [0, \infty]. \quad (3.34)$$

With respect to this measure, a quantum process Φ is called non-Markovian if and only if $\mathcal{N}(\Phi) > 0$.

I would like to emphasize that the existence of the maximum is not guaranteed in general. For infinite-dimensional systems, for example, the maximum might not be attained by some state pair. In addition, the integration which formally ranges to $t = \infty$ might yield that there is no maximizing pair of states. The value of \mathcal{N} is, however, approached by a sequence of state pairs. To be mathematically more precise, the maximum in (3.34) should thus be replaced by the supremum in order to take these cases into account.

This definition of a measure for non-Markovianity is in perfect accordance with the dynamics arising from a Lindblad master equation which is regarded to be the prototypical Markovian quantum process. Although any CPT-mapping is a contraction for the trace distance, this does not imply that the trace distance between two open system states is monotonically decreasing for all times.

However, a divisible process and, thus, in particular any semigroup evolution yields a continuous loss of distinguishability. This feature is due to the fact that for divisible quantum processes or semigroups the maps mediating between two points on the trajectory of a state are CPT and, therefore, contractions for the trace distance. One has

$$\Phi \text{ divisible} \quad \Rightarrow \quad \mathcal{N}(\Phi) = 0, \quad (3.35)$$

i.e. any divisible family of quantum maps is Markovian with respect to \mathcal{N} . The converse is not true [11, 35]: there are non-divisible quantum processes which are Markovian. Thus, non-divisibility is just necessary for non-Markovianity. The reason for this fact is two-folded. Even a merely P-divisible family of dynamical maps (cf. Sec. 3.2.3) may lead to a continuous loss of distinguishability of two states signifying Markovianity. Hence, there might be families of dynamical maps that are not divisible but still P-divisible (see [51] for an example). However, the trace distance might even not increase for a process which is not P-divisible. One concludes that there is a fundamental difference between the two presented concepts [5, 42] for quantum non-Markovianity. This aspect was discussed in [11] and a suggestion how to reconcile this approach with divisibility was made.

The maximization procedure included in the definition of \mathcal{N} makes this quantity difficult to evaluate and for this it has attracted criticism. However, I want to stress that this definition of non-Markovianity is much more feasible in experiments than those based on the divisibility of the dynamics. It solely requires state tomography while the other measures need a process tomography in order to be able to determine and study the connecting maps $\Phi_{t,s}$ for all $t, s > 0$. In principle, performing three state tomographies can be sufficient to draw a conclusion whether the dynamics is non-Markovian or not with respect to \mathcal{N} , i.e. it is a witness. The measure based on the information flux can thus be determined by observing the dynamical evolution of state pairs while the other approaches require the knowledge of the complete dynamics $\Phi_{t,0}$.

Chapter 4

Characterizing optimal pairs of quantum states

The maximization involved in definition 3.4 makes the measure \mathcal{N} difficult to evaluate. One has to maximize over the set $\mathcal{S}(\mathcal{H}_S) \times \mathcal{S}(\mathcal{H}_S)$ whose dimension is given by $2(\dim \mathcal{H}_S)^2 - 2$ and, thus, increases rapidly with the size of the underlying Hilbert space. Due to this, the approach based on the information flux is difficult to evaluate and for this it has attracted criticism. The main objective of this thesis is to characterize mathematically the maximizing set of states, i.e. the set of optimal pairs:

Definition 4.1. *For a non-Markovian process Φ , a pair of states ρ_1, ρ_2 is said to be optimal if and only if the maximum in equation (3.34) is attained for it, i.e. if and only if*

$$\mathcal{N}(\Phi) = \int_{\sigma>0} dt \sigma(t, \rho_1, \rho_2) \quad (4.1)$$

holds for this pair of initial states.

The definition of an optimal pair is only reasonable for non-Markovian dynamics, i.e. $\mathcal{N}(\Phi) \neq 0$, because otherwise any pair of states would be trivially optimal. Moreover, an optimal pair might not be unique and it is clear that the optimality property implies $\rho_1 \neq \rho_2$. From now on, I assume that the maximum in (3.34) exists which means that the set of optimal pairs is not empty. I will show in section 4.2.1 how the following results can also be used if there exist no optimal pair which occurs, for example, for infinite-dimensional systems.

In this section I present the major results of my work: I rigorously prove general statements about the mathematical properties of optimal state pairs. All my results are solely based on the linearity of dynamical maps and can therefore be applied to any dynamical process. As my first result (Sec. 4.1), I show that both states of an optimal pair must lie on the boundary (2.7) of the state space $\mathcal{S}(\mathcal{H}_S)$. In section 4.2 I then proceed to demonstrate that the states of any optimal pair must actually be orthogonal in order to give rise to the maximal possible degree of memory effects in their dynamics. At the end of this chapter (Sec. 4.4) I will present an alternative proof¹ of this result. The second proof employs the notion of joint translatability of two non-orthogonal

¹The second approach for a proof of the orthogonality of optimal states only holds for finite-dimensional systems whereas the first one holds for arbitrary systems.

states which gives some insight into the structure of state space. On the basis of the orthogonality of optimal states it is possible to resolve a second point of criticism of the measure \mathcal{N} : the maximization can be restricted to a single input state. I will show in section 4.3 how this can be done.

From now on, I will use \mathcal{H} instead of \mathcal{H}_S in order to simplify notation since I will exclusively talk about the Hilbert space of the open system and the corresponding state space.

4.1 Restriction to the boundary of state space

Theorem 4.1. *Let $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ be an optimal state pair. Then both states lie on the boundary of the states space, i.e. $\rho_1, \rho_2 \in \partial\mathcal{S}(\mathcal{H})$.*

Proof. Suppose that at least one state of the pair, say ρ_2 , does not belong to the boundary. Hence, ρ_2 is an interior point and by the definition of the interior $\dot{\mathcal{S}}(\mathcal{H})$ (cf. (2.6)) there exists $\lambda > 1$ such that

$$\rho_3 = (1 - \lambda)\rho_1 + \lambda\rho_2 \in \mathcal{S}(\mathcal{H}) , \quad (4.2)$$

is a quantum state (see Fig. 4.1 (a)). The time evolution of the three states according to the dynamical process Φ is given by $\rho_i(t) = \Phi_{t,0}(\rho_i)$, $i = 1, 2, 3$. By the linearity of the dynamical map one has

$$\rho_3(t) = (1 - \lambda)\rho_1(t) + \lambda\rho_2(t) , \quad (4.3)$$

and, hence,

$$\rho_1(t) - \rho_3(t) = \lambda(\rho_1(t) - \rho_2(t)) . \quad (4.4)$$

It follows that

$$\mathcal{D}(\rho_1(t), \rho_3(t)) = \lambda\mathcal{D}(\rho_1(t), \rho_2(t)) , \quad (4.5)$$

by the homogeneity of the trace and the continuous functional calculus which yields

$$|\rho_1(t) - \rho_3(t)| = |\lambda| |\rho_1(t) - \rho_2(t)| . \quad (4.6)$$

Note that λ is a fixed number strictly larger than 1. Thus, equation (4.5) states that the trace distance between $\rho_1(t)$ and $\rho_3(t)$ is always larger by the constant factor λ than the trace distance between $\rho_1(t)$ and $\rho_2(t)$. This implies that the quantity $\int_{\sigma>0} dt \sigma(t, \rho_1, \rho_3)$ is larger than $\int_{\sigma>0} dt \sigma(t, \rho_1, \rho_2)$ by the same factor λ as σ is homogeneous. It follows that ρ_1, ρ_2 cannot be an optimal pair which is a contradiction. Consequently, any optimal pair of states must belong to the boundary of the state space $\partial\mathcal{S}(\mathcal{H})$. \square

For any dynamical process Φ described by a one-parameter family of linear dynamical maps, the maximization over all initial state pairs in the definition 3.4 of the non-Markovianity measure $\mathcal{N}(\Phi)$ can thus be restricted to the boundary $\partial\mathcal{S}(\mathcal{H})$ of the state space,

$$\mathcal{N}(\Phi) = \max_{\rho_{1,2} \in \partial\mathcal{S}(\mathcal{H})} \int_{\sigma>0} dt \sigma(t, \rho_1, \rho_2) . \quad (4.7)$$

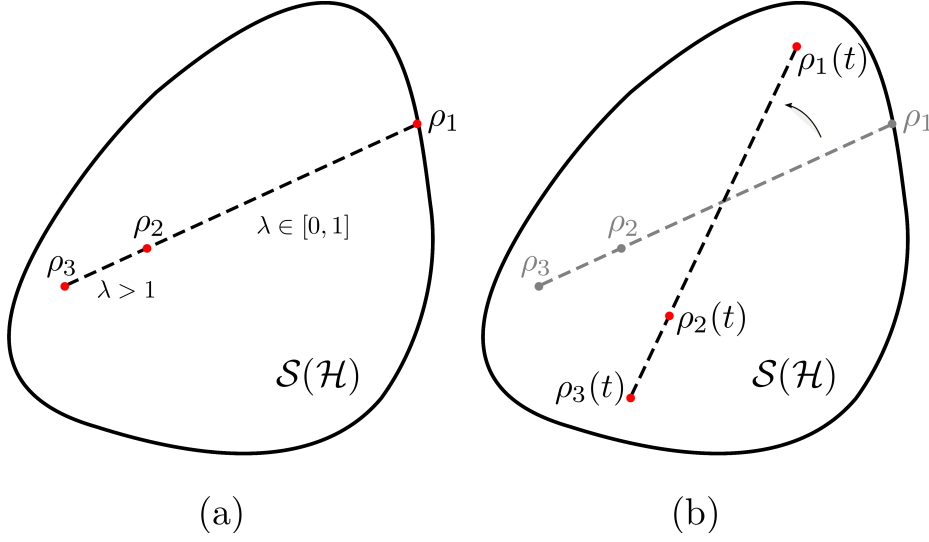


Figure 4.1: Illustration of the decomposition (4.2) (a) and of the corresponding time evolution (b) given by Eq. (4.3).

As the proof shows, this result is valid for any Hilbert space \mathcal{H} and for any family of linear dynamical maps $\Phi_{t,0}$. From the characterization of the boundary derived in section 2.1 it follows that the statement is trivial for infinite-dimensional systems. The only requirement on the structure of the dynamical maps is linearity which guarantees the invariance of the decomposition defined in (4.2) for all times t : lines remain lines within the dynamical evolution, see figure 4.1 (b). In addition, the theorem exploits the convex structure of the state space present in the characterization of the interior $\mathring{\mathcal{S}}(\mathcal{H})$ implying that an inner point is extendible in any direction.

As a consequence of this first characterization, optimal state pairs must be pure states for two-level systems since the set of pure states is identical to the boundary $\partial\mathcal{S}(\mathcal{H})$ in this case. However, this does not hold in general as it will be shown in chapter 5.

4.2 Orthogonality of optimal pairs

The physical content of the previous result is that having a zero eigenvalue is a necessary criterion for a state to be part of an optimal pair. However, this does not tell us anything about the relation of two optimal states. I will now demonstrate that optimal state pairs must be orthogonal, which strengthens the result of theorem 4.1 as it establishes a relation between the two partners of an optimal pair. The two states of an optimal pair are thus not chosen arbitrarily, as orthogonality implies that the states have a common spectral decomposition and their eigenvalues considered as a vector must be orthogonal with respect to the standard scalar product. By this, they must have a zero eigenvalue and, therefore, both states belong to the boundary $\partial\mathcal{S}(\mathcal{H})$. This result is particularly nice and physically very plausible as orthogonality is equivalent to unit trace distance [18, 40]: the largest flow of information from the environment back to

the open system emerges if the initial state pair is distinguishable with certainty, i.e. has the maximal information content.

The following theorem uses the well-known Jordan-Hahn decomposition [1, 40] which holds for arbitrary systems as it can be proven for C^* -algebras [2].

Lemma 4.1. *Let A be an Hermitian operator. Then there exist positive operators $A_+ \geq 0$ and $A_- \geq 0$ which satisfy $A_+A_- = A_-A_+ = 0$ and*

$$A = A_+ - A_- . \quad (4.8)$$

That is, A_+ and A_- are positive orthogonal operators whose difference is the given Hermitian operator A .

The idea of employing the Jordan-Hahn decomposition for the proof of the orthogonality of optimal pairs is due to *Antti Karlsson* [54]. Short time after I had given the first proof for this fact using the concept of joint-translatibility, which will be presented in section 4.4, he got the idea to employ this well-known decomposition to give a simpler proof for this property of optimal pairs. The proof of the following theorem has been then developed in close collaboration with the group of *Jyrki Piilo*.

Theorem 4.2. *Optimal state pairs are orthogonal.*

Proof. Let $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ be an optimal pair of states, and suppose that the states are not orthogonal, $\rho_1 \not\perp \rho_2$. According to the Jordan-Hahn decomposition there exist positive and orthogonal operators P_1 and P_2 such that the traceless Hermitian operator $\rho_1 - \rho_2$ can be represented by

$$\rho_1 - \rho_2 = P_1 - P_2 . \quad (4.9)$$

Taking the trace of this equation, one obtains $\lambda \equiv \text{Tr}P_1 = \text{Tr}P_2 \geq 0$ by positivity of the P_i . From $\rho_1 \neq \rho_2$ it follows that $P_1, P_2 \neq 0$ and, therefore, $\lambda > 0$. Using equation (4.9), the orthogonality of P_1 and P_2 , and the fact that the trace distance between non-orthogonal states is always strictly smaller than 1, one finds

$$1 > \mathcal{D}(\rho_1, \rho_2) = \mathcal{D}(P_1, P_2) = \frac{1}{2} (\text{Tr}P_1 + \text{Tr}P_2) = \lambda . \quad (4.10)$$

Thus, one has $0 < \lambda < 1$. Now one defines the operators $\sigma_1 \equiv P_1/\lambda$ and $\sigma_2 \equiv P_2/\lambda$. Being positive and of unit trace, these operators represent quantum states. Moreover, they obey

$$\sigma_1 - \sigma_2 = \frac{1}{\lambda} (\rho_1 - \rho_2) . \quad (4.11)$$

By use of the linearity of the dynamical maps, this relation is preserved under time evolution, i.e.

$$\sigma_1(t) - \sigma_2(t) = \frac{1}{\lambda} (\rho_1(t) - \rho_2(t)) , \quad (4.12)$$

from which it follows that

$$\mathcal{D}(\sigma_1(t), \sigma_2(t)) = \frac{1}{\lambda} \mathcal{D}(\rho_1(t), \rho_2(t)) , \quad (4.13)$$

by the same arguments as in the proof of theorem 4.1. Since $\lambda^{-1} > 1$ one concludes from the last equation that the pair σ_1, σ_2 yields a non-Markovianity which is strictly larger than that of the pair ρ_1, ρ_2 , which contradicts the assumption that ρ_1, ρ_2 is an optimal pair. Hence, ρ_1 and ρ_2 must be orthogonal. \square

The maximization in the definition (3.34) of the measure $\mathcal{N}(\Phi)$ for quantum non-Markovianity can thus be restricted to orthogonal initial state pairs,

$$\mathcal{N}(\Phi) = \max_{\rho_1 \perp \rho_2} \int_{\sigma > 0} dt \, \sigma(t, \rho_1, \rho_2) . \quad (4.14)$$

Again, this result holds for any Hilbert space \mathcal{H} (finite or infinite) and any family of linear dynamical maps $\Phi_{t,0}$ representing the dynamical process Φ . Returning to a two-dimensional Hilbert space, this result implies that the states of an optimal pair must be pure, antipodal states (cf. Sec. 2.3.1).

4.2.1 Existence of an optimal pair

I have assumed in theorem 4.1 and 4.2 that an optimal pair of states does exist. As mentioned previously the existence of these pairs is not ensured in general. If there is no such pair and the maximum is thus a supremum, there is a sequence of state pairs ρ_1^n, ρ_2^n such that $\int_{\sigma > 0} dt \, \sigma(t, \rho_1^n, \rho_2^n)$ converges to $\mathcal{N}(\Phi)$ for $n \rightarrow \infty$. Employing the construction used in the proof of theorem 4.2, one can show that the pairs ρ_1^n, ρ_2^n can always be taken to be orthogonal. This means that the non-Markovianity measure can be approximated with arbitrary precision by orthogonal state pairs and that one can write

$$\mathcal{N}(\Phi) = \sup_{\rho_1 \perp \rho_2} \int_{\sigma > 0} dt \, \sigma(t, \rho_1, \rho_2) . \quad (4.15)$$

4.3 A new representation of the measure

I will now use the mathematical characterization of optimal states for non-Markovian dynamics obtained in theorem 4.2 in order to determine a new and more convenient representation of the measure \mathcal{N} . I will show in theorem 4.3 that the set of orthogonal state pairs of any finite-dimensional system can be represented by states of an appropriate set and a second, fixed state in the interior $\mathring{\mathcal{S}}(\mathcal{H})$. This yields a new representation of the measure \mathcal{N} where the maximization is reduced to a single input state while the other state is kept fixed. The result strongly uses the Jordan-Hahn decomposition (cf. lemma 4.1). To make the statement more precise I first define

$$\mathcal{E}_0(\mathcal{H}) = \{A \in \mathcal{B}(\mathcal{H}) \mid A \neq 0, A = A^\dagger, \text{Tr} A = 0\} , \quad (4.16)$$

to be the set of non-zero, Hermitian and traceless operators on \mathcal{H} . Using this set I introduce a particular kind of sets for a state of the interior. Let $\rho_0 \in \mathring{\mathcal{S}}(\mathcal{H})$ be an interior point of a finite-dimensional state space $\mathcal{S}(\mathcal{H})$.

Definition 4.2. A set $\partial U(\rho_0) \subset \mathcal{S}(\mathcal{H})$ is called an enclosing surface of ρ_0 if and only if for any operator $A \in \mathcal{E}_0(\mathcal{H})$ there exists a real number $\lambda > 0$ such that

$$\rho_0 + \lambda A \in \partial U(\rho_0) . \quad (4.17)$$

It follows that $\rho_0 \notin \partial U(\rho_0)$ by definition as A cannot be trivial and $\lambda > 0$ for any A . Moreover, one observes that $\partial U(\rho_0) \subset \mathcal{S}(\mathcal{H})$ holds by definition. An enclosing surface corresponds to the boundary of a neighbourhood of ρ_0 (or $\vec{v}^{(\rho_0)}$),

respectively) with respect to the Euclidean distance if the state space is identified with a subset of Euclidean space using the generalized Bloch representation. This is easily determined from the fact that the set $\mathcal{E}_0(\mathcal{H})$ of non-trivial, Hermitian and traceless operators corresponds to all non-trivial vectors in \mathbb{R}^{N^2-1} for an N -level system. In this case, an $N^2 - 2$ -dimensional sphere having $\vec{v}^{(\rho_0)}$ in its center is an example for an enclosing surface of ρ_0 . One observes that the convex hull of an enclosing surface contains its inner point ρ_0 . Therefore, an enclosing surface can also be seen as the boundary of the convex hull of a set which contains the reference state.

It can be easily seen from the definition of the interior $\mathring{\mathcal{S}}(\mathcal{H})$ (cf. (2.6)) that any interior point has an enclosing surface. On the other hand it is clear that no point on the (intrinsic) boundary has an enclosing surface. For such points there exist operators $A \in \mathcal{E}_0(\mathcal{H})$ such that $\rho_0 + \lambda A \notin \mathcal{S}(\mathcal{H})$ for all $\lambda > 0$ by definition. For the same reason this new representation is only valid for finite systems. In theorem 2.2 it has been shown that for any state ρ_0 there exists an operator $A \in \mathcal{E}_0(\mathcal{H})$ such that $\rho_0 + \lambda A \notin \mathcal{S}(\mathcal{H})$ for any $\lambda > 0$.

I emphasize that an enclosing surface $\partial U(\rho_0)$ can be of any shape such that its convex hull contains ρ_0 . Using this definitions, it is possible to prove the following theorem:

Theorem 4.3. *Let $\rho_0 \in \mathring{\mathcal{S}}(\mathcal{H})$ be any fixed state of the interior of a finite-dimensional state space and $\partial U(\rho_0)$ an arbitrary enclosing surface of ρ_0 . For a dynamical process Φ , the measure for quantum non-Markovianity \mathcal{N} (3.4) is then given by*

$$\mathcal{N}(\Phi) = \max_{\rho \in \partial U(\rho_0)} \int_{\bar{\sigma} > 0} dt \, \bar{\sigma}(t, \rho, \rho_0), \quad (4.18)$$

where

$$\bar{\sigma}(t, \rho, \rho_0) \equiv \frac{\frac{d}{dt} \mathcal{D}(\Phi_{t,0}(\rho), \Phi_{t,0}(\rho_0))}{\mathcal{D}(\rho, \rho_0)}. \quad (4.19)$$

Proof. Let $\rho \in \partial U(\rho_0)$. Applying the Jordan-Hahn decomposition, there exists an orthogonal pair of states ρ_1, ρ_2 such that (cf. the proof of theorem 4.2)

$$\rho_1 - \rho_2 = \frac{\rho - \rho_0}{\mathcal{D}(\rho, \rho_0)}, \quad (4.20)$$

and, hence,

$$\rho_1(t) - \rho_2(t) = \frac{\rho(t) - \rho_0(t)}{\mathcal{D}(\rho, \rho_0)}, \quad (4.21)$$

by linearity of the dynamical maps. Employing homogeneity of the trace distance and the derivative, this shows that the right-hand side of (4.18) is not larger than \mathcal{N} when it is maximized over pairs of orthogonal states, see (4.15). However, the right-hand side of (4.18) is actually equal to the originally defined measure \mathcal{N} . In order to prove this, suppose ρ_1, ρ_2 are two orthogonal states. As $\rho_1 - \rho_2 \in \mathcal{E}_0(\mathcal{H})$, there exists a $\lambda > 0$ such that

$$\rho \equiv \rho_0 + \lambda(\rho_1 - \rho_2) \in \partial U(\rho_0), \quad (4.22)$$

by definition of an enclosing surface of ρ_0 . Thus, one obtains

$$\rho_1 - \rho_2 = \frac{\rho - \rho_0}{\lambda} , \quad (4.23)$$

and $\lambda = \mathcal{D}(\rho, \rho_0)$, since $\rho_1 \perp \rho_2$, so that one has again

$$\rho_1 - \rho_2 = \frac{\rho - \rho_0}{\mathcal{D}(\rho, \rho_0)} . \quad (4.24)$$

This equation shows that the right-hand side of equation (4.18) is larger than or equal to \mathcal{N} which finally establishes equality between these two terms showing that (4.18) holds. \square

This surprising result reveals the fact that an inner point and an enclosing surface contain all *directions*, that is, all traceless, Hermitian operators. If the difference of the reference state $\rho_0 \in \mathcal{S}(\mathcal{H})$ and its surrounding states of an enclosing surface is considered, one obtains all operators in $\mathcal{E}_0(\mathcal{H})$ by the very definition of the surface. These operators are the relevant input for non-Markovianity regarding the backflow of information defined by \mathcal{N} . Thus, all information needed for the calculation of the measure enter the pair $(\rho_0, \partial U(\rho_0))$ of a reference state and an enclosing surface. Moreover, even this pair contains too much information: for a traceless, Hermitian operator A , its reflection $B = -A$ is also in $\mathcal{E}_0(\mathcal{H})$, but the trace norm is not sensitive to different signs, i.e. $\text{Tr}|A| = \text{Tr}|B|$. In addition, an enclosing surface might be curved which means that there exist several $\lambda > 0$ for an operator $A \in \mathcal{E}_0(\mathcal{H})$ that yield a point on the surface. This is again dispensable information regarding the evaluation of non-Markovianity. Due to these effects, it suffices to maximize (4.18) over a hemispherical enclosing surface defined by:

Definition 4.3. A set $\partial \tilde{U}(\rho_0) \subset \mathcal{S}(\mathcal{H})$ is said to be an hemispherical enclosing surface of ρ_0 if and only if for any $A \in \mathcal{E}_0(\mathcal{H})$ there exists exactly one real number $\lambda > 0$ such that either

$$\rho_0 + \lambda A \in \partial \tilde{U}(\rho_0) , \quad \text{or} \quad \rho_0 - \lambda A \notin \partial \tilde{U}(\rho_0) \quad (4.25)$$

holds.

Figure 4.2 provides an example for an enclosing and a hemispherical enclosing surface of an inner point ρ_0 . A hemispherical enclosing surface thus contains any *direction*, given by operators $A \in \mathcal{E}_0(\mathcal{H})$, only once. Moreover, an (hemispherical) enclosing surface must neither be smooth and a hemispherical enclosing surface must even not be connected (see Fig. 4.3). This characterization is thus very useful for noisy experiments.

The proof of theorem 4.3 relies on an alternative characterization of orthogonal state pairs which is fundamental in three ways. First, it allows to fix one input state to be some inner point and to sample the second initial state over any (hemispherical) enclosing surface of the fixed state. A convenient choice for an enclosing surface for an N -level system is certainly any $(N^2 - 2)$ -dimensional sphere (hemisphere) in \mathbb{R}^{N^2-1} containing the interior point. In particular, when doing a Monte Carlo simulation, this allows to use gradient methods more easily which increases the efficiency of sampling. Theorem 4.3 is particularly advantageous when dealing with a dynamical process that has an invariant state which

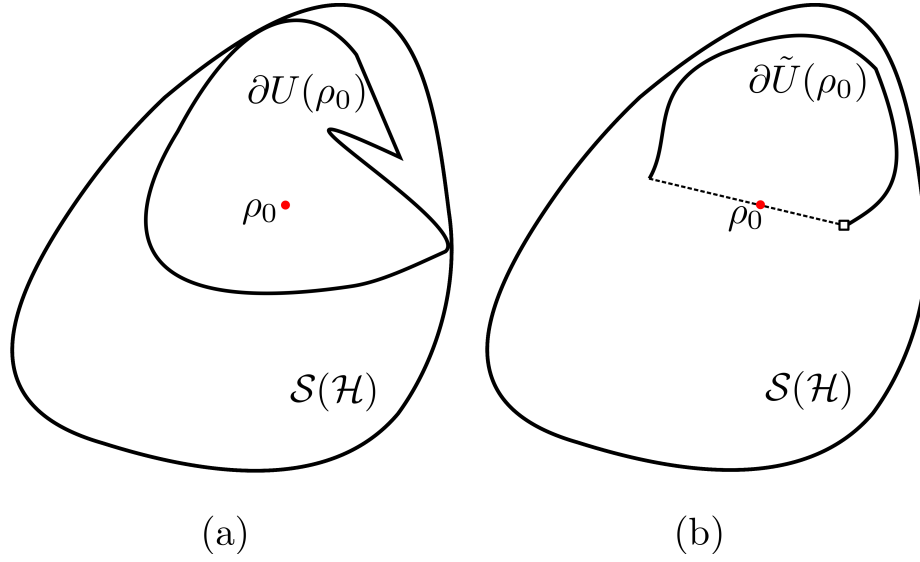


Figure 4.2: Illustration of an enclosing surface with curved boundary (a) and of a hemispherical enclosing surface (b) of an inner point ρ_0 .

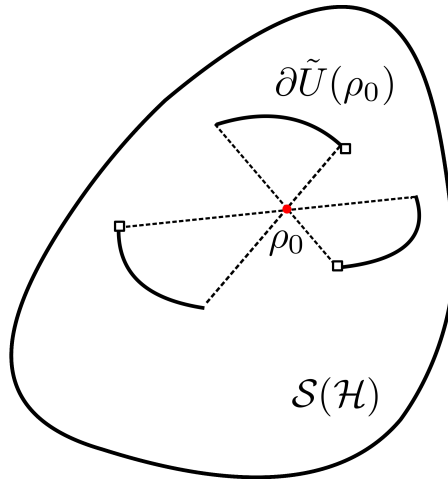


Figure 4.3: Illustration of a hemispherical enclosing surface of an inner point ρ_0 which is not connected.

lies in the interior. Thermalization processes where the system reaches a thermal equilibrium state provide an example for a dynamics with an invariant state in the interior. For the sake of convenience, one can then choose the invariant state of the dynamics to be the reference state so that only the sampled states evolve non-trivially.

Second, apart from the technical improvements, theorem 4.3 shows that (non-)Markovianity of a dynamical process is indeed a universal property. The information about the dynamics regarding memory effects is contained in any part of the state space as the result shows that \mathcal{N} can be evaluated everywhere in the state space. This behaviour is very plausible and supports the intuitive idea that memory effects are an intrinsic property of the dynamical process.

Last but not least, the result shows that the total backflow of information from the environment to the open system depends significantly on the initial distinguishability of two states which is given by their trace distance. Theorem 4.3 proves that the maximal backflow of information is linked to the information flow for states relative to their initial distinguishability. This shows that the backflow of information relative to the initial information content is the universal quantity which determines the dynamics. Rescaling the measure for the information flow, it is thus possible to sample also over non-orthogonal states in order to determine the maximal backflow during the dynamics.

4.4 The notion of joint translatability

In this section I present an alternative proof for the orthogonality of optimal state pairs for finite-dimensional Hilbert spaces. Linearity of the dynamical map is once more the only requirement which is needed. For the proof I establish the notion of joint translatability which characterizes the behaviour of pairs of states under parallel translations, elucidating the structure of the state space for finite systems. Due to this, the results could be of interest also in other contexts.

The idea of the proof is based on the observation gained from two-level systems that non-orthogonal states on the boundary of state space can be simultaneously translated by a traceless Hermitian operator to yield a pair of mixed states, while the trace distance of the pair is invariant under such translations. Recall that $\mathcal{E}_0(\mathcal{H})$ denotes the set of non-trivial, Hermitian and traceless operators on \mathcal{H} .

Definition 4.4. *Two states $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ are called jointly translatable if and only if there exists an operator $A \in \mathcal{E}_0(\mathcal{H})$ such that $\rho_k - A \in \mathcal{S}(\mathcal{H})$ for $k = 1, 2$.*

Hence, two states are said to be jointly translatable if and only if there is a non-trivial, Hermitian and traceless operator A which can be subtracted from the states without leaving the state space. It is clear that Hermiticity and the trace of the translated states is preserved by the choice of the operator A so that the crucial point is positivity. For finite-dimensional systems, I prove that any pair of non-orthogonal states is jointly translatable in such a way that both translated states do not belong to the boundary of the state space. In the following considerations, \mathcal{H} refers to a Hilbert space with dimension $\dim \mathcal{H} = N$.

Theorem 4.4. *If $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ and $\rho_1 \not\prec \rho_2$, then ρ_1, ρ_2 are jointly translatable. Moreover, there exists an operator $A \in \mathcal{E}_0(\mathcal{H})$ such that $\rho_k - A \notin \partial\mathcal{S}(\mathcal{H})$ for $k = 1, 2$.*

Proof. Let ρ_1, ρ_2 be given with respect to their spectral decomposition,

$$\rho_k = \sum_{i=1}^N p_i^{(k)} |\psi_i^{(k)}\rangle \langle \psi_i^{(k)}|, \quad (4.26)$$

where $p_i^{(k)}$, $i = 1, \dots, N$, denote the eigenvalues and $|\psi_i^{(k)}\rangle$ the corresponding eigenvectors of ρ_k . The projection onto the eigenvectors $|\psi_i^{(k)}\rangle$ will be denoted by $P_i^{(k)}$. The assumption $\rho_1 \not\prec \rho_2$ implies that both ρ_1 and ρ_2 have at least one eigenvector with non-zero eigenvalue and that these vectors are not orthogonal. After possible relabeling one can assume that $\alpha \equiv \langle \psi_1^{(1)} | \psi_1^{(2)} \rangle \neq 0$ and $p_1^{(1)}, p_1^{(2)} \neq 0$ holds. Moreover, by an appropriate choice of the phases of the eigenstates one can assume without restriction that α is real and positive, i.e. $0 < \alpha \leq 1$.

Consider the following superpositions of the two overlapping eigenvectors,

$$|\psi_{\pm}\rangle = c_{\pm} \left(|\psi_1^{(1)}\rangle \pm |\psi_1^{(2)}\rangle \right), \quad (4.27)$$

where the normalization constants obey $c_{\pm}^{-1} = \sqrt{2(1 \pm \alpha)}$. The projections onto these states are denoted by P_{\pm} . Note that $c_+ < c_-$ by positivity of the overlap α . Now, I define

$$\begin{aligned} A_{\epsilon} &\equiv \epsilon \cdot B, \\ B &= P_+ - \left(\frac{c_+}{c_-} \right)^2 P_- - \left[1 - \left(\frac{c_+}{c_-} \right)^2 \right] \cdot \frac{1}{N} \mathbb{1}_N, \end{aligned} \quad (4.28)$$

where $\epsilon > 0$ is a real number to be chosen later. Clearly, $B^{\dagger} = B$, $B \neq 0$ and $\text{Tr} B = 0$ so that A_{ϵ} is a candidate for the traceless Hermitian operator which simultaneously shifts both states. Furthermore, as $c_+ < c_-$, one recognizes that the two last terms are negative semi-definite while the first one is positive semi-definite. Note that for $\alpha = 1$, that is ρ_1 and ρ_2 have a common eigenvector, definition (4.28) reduces to $A_{\epsilon} = \epsilon(P_1^{(1)} - \frac{1}{N}\mathbb{1}_N)$. It can be readily seen that this operator jointly translates ρ_1, ρ_2 into the interior of $\mathcal{S}(\mathcal{H})$ for all $0 < \epsilon \leq \min_{k=1,2} p_1^{(k)}$. In order to show positivity of $\hat{\rho}_k \equiv \rho_k - A_{\epsilon}$ for an appropriate choice of ϵ in general, I consider the quantity $\langle \chi | \hat{\rho}_k | \chi \rangle$ for an arbitrary normalized vector $|\chi\rangle \in \mathcal{H}$. One gets

$$\begin{aligned} \langle \chi | \hat{\rho}_k | \chi \rangle &= \langle \chi | \rho_k | \chi \rangle - \epsilon \langle \chi | P_+ | \chi \rangle + \epsilon \left(\frac{c_+}{c_-} \right)^2 \langle \chi | P_- | \chi \rangle + \frac{\epsilon}{N} \left[1 - \left(\frac{c_+}{c_-} \right)^2 \right] \\ &= B_k(|\chi\rangle) + p_1^{(k)} |\langle \chi | \psi_1^{(k)} \rangle|^2 + \frac{4\alpha c_+^2 \epsilon}{N} - \dots \\ &\quad c_+^2 \epsilon \left\{ |\langle \chi | \psi_1^{(1)} \rangle + \langle \chi | \psi_1^{(2)} \rangle|^2 - |\langle \chi | \psi_1^{(1)} \rangle - \langle \chi | \psi_1^{(2)} \rangle|^2 \right\} \\ &= B_k(|\chi\rangle) + p_1^{(k)} |\langle \chi | \psi_1^{(k)} \rangle|^2 + \dots \\ &\quad 4c_+^2 \epsilon \left\{ \frac{\alpha}{N} - \text{Re}(\langle \psi_1^{(1)} | \chi \rangle \langle \chi | \psi_1^{(2)} \rangle) \right\} \\ &\geq B_k(|\chi\rangle) + p_1^{(k)} |\langle \chi | \psi_1^{(k)} \rangle|^2 + 4c_+^2 \epsilon \left\{ \frac{\alpha}{N} - |\langle \chi | \psi_1^{(k)} \rangle| \right\}, \end{aligned} \quad (4.29)$$

where $B_k(|\chi\rangle) \equiv \sum_{i=2}^N p_i^{(k)} |\langle \chi | \psi_i^{(k)} \rangle|^2 \geq 0$ and since $c_+^{-2} - c_-^{-2} = 4\alpha$ by definition of c_\pm . In the last step one uses the fact that $\text{Re}(z) \leq |z|$ for all complex numbers z , and that $|\langle \psi_1^{(m)} | \chi \rangle| \leq 1$ for all normalized vectors by the Cauchy-Schwarz inequality. Consider now the quadratic function

$$g_\epsilon^{(k)}(x) = p_1^{(k)} x^2 + 4c_+^2 \epsilon \left\{ \frac{\alpha}{N} - x \right\}. \quad (4.30)$$

One can show that this function is strictly positive for $k = 1, 2$ if ϵ satisfies

$$0 < \epsilon < \frac{\alpha}{N c_+^2} \min_{k=1,2} p_1^{(k)}. \quad (4.31)$$

The derivatives of $g_\epsilon^{(k)}$ (with respect to x) are given by

$$g_\epsilon^{(k)'}(x) = 2p_1^{(k)} x - 4c_+^2 \epsilon, \quad g_\epsilon^{(k)''}(x) = 2p_1^{(k)} > 0, \quad (4.32)$$

so that the function attains its minimal value² at $x_{\min} = 2c_+^2 \epsilon p_1^{(k)-1}$ and

$$g_\epsilon^{(k)}(x_{\min}) = 4c_+^2 \epsilon \left\{ \frac{\alpha}{N} - \frac{c_+^2 \epsilon}{p_1^{(k)}} \right\}, \quad (4.33)$$

which is strictly positive if and only if $0 < \epsilon < \alpha p_1^{(k)} (N c_+^2)^{-1}$ for a given k . Hence, $g_\epsilon^{(k)}$ is a strictly positive function for all $k \in \{1, 2\}$ if ϵ satisfies (4.31). Choosing ϵ according to this, I then obtain $g_\epsilon^{(k)}(|\langle \chi | \psi_1^{(k)} \rangle|) > 0$ for all normalized vectors $|\chi\rangle \in \mathcal{H}$ and $k = 1, 2$ which yields $\langle \chi | \hat{\rho}_{1,2} | \chi \rangle > 0$ as $B_k(|\chi\rangle) \geq 0$ is positive semi-definite. This demonstrates that $\hat{\rho}_{1,2}$ is positive and has no zero eigenvalue, i.e. $\hat{\rho}_{1,2} \in \mathring{\mathcal{S}}(\mathcal{H})$ due to the characterization of the boundary in terms of the eigenvalues given in section 2.1. In particular, ρ_1 and ρ_2 are jointly translatable. \square

The proof of theorem 4.4 obviously holds solely for finite-dimensional Hilbert spaces since the identity is not a trace class operator for infinite systems. If the system is finite-dimensional, theorem 4.2 can then also be proven as follows:

Proof. Let ρ_1, ρ_2 be an optimal pair, and suppose that $\rho_1 \not\perp \rho_2$. Then by theorem 4.4 there exists an operator $A \in \mathcal{E}_0(\mathcal{H})$ such that $\hat{\rho}_k \equiv \rho_k - A \notin \partial\mathcal{S}(\mathcal{H})$. Applying theorem 4.1, I conclude that the states $\hat{\rho}_k$ are not optimal. Since $\rho_1 - \rho_2 = \hat{\rho}_1 - \hat{\rho}_2$ it follows that the states ρ_k are not optimal either, which represents a contradiction. The optimal pair must therefore be orthogonal. \square

Since this statement holds for arbitrary dynamical processes described by a one-parameter family of linear maps as mentioned in the beginning, it mainly reveals the structure of the state space. The notion of joint translatability gives indeed some insight into the structural properties of state space as the converse of the statement of theorem 4.4 holds, too.

²The equation $g_\epsilon^{(k)'}(x_{\min}) = 2p_1^{(k)} x_{\min} - 4c_+^2 \epsilon \stackrel{!}{=} 0$ defines the position of the global minimum of $g_\epsilon^{(k)}$ as the second derivative is strictly positive.

Proposition 4.1. $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ are jointly translatable if and only if $\rho_1 \not\perp \rho_2$.

Proof. It remains to show that all pairs of jointly translatable states are non-orthogonal. To this end, I suppose $\rho_1 \perp \rho_2$ and prove that they are not jointly translatable.

Due to this assumption, $\rho_1 \perp \rho_2$, these states have a common spectral decomposition

$$\rho_k = \sum_{i=1}^N p_i^{(k)} |\psi_i\rangle \langle \psi_i| , \quad (4.34)$$

where $|\psi_i\rangle$ are their common eigenvectors, forming an orthonormal basis of \mathcal{H} , and $p_i^{(k)}$, $i = 1, \dots, N$, denote the eigenvalues which satisfy $\sum_i p_i^{(1)} \cdot p_i^{(2)} = 0$. As $p_i^{(k)} \geq 0$ for all i and k due to the positivity of states, it then follows that

$$\nexists k \in \{1, \dots, N\} \text{ such that } p_k^{(1)}, p_k^{(2)} \neq 0 . \quad (4.35)$$

Let $A \in \mathcal{E}_0(\mathcal{H})$ be an arbitrary non-trivial, Hermitian and traceless operator which is given in terms of the spectral decomposition by

$$A = \sum_{i=1}^N a_i |\chi_i\rangle \langle \chi_i| . \quad (4.36)$$

The eigenvalues a_i are thus real-valued and obey $\sum_{i=1}^N a_i = 0$. Representing A with respect to the eigenbasis of $\rho_{1,2}$, one obtains

$$A = \sum_{m,n=1}^N \tilde{a}_{mn} |\psi_m\rangle \langle \psi_n| , \quad (4.37)$$

where $\tilde{a}_{mn} = \sum_{i=1}^N a_i \langle \psi_m | \chi_i \rangle \langle \chi_i | \psi_n \rangle$. The vanishing trace, $\text{Tr} A = 0$, then implies $\sum_{m=1}^N \tilde{a}_{mm} = 0$. If not all terms of this sum vanish separately, there exists $k \in \{1, \dots, N\}$ such that $\tilde{a}_{kk} > 0$. One thus has

$$\langle \psi_k | \rho_{1,2} - A | \psi_k \rangle = p_k^{(1,2)} - \tilde{a}_{kk} < p_k^{(1,2)} , \quad (4.38)$$

from which it follows that at least one of the shifted operators $\rho_{1,2} - A$ is not positive due to (4.35).

Thus, I can restrict my considerations to operators A with zero diagonal elements with respect to the eigenbasis of $\rho_{1,2}$, i.e. $\tilde{a}_{kk} = 0$ for all $k \in \{1, \dots, N\}$. However, since $A \neq 0$, there exist $k, l \in \{1, \dots, N\}$ such that $\tilde{a}_{kl} \neq 0$. The expectation value of the operator $\rho_{1,2} - A$ in the state

$$|\tilde{\psi}_{kl}\rangle = d \tilde{a}_{kl} |\psi_k\rangle + |\psi_l\rangle , \quad (4.39)$$

where

$$d = \frac{\sqrt{(p_k^{(1,2)})^2 + 4|\tilde{a}_{kl}|^2} - p_k^{(1,2)}}{2|\tilde{a}_{kl}|^2} > 0 , \quad (4.40)$$

is given by

$$\begin{aligned}
& \langle \tilde{\psi}_{kl} | \rho_{1,2} - A | \tilde{\psi}_{kl} \rangle \\
&= d^2 |\tilde{a}_{kl}|^2 p_k^{(1,2)} + p_l^{(1,2)} - 2d |\tilde{a}_{kl}|^2 \\
&= p_l^{(1,2)} + \underbrace{\frac{d}{2} \left\{ p_k^{(1,2)} \sqrt{(p_k^{(1,2)})^2 + 4|\tilde{a}_{kl}|^2} - ((p_k^{(1,2)})^2 + 4|\tilde{a}_{kl}|^2) \right\}}_{<0}, \quad (4.41)
\end{aligned}$$

where the expression within the curly brackets is negative for all possible values of $p_k^{(1,2)}$: if $p_k^{(1,2)} = 0$, this follows from $-|\tilde{a}_{kl}|^2 < 0$ and for non-zero k 'th eigenvalue of $\rho_{1,2}$ one observes that $0 < y^2 + y^4/x^2$ for $x, y > 0$ which yields the inequality $x\sqrt{x^2 + y^2} < x^2 + y^2$. Thus again, there is at least one operator $\rho_{1,2} - A$ which is not positive due to (4.35). Hence, there exists no non-trivial, Hermitian and traceless operator $A \in \mathcal{E}_0(\mathcal{H})$ such that $\rho_{1,2} - A \geq 0$ for orthogonal states $\rho_1 \perp \rho_2$. That is, orthogonal states are not jointly translatable. \square

Given two orthogonal states, the proof demonstrates that at least one state is shifted outside the state space if any operator in $\mathcal{E}_0(\mathcal{H})$ is applied. This happens because orthogonal states cannot have non-zero eigenvalues to the same eigenvector. Moreover, this result partly reveals the basic properties of an $(N - 1)$ -simplex which describes the eigenvalue distribution of a state of an N -dimensional system. Orthogonality implies that the two states can be represented by two points in the same simplex and that they must lie on opposing sides of the simplex. By this, one easily observes that for any shift operator A with the same eigenbasis as the states, at least one of the states will leave the simplex. In other words and more figuratively (cf. Fig. 4.4), there is no possibility to translate the line defined by the two orthogonal states without leaving the simplex. Proposition 4.1 shows that this also holds for operators $A \in \mathcal{E}_0(\mathcal{H})$ which have a different eigenbasis. In this way, this result provides new insight in the structure of the state space of quantum systems.

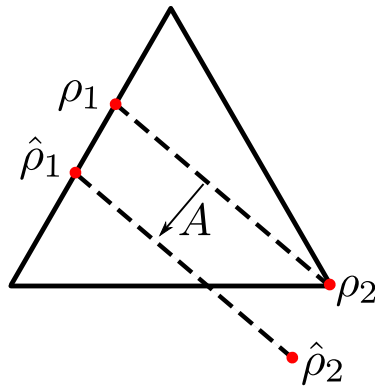


Figure 4.4: Illustration of orthogonal 3-level states $\rho_1 \perp \rho_2$ and of the action of an operator $A \in \mathcal{E}_0(\mathcal{H})$ with the same eigenbasis as $\rho_{1,2}$. The vertices of this 2-simplex (equilateral triangle) correspond to pure states.

4.4.1 Illustration in the Bloch ball

In this section I illustrate theorem 4.4 by showing explicitly the action of the translation operator A_ϵ (4.28) on states of a two-level system. The mode of operation will be demonstrated using the Bloch representation (cf. Sec. 2.3). To this end, I firstly determine the eigenvalues and eigenvectors of two-level states with respect to the entries of their associated Bloch vectors.

Let $\rho_{1,2} \in \mathcal{S}(\mathbb{C}^2)$ be two unequal states whose corresponding Bloch vectors are denoted by $\vec{v}^{(1,2)}$. The eigenvalues are given by

$$\lambda_{\pm}^{(1,2)} = \frac{1}{2}(1 \pm \|\vec{v}^{(1,2)}\|) , \quad (4.42)$$

and the corresponding eigenvectors have to obey

$$\rho_{1,2} |\chi_{\pm}^{(1,2)}\rangle = \lambda_{\pm}^{(1,2)} |\chi_{\pm}^{(1,2)}\rangle , \quad (4.43)$$

which yields two coupled linear equations

$$a_{\pm}^{(1,2)} (\pm \|\vec{v}^{(1,2)}\| - v_z^{(1,2)}) = b_{\pm}^{(1,2)} (v_x^{(1,2)} - i v_y^{(1,2)}) , \quad (4.44)$$

$$b_{\pm}^{(1,2)} (\pm \|\vec{v}^{(1,2)}\| + v_z^{(1,2)}) = a_{\pm}^{(1,2)} (v_x^{(1,2)} + i v_y^{(1,2)}) . \quad (4.45)$$

Henceforth, I assume that ρ_1 and ρ_2 are pure which means that their Bloch vectors have length one. As one can see, there exist different solutions depending on the range of $v_z^{(1,2)}$. This is related to the fact that two charts are needed to cover a sphere completely. The normalized eigenvectors are determined by

$$|\chi_{\pm}^{(1,2)}\rangle_{|v_z^{(1,2)} \neq -1} = \sqrt{\frac{\beta_{\pm}^{(1,2)}}{2}} \left(\pm \frac{\alpha_{\pm}^{(1,2)}}{\beta_{\pm}^{(1,2)}} e_{2 \mp 1 \bmod 3} + e_{2 \pm 1 \bmod 3} \right) , \quad (4.46)$$

$$|\chi_{\pm}^{(1,2)}\rangle_{|v_z^{(1,2)} \neq 1} = \sqrt{\frac{\beta_{\mp}^{(1,2)}}{2}} \left(\pm \frac{\alpha_{\mp}^{(1,2)}}{\beta_{\mp}^{(1,2)}} e_{2 \pm 1 \bmod 3} + e_{2 \mp 1 \bmod 3} \right) , \quad (4.47)$$

where $e_0 = (1, 0)^T$, $e_1 = (0, 1)^T$ defines the canonical basis of \mathbb{R}^2 . In addition, I used $\alpha_{\pm}^{(1,2)} = v_x^{(1,2)} \pm i v_y^{(1,2)}$ and $\beta_{\pm}^{(1,2)} = \|\vec{v}^{(1,2)}\| \pm v_z^{(1,2)} = 1 \pm v_z^{(1,2)}$.

Now, suppose $\rho_1 \not\perp \rho_2$. For the sake of convenience, I consider ρ_1 to have the associated Bloch vector $\vec{v}^{(1)} = (0, 0, 1)^T$. Because the states are neither equal nor orthogonal the z-component of the assigned Bloch vector of ρ_2 obeys $v_z^{(2)} \neq -1, 1$. Using equation (4.46), it thus follows for the eigenvectors of ρ_1 and ρ_2

$$|\chi_+^{(1)}\rangle = e_0 , \quad |\chi_+^{(2)}\rangle = \sqrt{\frac{\beta_+}{2}} \left(1, \frac{\alpha_+}{\beta_+} \right)^T , \quad (4.48)$$

$$|\chi_-^{(1)}\rangle = e_1 , \quad |\chi_-^{(2)}\rangle = \sqrt{\frac{\beta_-}{2}} \left(-\frac{\alpha_-}{\beta_-}, 1 \right)^T , \quad (4.49)$$

where I used the replacements $\beta_+ = \beta_+^{(2)}$ and $\alpha_{\pm} = \alpha_{\pm}^{(2)}$ in order to simplify notation. Clearly, any pair of eigenvectors of (4.48) and (4.49) is non-orthogonal. I choose the eigenvectors $|\chi_+^{(1)}\rangle, |\chi_+^{(2)}\rangle$ for the construction of A_ϵ . Their overlap is given by

$$\alpha \equiv \langle \chi_+^{(2)} | \chi_+^{(1)} \rangle = \sqrt{\frac{\beta_+}{2}} \in (0, 1) . \quad (4.50)$$

Thus, there is no need to add a phase to the eigenvectors so that I can directly start with the calculation of the shift operator A_ϵ (4.28). I obtain

$$|\psi_\pm\rangle = c_\pm(|\chi_+^{(1)}\rangle \pm |\chi_+^{(2)}\rangle) = c_\pm(1 \pm \alpha, \pm \frac{\alpha_\pm}{2\alpha})^T, \quad (4.51)$$

where $c_\pm = \sqrt{2(1 \pm \alpha)}^{-1}$. This yields

$$P_\pm = c_\pm^2 \begin{pmatrix} (1 \pm \alpha)^2 & \pm(1 \pm \alpha)\frac{\alpha}{\beta_+}\alpha_- \\ \pm(1 \pm \alpha)\frac{\alpha}{\beta_+}\alpha_+ & 1 - \alpha^2 \end{pmatrix}, \quad (4.52)$$

for the corresponding projections when the relations $|\alpha_\pm|^2 = \beta_+\beta_-$ and $\beta_- = 2 - \beta_+ = 2(1 - \alpha^2)$ are used. Applying this, one obtains for the shift operator A_ϵ

$$\begin{aligned} A_\epsilon &= 2c_+^2\epsilon \begin{pmatrix} 2\alpha & \frac{\alpha}{\beta_+}\alpha_- \\ \frac{\alpha}{\beta_+}\alpha_+ & 0 \end{pmatrix} - 2\alpha c_+^2\epsilon \mathbb{1}_2 \\ &= \frac{\alpha\epsilon}{1 + \alpha} \begin{pmatrix} 1 & \frac{\alpha_-}{\beta_+} \\ \frac{\alpha_+}{\beta_+} & -1 \end{pmatrix}. \end{aligned} \quad (4.53)$$

The Bloch vector corresponding to this traceless Hermitian operator is given as usual by the expectation values of the Pauli spin operators, i.e. one has

$$w_{A_\epsilon, x} = \text{Tr}(A_\epsilon \sigma_x) = \frac{\alpha\epsilon}{1 + \alpha} \frac{1}{\beta_+} (\alpha_+ + \alpha_-), \quad (4.54)$$

$$w_{A_\epsilon, y} = \text{Tr}(A_\epsilon \sigma_y) = \frac{\alpha\epsilon}{1 + \alpha} \frac{1}{\beta_+} i(\alpha_- - \alpha_+), \quad (4.55)$$

$$w_{A_\epsilon, z} = \text{Tr}(A_\epsilon \sigma_z) = 2 \frac{\alpha\epsilon}{1 + \alpha}. \quad (4.56)$$

As both states are pure (which means that the relevant eigenvalues are one), ϵ must satisfy $0 < \epsilon < \alpha(2c_+^2)^{-1} = \alpha(1 + \alpha)$ (cf. Eq. (4.31)) in order to guarantee positivity of the shifted states $\hat{\rho}_1$ and $\hat{\rho}_2$. Rewriting this parameter by $\epsilon = c\alpha(1 + \alpha)$ with $c \in (0, 1)$, the Bloch vector of A_ϵ parametrized by c reads

$$\vec{w}_{A_c} = c \begin{pmatrix} v_x^{(2)} \\ v_y^{(2)} \\ 1 + v_z^{(2)} \end{pmatrix} = c \left(\vec{v}^{(1)} + \vec{v}^{(2)} \right). \quad (4.57)$$

Thus, the Bloch vectors of the shifted states $\hat{\rho}_k \equiv \rho_k - A_\epsilon$ are given by

$$\vec{\hat{v}}^{(k)} = \vec{v}^{(k)} - \vec{w}_{A_c} = (1 - c)\vec{v}^{(k)} - c\vec{v}^{(l \neq k)}, \quad (4.58)$$

that is,

$$\vec{\hat{v}}^{(1)} = \begin{pmatrix} -cv_x^{(2)} \\ -cv_y^{(2)} \\ (1 - c) - cv_z^{(2)} \end{pmatrix}, \quad \vec{\hat{v}}^{(2)} = \begin{pmatrix} (1 - c)v_x^{(2)} \\ (1 - c)v_y^{(2)} \\ (1 - c)v_z^{(2)} - c \end{pmatrix}. \quad (4.59)$$

It can be readily shown that the norm of these vectors is

$$\|\vec{\hat{v}}^{(k)}\|^2 = (1 - c)^2 + c^2 - 2c(1 - c)v_z^{(2)}, \quad (4.60)$$

which is strictly smaller than one for all $c \in (0, 1)$. Thus, both states lie on the same shell in the interior of the Bloch ball for all possible values of c . For $c = 0, 1$ one has $\|\vec{\hat{v}}^{(k)}\| = 1$, i.e. the shifted states are on the Bloch sphere again and, therefore, pure.

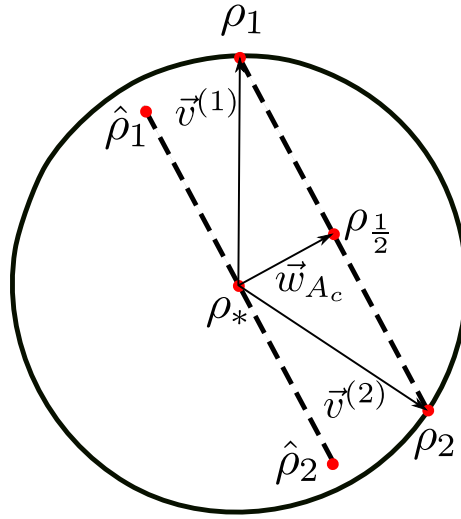


Figure 4.5: Scheme of the action of the shift operator A_ϵ on non-orthogonal two-level states ρ_1, ρ_2 . The Bloch vector of ρ_1 is $\vec{v}^{(1)} = (0, 0, 1)^T$. ρ_* denotes the maximally mixed state and $\hat{\rho}_{1,2}$ refer to the parameter $c = \frac{1}{2}$ (c.f. (4.62)).

If one considers the states

$$\rho_\lambda = (1 - \lambda)\rho_1 + \lambda\rho_2 \ , \quad (4.61)$$

with $\lambda \in [0, 1]$, the Bloch vector of $\rho_{\frac{1}{2}}$ is given by

$$\vec{v}_{\frac{1}{2}} \equiv \frac{1}{2}(\vec{v}^{(1)} + \vec{v}^{(2)}) = \frac{1}{2c}\vec{w}_{A_c} \ , \quad (4.62)$$

which is proportional to \vec{w}_{A_c} . Moreover, this Bloch vector is perpendicular to the one-dimensional subspace spanned by $\vec{v}^{(1)} - \vec{v}^{(2)}$ which describes the orientation of the line connecting ρ_1 and ρ_2 . Any point of the line can thus be written as the direct sum of $\vec{v}_{\frac{1}{2}}$ and $\mu\{\vec{v}^{(1)} - \vec{v}^{(2)}\}$ for $-\frac{1}{2} \leq \mu \leq \frac{1}{2}$. Due to this, the shift induced by A_ϵ corresponds to a translation perpendicular to the straight line connecting ρ_1 and ρ_2 (c.f. Fig. 4.5). For $c = \frac{1}{2}$, implying $\vec{w}_{A_c} = \vec{v}_{\frac{1}{2}}$, the translated line runs through the maximally mixed state so that an extension of the line towards the boundary according to theorem 4.1 yields a pair of orthogonal, antipodal states. In this case, the Bloch vectors of $\rho_{1,2}$ are replaced by their contributions parallel to the line $\vec{v}^{(1)} - \vec{v}^{(2)}$ connecting these points. Furthermore, for $c = 1$, the line defined by the translated states is just the initial line reflected along the plane defined by \vec{w}_{A_c} (or $\vec{v}_{\frac{1}{2}}$, respectively). This shows that the proof of theorem 4.4 is a generalization of the figurative idea of translating lines in the Bloch ball for two-level systems.

Chapter 5

Purity of the optimal pair

5.1 The Λ -model

As a simple application of theorem 4.2, one obtains the result that for all non-Markovian quantum processes of a two-dimensional system (qubit) the maximal backflow of information occurs for a pair of pure, orthogonal initial states, corresponding to antipodal points on the surface of the Bloch sphere. This follows immediately from the fact that for qubits the set of pure states is identical to the boundary $\partial\mathcal{S}(\mathcal{H})$ of the state space and orthogonal states have antipodal corresponding Bloch vectors. For higher-dimensional systems, however, the set of pure states represents a proper subset of the boundary. In this section I will construct an explicit example for an open system dynamics of a three-level system for which the optimal pair is not a pair of pure states.

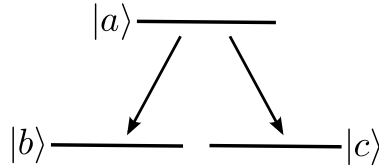


Figure 5.1: Scheme of the Λ -model.

I consider a Λ -system which interacts with an off-resonant cavity field. The weak-coupling master equation of this model is given by

$$\begin{aligned}
 \frac{d}{dt}\rho(t) &= -i\lambda_1(t)[|a\rangle\langle a|, \rho(t)] - i\lambda_2(t)[|a\rangle\langle a|, \rho(t)] \\
 &+ \gamma_1(t)\left[|b\rangle\langle a|\rho(t)|a\rangle\langle b| - \frac{1}{2}\{\rho(t), |a\rangle\langle a|\}\right] \\
 &+ \gamma_2(t)\left[|c\rangle\langle a|\rho(t)|a\rangle\langle c| - \frac{1}{2}\{\rho(t), |a\rangle\langle a|\}\right], \quad (5.1)
 \end{aligned}$$

where $|a\rangle$ refers to the excited and $|b\rangle, |c\rangle$ to the two ground states [29]. The coefficients $\lambda_{1,2}(t)$ and $\gamma_{1,2}(t)$ are determined by the spectral density of the

cavity field $J(\omega)$:

$$\lambda_i(t) = \int_0^t ds \int_0^\infty d\omega J(\omega) \sin((\omega - \omega_i)s) , \quad (5.2)$$

$$\gamma_i(t) = \int_0^t ds \int_0^\infty d\omega J(\omega) \cos((\omega - \omega_i)s) . \quad (5.3)$$

The generator of the master equation is thus of the type of (3.16) with two time-independent Lindblad operators $|b\rangle\langle a|$ and $|c\rangle\langle a|$, and two time-dependent decay rates $\gamma_1(t)$ and $\gamma_2(t)$. Introducing the functions

$$f(t) = e^{-(D_1(t)+D_2(t))/2} e^{-i(L_1(t)+L_2(t))} , \quad (5.4)$$

$$g_i(t) = \int_0^t ds \gamma_i(s) e^{-(D_1(s)+D_2(s))} , \quad (5.5)$$

where

$$D_i(t) = \int_0^t ds \gamma_i(s) , \quad L_i(t) = \int_0^t ds \lambda_i(s) , \quad (5.6)$$

one finds that the solution of the master equation yields the dynamical map

$$\Phi_{t,0}^\Lambda(\rho) = \begin{pmatrix} |f(t)|^2 \rho_{aa} & f(t) \rho_{ab} & f(t) \rho_{ac} \\ f(t)^* \rho_{ab}^* & g_1(t) \rho_{aa} + \rho_{bb} & \rho_{bc} \\ f(t)^* \rho_{ac}^* & \rho_{bc}^* & g_2(t) \rho_{aa} + \rho_{cc} \end{pmatrix} , \quad (5.7)$$

and the described dynamical process is non-divisible if and only if a decay rate $\gamma_i(t)$ is negative for some time t . The functions f , g_1 and g_2 have to obey the following relations which guarantee that $\Phi_{t,0}^\Lambda$ is trace preserving (5.8) and completely positive (5.9),

$$g_1(t) + g_2(t) + |f(t)|^2 = 1 , \quad (5.8)$$

$$g_{1,2}(t) \geq 0 . \quad (5.9)$$

Furthermore, one has to require $f(0) = 1$ and $g_{1,2}(0) = 0$ in order to satisfy $\Phi_{0,0}^\Lambda = \mathbb{1}_3$. One easily infers from equation (5.8) and (5.9) that $|f(t)| \leq 1$ and, in addition, from (5.7), that all states whose support is in the two-dimensional linear subspace $\mathcal{U}_{bc} = \text{span}_{\mathbb{C}}\{|b\rangle, |c\rangle\}$, spanned by the system's ground states, are invariant under the action of the dynamical map $\Phi_{t,0}^\Lambda$.

As there is no possibility to transform the ground states directly into each other, such a quantum mechanical three-level system is called a Λ -model in the literature. This type of system occurs in various applications in quantum optics, see [46].

5.1.1 Particular pairs of states

I will derive an analytic expression for the trace distance of particular pairs of three-level states evolving according to the dynamics of the Λ -system. Firstly however, I present a general expression for arbitrary initial pairs of states.

Let $\rho, \sigma \in \mathcal{S}(\mathbb{C}^3)$. The eigenvalues of $\Delta(t) \equiv \rho(t) - \sigma(t)$ are determined by the roots of the polynomial

$$p(\lambda, t) \equiv a_0(t) + a_1(t)\lambda - a_3(t)\lambda^3 , \quad (5.10)$$

where

$$a_0(t) = |f(t)|^2 \left[2\text{Re}(\Delta_{ab}\Delta_{ac}\Delta_{bc}^*) - |\Delta_{ab}|^2(g_2(t)\Delta_{aa} + \Delta_{cc}) - |\Delta_{ac}|^2(g_1(t)\Delta_{aa} + \Delta_{bb}) + \Delta_{aa}\{(g_1(t)\Delta_{aa} + \Delta_{bb}) \cdot (g_2(t)\Delta_{aa} + \Delta_{cc}) - |\Delta_{bc}|^2\} \right], \quad (5.11)$$

$$a_1(t) = |f(t)|^2 (|\Delta_{ab}|^2 + |\Delta_{ac}|^2) - (g_1(t)\Delta_{aa} + \Delta_{bb}) \cdot (g_2(t)\Delta_{aa} + \Delta_{cc}) + |\Delta_{bc}|^2 - |f(t)|^2 \Delta_{aa}((g_1(t) + g_2(t))\Delta_{aa} + \Delta_{bb} + \Delta_{cc}), \quad (5.12)$$

$$a_3(t) = 1. \quad (5.13)$$

One directly observes that the polynomial (5.10) does not depend on the phase of the function f so that the eigenvalues of $\Delta(t)$ do not depend either on the phase. For simplicity, one can thus restrict oneself to solely real-valued functions. There is no quadratic contribution to the characteristic polynomial $p(\lambda, t)$ due to the fact that $\Delta(t)$ is a traceless operator. This property holds in general: the sum of the roots of a polynomial is zero if and only if the quadratic term of the polynomial vanishes.

Using Cardano's formula [21] for the roots of a third degree polynomial (without quadratic term), the eigenvalues of (5.10) are given by

$$\lambda_1(t) = S(t) + T(t), \quad (5.14)$$

$$\lambda_2(t) = e^{-i\frac{2}{3}\pi}S(t) + e^{i\frac{2}{3}\pi}T(t), \quad (5.15)$$

$$\lambda_3(t) = e^{i\frac{2}{3}\pi}S(t) + e^{-i\frac{2}{3}\pi}T(t), \quad (5.16)$$

where the functions $S(t)$ and $T(t)$ can be written as

$$S(t) = \sqrt[3]{\frac{a_0(t)}{2} \pm i|D_t|^{1/2}}, \quad T(t) = \sqrt[3]{\frac{a_0(t)}{2} \mp i|D_t|^{1/2}}, \quad (5.17)$$

since the discriminant $D_t \equiv -(1/27)a_1(t)^3 + (1/4)a_0(t)^2 \leq 0$ is non-positive. This holds due to the fact that the eigenvalues are real-valued. If $D_t < 0$, then it follows that

$$S(t) = T(t)^* = \sqrt{\frac{a_1(t)}{3}} e^{\pm i\alpha(t)}, \quad (5.18)$$

where $\alpha(t) \equiv \frac{1}{3}\arg\{\frac{a_0(t)}{2} \pm i|D_t|^{1/2}\}$. If $D_t = 0$ for some t , one clearly has $S(t) = T(t) = \sqrt{a_1(t)/3}$. Applying this description for the eigenvalues, the trace distance of two states $\rho, \sigma \in \mathcal{S}(\mathbb{C}^3)$ of the treated Λ -model can be written as follows

$$\begin{aligned} \mathcal{D}(\rho(t), \sigma(t)) &= \frac{1}{2} \left\{ |2\text{Re}(S(t))| + |2\text{Re}(e^{i\frac{2}{3}\pi}S(t))| + |2\text{Re}(e^{-i\frac{2}{3}\pi}S(t))| \right\} \\ &= \sqrt{\frac{a_1(t)}{3}} \left\{ |\cos \alpha(t)| + \left| \cos\left(\alpha(t) + \frac{2\pi}{3}\right) \right| + \left| \cos\left(\alpha(t) - \frac{2\pi}{3}\right) \right| \right\}. \end{aligned} \quad (5.19)$$

However, it is possible to derive even simpler expressions for the trace distance of some particular initial state pairs:

(A) Consider the orthogonal states $\rho_{\pm} = |\psi_{ab}^{\pm}\rangle\langle\psi_{ab}^{\pm}|$ where

$$|\psi_{ab}^{\pm}\rangle = \sqrt{\frac{1}{2}}e^{i\phi}|a\rangle \pm \sqrt{\frac{1}{2}}e^{i\vartheta}|b\rangle, \quad (5.20)$$

with $\phi, \vartheta \in [0, 2\pi)$. Their support is contained in the two-dimensional subspace $\mathcal{U}_{ab} = \text{span}_{\mathbb{C}}\{|a\rangle, |b\rangle\}$ which is spanned by the excited state $|a\rangle$ and the ground state $|b\rangle$. The operator $\Delta(t) \equiv \rho_+(t) - \rho_-(t)$ is given by

$$\Delta(t) = \begin{pmatrix} 0 & f(t)e^{i\omega} & 0 \\ f(t)e^{-i\omega} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (5.21)$$

where $\omega = \phi - \theta$ denotes the difference of the phases. It follows that the trace distance for this initial state pair has the simple dynamics¹

$$\mathcal{D}_I(t) \equiv \mathcal{D}(\rho_+(t), \rho_-(t)) = |f(t)|. \quad (5.22)$$

(B) As a second type of initial states, I consider classical mixtures of the three levels $|a\rangle$, $|b\rangle$ and $|c\rangle$. More precisely, the trace distance for pairs consisting of the excited state $\rho_a = |a\rangle\langle a|$ and classical mixtures of the three levels of the system $\rho_{\{q\}} = q_0|a\rangle\langle a| + q_1|b\rangle\langle b| + q_2|c\rangle\langle c|$ is determined². For such states the operator $\Delta(t)$ is diagonal for all times t and obeys

$$\Delta(t) = \text{diag}\{f(t)^2(q_1 + q_2), g_1(t)(q_1 + q_2) - q_1, g_2(t)(q_1 + q_2) - q_2\}, \quad (5.23)$$

which yields

$$\mathcal{D}(\rho_a(t), \rho_{\{q\}}(t)) = \sum_{i=1}^2 (q_i - (q_1 + q_2)g_i(t))\Theta(q_i - (q_1 + q_2)g_i(t)), \quad (5.24)$$

for the trace distance. Here, Θ refers to the Heaviside step function. For the derivation I used the trace condition (5.8). For the probability distributions $\{q\}$,

$$\{q\}_{II} = \{0, 1, 0\}, \quad \{q\}_{III} = \{0, 0, 1\}, \quad \{q\}_{IV} = \{0, \frac{1}{2}, \frac{1}{2}\}, \quad (5.25)$$

one thus gets the following analytic expressions for the trace distance

$$\mathcal{D}_{II}(t) = 1 - g_1(t), \quad \mathcal{D}_{III}(t) = 1 - g_2(t), \quad (5.26)$$

and

$$\mathcal{D}_{IV}(t) = (\frac{1}{2} - g_1(t))\Theta(\frac{1}{2} - g_1(t)) + (\frac{1}{2} - g_2(t))\Theta(\frac{1}{2} - g_2(t)). \quad (5.27)$$

If $q_0 = 0$, the states are orthogonal, $\rho_a \perp \rho_{\{q\}}$. Moreover, the states corresponding to \mathcal{D}_{IV} define an antipodal pair which is thus not a pure state pair³.

¹A similar pair of states in the other subspace \mathcal{U}_{ac} yield the same expression for the trace distance.

²The q_i 's define a probability distribution which means that $q_0 + q_1 + q_2 \equiv 1$.

³ $\rho_{\{q\}_{IV}}$ is the equal mixture of the ground states $|b\rangle$ and $|c\rangle$.

5.2 A non-pure optimal pair

On the basis of the trace distance of the considered special initial state pairs, I implement a particular dynamics for the Λ -model by choosing the functions g_1 and g_2 to obey

$$g_1(t) = g_{\text{int}}(t)\Theta(t_0 - t) + \Theta(t - t_0) \left\{ 8(t - (t_0 + \frac{1}{2}t_1))^2 \Theta(\sum_{i=0}^1 t_i - t) + (t - \sum_{i=0}^1 t_i) \Theta(\sum_{i=0}^2 t_i - t) \Theta(t - \sum_{i=0}^1 t_i) + \Theta(t - \sum_{i=0}^2 t_i) \right\}, \quad (5.28)$$

$$g_2(t) = g_{\text{int}}(t)\Theta(t_0 - t) + \Theta(t - t_0) \left\{ \frac{1}{2} \Theta(\sum_{i=0}^1 t_i - t) + (1 + \sum_{i=0}^1 t_i - t) \Theta(\sum_{i=0}^2 t_i - t) \Theta(t - \sum_{i=0}^1 t_i) \right\}, \quad (5.29)$$

where $0 < t_0 < t_1 < t_2$ and $g_{\text{int}}(t) = \frac{1}{2} \sin((2t_0)^{-1}\pi t)$. As stated in section 5.1.1, the function f can be chosen real-valued so that f is determined by the condition (5.8) which yields $f(t) = \sqrt{1 - (g_1(t) + g_2(t))}$. The shape of these functions is depicted in figure 5.2. By construction, all three functions are continuous and satisfy the conditions (5.8), (5.9) and $f(0) = 1$. Moreover, the functions are taken so that the antipodal state pair defining \mathcal{D}_{IV} increases most compared to the other special states defined above (cf. Fig. 5.3).

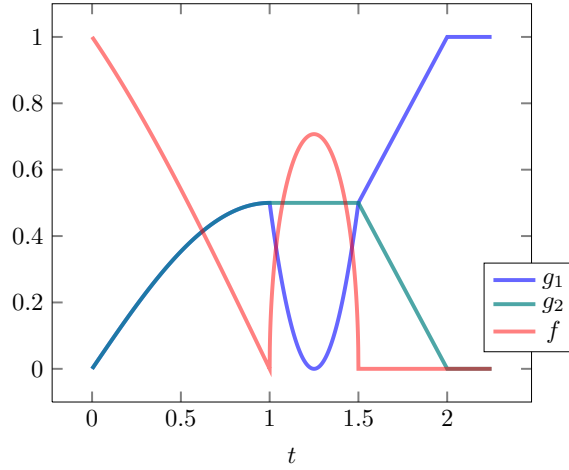


Figure 5.2: Plot of the functions f , g_1 and g_2 for $t_0 = 1$, $t_1 = 1.5$ and $t_2 = 2$.

I emphasize that the functions g_1 and g_2 (and then f) are determined directly. It is not clear whether there exists a spectral density $J(\omega)$ of the cavity field which yields this dynamics. However, the chosen functions satisfy the requirements and, therefore, the implemented dynamics in the Λ -model defines a dynamical process. Going back to the definition of the measure for the quantum non-Markovianity (3.34), one recognizes that \mathcal{N} solely measures the total increase. Thus, there are yet many possibilities to manipulate g_1 and g_2 in order

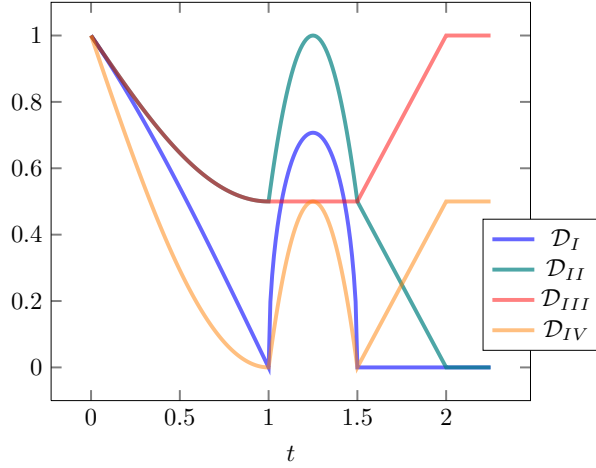


Figure 5.3: The shape of the trace distance for the four special initial state pairs \mathcal{D}_i for $t_0 = 1$, $t_1 = 1.5$ and $t_2 = 2$. The respective total increase is given by: $\mathcal{D}_I \rightarrow \frac{1}{\sqrt{2}}$, $\mathcal{D}_{II} \rightarrow \frac{1}{2}$, $\mathcal{D}_{III} \rightarrow \frac{1}{2}$, $\mathcal{D}_{IV} \rightarrow 1$.

to find a dynamics which is indeed associated to a spectral density and preserves the basic features of the counterexample.

The implemented dynamics can be divided into four parts and has the following fundamental properties:

During the first time interval, i.e. $t \leq t_0$, the dynamics is governed by identical dissipation via the two channels which is described by the increasing function g_{int} . Within the interval $[t_1, t_2]$, however, the populations are entirely swapped to the ground state $|b\rangle$ and in the subsequent part the dynamics stops completely. In between, there is a revival of the excitation from ground state $|b\rangle$ while the other ground state remains unchanged. I emphasize that the population is swapped to the same ground state from which the excitation is also taken in the second interval. By symmetry, the ground state $|c\rangle$ could also be the preferred one.

Despite of the simplicity of the dynamics for the Λ -model it seems to be impossible to determine analytically the optimal pair. Due to this, I have carried out a Monte Carlo simulation, drawing random pairs of pure, orthogonal, and antipodal initial states and determining the corresponding increase of the trace distance for each initial pair. The simulation was performed in *Mathematica* [57]. I applied a generator for random unitary matrices included in [37, 38] to sample pairs of pure, orthogonal, and antipodal states. The algorithm generates random unitaries with respect to the Haar measure [36] using *QR decomposition*. That is, a decomposition of a matrix A into a product $A = QR$ of an orthogonal matrix Q and an upper triangular matrix R . To each basis corresponding to a randomly drawn unitary, I evaluated all possible combinations of the eigenvalue distributions of pure, orthogonal, and antipodal states.

The results are shown in figure 5.4. One can see from the figure that there is a finite gap between the maximal possible increase of the trace distance for pure, orthogonal initial pairs, and the increase of the trace distance corresponding to the antipodal initial pair defining \mathcal{D}_{IV} . The largest total increase for pairs of

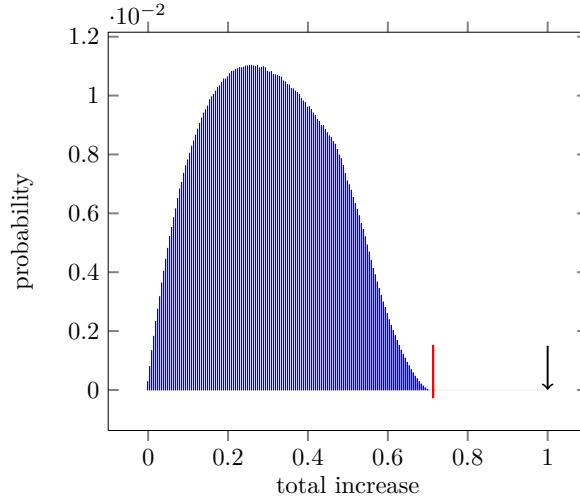


Figure 5.4: Probability of the total increase of the trace distance for randomly drawn pure, orthogonal states evolving according to the dynamics (5.7). The red line indicates the total increase of \mathcal{D}_I ($\frac{1}{\sqrt{2}}$) while the arrow refers to the maximal increase for this dynamics given by \mathcal{D}_{IV} (1). The sample size of pairs of pure, orthogonal states is equal to 10^7 .

pure, orthogonal states was obtained for states whose support is contained in the subspace $\mathcal{U}_{ab} = \text{span}_{\mathbb{C}}\{|a\rangle, |b\rangle\}$ or $\mathcal{U}_{ac} = \text{span}_{\mathbb{C}}\{|a\rangle, |c\rangle\}$, respectively. That is, the increase of \mathcal{D}_I , which is $\frac{1}{\sqrt{2}}$, yields the maximum for pure, orthogonal states. Performing an additional variation around these state pairs, one gets only smaller values for the increase which shows that these pairs constitute at least a local maximum of the trace distance for pure initial states. However, sampling instead merely antipodal states yields a probability distribution which continuously approaches the maximal increase given by \mathcal{D}_{IV} (cf. Fig. 5.5). Thus, there is strong numerical evidence that the optimal pair is indeed given by the antipodal initial states

$$\rho_1 = |a\rangle\langle a|, \quad \rho_2 = \frac{1}{2}(|b\rangle\langle b| + |c\rangle\langle c|). \quad (5.30)$$

Hence, this example demonstrates that for Hilbert spaces with dimension larger than two, the optimal initial state pair can indeed contain a mixed state for certain non-Markovian dynamical processes. By this, the considered dynamics constitutes a counterexample for the hypothesis that the optimal pair must be pure in general and, therefore, the maximization procedure (cf. Sec. 4) can not be tightened further to the extreme points of the state space, i.e. the pure states.

I want to stress that the same pair (5.30) is also the optimal pair for a simpler dynamics for the Λ -model [54]: If the rates of the Lamb-shifts (5.2) are zero and the decay rates (5.3) in the dissipator of the master equation, from which the dynamics of the Λ -model is derived, are chosen to obey small oscillations, one obtains also a finite gap between the maximal increase of the trace distance for pure, orthogonal states and the increase of \mathcal{D}_{IV} . That is, for

$$\lambda_{1,2}(t) = 0, \quad \gamma_{1,2}(t) = 0.3 \cdot \sin(\pi t) \quad (5.31)$$

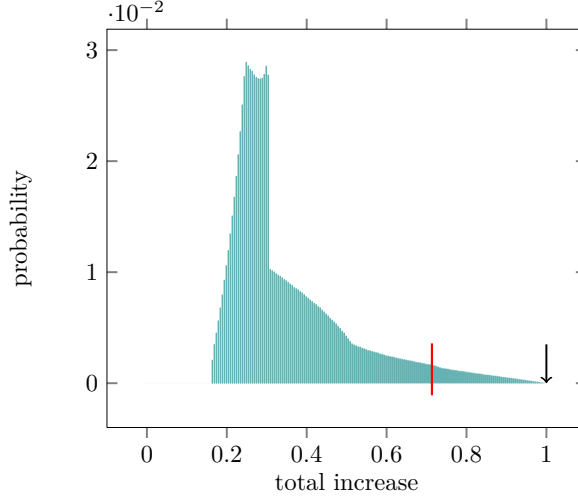


Figure 5.5: Probability distribution of the total increase of the trace distance for randomly drawn antipodal states evolving according to the dynamics (5.7) (sample size: 10^7). The red line indicates the total increase of \mathcal{D}_I while the arrow refers to the increase of \mathcal{D}_{IV} .

one obtains the distribution depicted in figure 5.6 for the total increase within one period for pure, orthogonal, and antipodal states. It is readily shown that also for this choice the conditions (5.8) and (5.9) are satisfied.

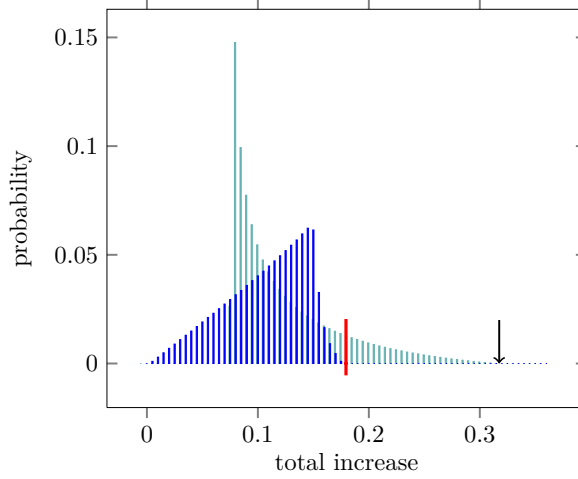


Figure 5.6: Probability distribution of the total increase of the trace distance for randomly drawn pure, orthogonal pairs (blue) and antipodal pairs of states (teal) evolving according to the dynamics given by (5.31). The arrow indicates the total increase of the trace distance for the antipodal states ρ_1, ρ_2 (5.30) which yields the maximum (≈ 0.317). The total increase of \mathcal{D}_I for this dynamics is 0.174 described by the red line. It is an upper bound for the increase of pure, orthogonal state pairs for this dynamics, too. The sample size used to determine the two distributions is again about 10^7 each.

The shape of the probability distributions is very special, see figure 5.4, 5.5 and 5.6. In particular, the probability distribution for antipodal states evolving according to the dynamics specified by (5.7) is interesting: it seems to consist of different parts (cf. the slope of the distribution) and it has an offset so that there exists no pair of antipodal initial states whose distinguishability has no revival during the dynamics. For these kinds of pairs one also obtains an offset for the dynamics (5.31). It might be interesting to study the Λ -system and the implemented dynamics again and in more detail in order to find an explanation for this behaviour.

Chapter 6

Summary and conclusion

In this thesis I have developed a mathematical characterization of optimal initial state pairs for the measure for quantum non-Markovianity [5, 29]. Due to my studies, the maximization involved in \mathcal{N} (cf. (3.34)) can be reduced to an $(N^2 - 2)$ -dimensional set for a Hilbert space with dimension N whereas the maximization involved in the original definition was performed over a set with dimension $2N^2 - 2$. The obtained results rely solely on the convexity of the state space and on the linearity of the dynamical maps. The characterization of optimal pairs thus applies to any open system dynamics which is determined by a one-parameter family of linear, completely positive and trace preserving maps. In addition, all the developed constructions can be applied to any homogeneous measure which evaluates the difference of two states (operators), for example to a metric arising from a norm.

After having shown that the states of optimal pairs must be on the boundary of the state space, I have proven that they in addition must be orthogonal. This is very plausible since it implies that these states can be distinguished with certainty by a single measurement. Optimal state pairs thus have the maximal possible amount of initial information and are therefore capable of emitting and reabsorbing the maximal amount of information during the non-Markovian dynamics. Introducing the notion of joint translatability, an alternative proof of this result for finite-dimensional systems has been obtained. Moreover, this concept gives insight into the structure of the state space and might serve also for other applications.

Based on the orthogonality of states of an optimal pair, it has been possible to derive a new representation of the measure \mathcal{N} for finite systems. I have shown that it is possible to fix one of the input states to be any point in the interior of the state space and to maximize the quantity solely over the states of an enclosing surface of the inner point. Hence, the information about the dynamics regarding memory effects is contained in any part of the state space which supports the intuitive idea that memory effects are an intrinsic property of the dynamical process. In order to obtain this representation, the information flow must be rescaled by the initial distinguishability of the considered state pair showing that the backflow of information relative to the initial information content is the universal quantity which determines the dynamics. This result allows to apply gradient methods more easily in the sampling process so that the numerical efficiency increases. In particular, this characterization makes the

evaluation of the measure \mathcal{N} in an experiment more feasible. On the basis of an already existing optical experiment regarding non-Markovianity [28, 32] and the present results, experimental realizations of this scheme are currently under construction.

I have further demonstrated that for Hilbert spaces with dimensions of at least three, optimal state pairs need not consist of pure states, in contrast to two-level systems where optimal pairs are always antipodal points on the Bloch sphere, and as such pure. The example constructed here leads to an optimal pair consisting of antipodal states, that is, a pure and a mixed quantum state. Although based on a master equation and in agreement with the general requirements on dynamical maps, the implemented dynamics is artificial and might therefore not be realizable experimentally. An experimental realization of such a counterexample regarding the purity of optimal states might be an objective of further studies. The special shape of the probability distributions regarding the total increase of the trace distance (in particular, see Fig. 5.5) might also be an interesting subject of further studies of the Λ -system and the implemented dynamics. Moreover, I conjecture that for even larger Hilbert spaces one can also construct quantum processes for which both states of the optimal pair are mixed. Finally, I mention that on the basis of the present results more specific statements could be proven if one assumes additional properties of the quantum process: invariance under certain symmetry groups, or the existence of invariant states might yield even further statements on the optimal states implying a further reduction of the set of optimal states.

There has been a significant progress in developing a general theory of non-Markovian quantum processes over the past years [4, 14, 39, 41, 58]. Moreover, a better understanding of the fundamental properties of these kind of open system quantum dynamics was gained and yet several experiments [32, 33, 50] have been carried out demonstrating the experimental accessibility of the studied measure \mathcal{N} for quantum non-Markovianity. A major point of the entire non-Markovianity business is that the influence of these memory effects on physical systems and, therefore, its exploit for applications is not yet known in detail. Several steps towards this direction were made quite recently: In [27] the authors show that non-local memory effects allow to perform perfect quantum teleportation with mixed photon polarization states. Moreover, in [28, 32], it was demonstrated how an open quantum system can be used as a probe of the environment determining its correlations. These first experimental results yield a promising outlook for future applications of non-Markovian dynamics. However, further progress in understanding the physical cause of non-Markovianity and its impact on actual systems must be made so that the relevance of this mathematical classification of dynamical processes will be clarified completely. This might also resolve the conflict concerning the different definitions.

Parts of the results of this thesis were published in [54].

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Erklärung zur Urheberschaft

Ich erkläre hiermit, dass ich die vorliegende Diplomarbeit selbständig verfasst und keine außer den angegebenen Quellen und Hilfsmittel benutzt habe, und dass ich diese Arbeit, in gleicher oder ähnlicher Form, nicht anderweitig für Prüfungszwecke vorgelegt habe.

Ort, Datum

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