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## QUANTUM MARKOVIAN DYNAMICS AND BIPARTITE ENTANGLEMENT

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# Contents

<b>Introduction</b>	<b>4</b>
<b>1 Entanglement</b>	<b>9</b>
1.1 Compound systems . . . . .	9
1.1.1 Bipartite systems . . . . .	10
1.1.2 Entanglement . . . . .	11
1.2 Positivity and complete positivity . . . . .	11
1.2.1 Definitions . . . . .	11
1.2.2 Positive maps and separability criteria . . . . .	13
1.3 Entanglement measures . . . . .	15
1.3.1 Definitions and properties . . . . .	15
1.3.2 Relative entropy of entanglement . . . . .	20
1.3.3 Concurrence . . . . .	20
<b>2 Open Quantum Systems</b>	<b>23</b>
2.1 Reversible and irreversible dynamics . . . . .	23
2.2 Reduced dynamics . . . . .	26
2.2.1 Abstract form of the generators of dynamical semigroups . . . . .	27
2.2.2 Master equation and Markovian approximations . . . . .	29
2.2.3 One- and two-qubit systems . . . . .	32
2.3 Asymptotic states . . . . .	35
2.3.1 One-qubit case . . . . .	36
2.3.2 Two-qubit case . . . . .	37
<b>3 Determination of the noise parameters in a one-dimensional open quantum system</b>	<b>41</b>
3.1 Introduction . . . . .	41
3.2 Determination of the Kossakowski matrix elements . . . . .	42
3.3 Complete positivity . . . . .	47
3.4 Conclusions . . . . .	49

<b>4</b>	<b>Open quantum systems and entanglement</b>	<b>51</b>
4.1	Entanglement generation in a two-qubit system . . . . .	52
4.2	Asymptotic entanglement . . . . .	56
<b>5</b>	<b>Environment-Induced Bipartite Entanglement</b>	<b>59</b>
5.1	Introduction . . . . .	59
5.2	Entanglement generation between two qubits . . . . .	60
5.3	Entanglement generation in higher dimensional bipartite systems . . . . .	67
5.4	Conclusions . . . . .	71
<b>6</b>	<b>Entanglement and entropy rates in open quantum systems</b>	<b>73</b>
6.1	Introduction . . . . .	73
6.2	The Reduced Dynamics . . . . .	74
6.3	Entropy and Entanglement Rates . . . . .	77
6.4	Results . . . . .	80
6.5	Conclusions . . . . .	85
	<b>Summary and Outlook</b>	<b>87</b>
	<b>Acknowledgements</b>	<b>89</b>
<b>A</b>	<b>Calculation of transmission and reflection coefficients</b>	<b>91</b>
<b>B</b>	<b>Integration of the master equation</b>	<b>93</b>
<b>C</b>	<b>Solution of the maximization problem</b>	<b>95</b>
	<b>Bibliography</b>	<b>98</b>

# Introduction

The focus of this PhD work is two-fold: on one hand, *open quantum systems*, i.e. systems whose interactions with the external environment cannot be neglected, are studied, and a way of characterizing the bath is found in terms of physical quantities of the subsystem immersed within it; on the other hand *bipartite entanglement* in open quantum systems is analyzed in detail, from the point of view both of environment-induced entanglement generation and of the time-evolution of entanglement under particular dissipative dynamics together with the possibility of its asymptotic persistence.

The importance of the purely quantum phenomenon of entanglement as a physical resource for performing informational tasks which would be classically impossible [1] has spurred the study of its dynamical behavior in many different systems. The time-evolution of most of these is reversible and generated by a Hamiltonian. Many realistic systems, however, interact with the external environment in a non-negligible way and thus undergo dissipative irreversible dynamics. Therefore, since the aim is to be able to use entanglement as an efficient physical resource in realistic systems that can be experimentally implemented, it is important that the temporal behavior of this purely quantum phenomenon should be studied also in systems that are driven by noisy environments.

In standard quantum mechanics the focus is mainly upon *closed* physical systems, i.e. systems which can be considered isolated from the external environment and whose reversible time-evolution is described by one-parameter groups of unitary operators. On the other hand, when a system  $S$  interacts with an environment  $E$ , it must be considered as an *open* quantum system whose time-evolution is irreversible and exhibits dissipative and noisy effects. A standard way of obtaining a manageable dissipative time-evolution of the density matrix  $\rho_t$  describing the state of  $S$  at time  $t$  is to construct it as the solution of a Liouville-type master equation  $\partial_t \rho_t = \mathbf{L}[\rho_t]$ . This can be done by tracing away the environment degrees of freedom [2, 3] and by performing a Markovian approximation [4, 5], i.e. by studying the evolution on a slow time-scale and neglecting fast decaying memory effects. Then the irreversible reduced dynamics of  $S$  is described by one-parameter semi-groups of linear maps obtained by exponentiating the generator  $\mathbf{L}$  of Lindblad type [6, 7]:  $\gamma_t = e^{t\mathbf{L}}$ ,  $t \geq 0$ , such that  $\gamma_{t+s} = \gamma_t \circ \gamma_s = \gamma_s \circ \gamma_t$  ( $s, t \geq 0$ ) and  $\rho_t \equiv \gamma_t[\rho]$ .

In order to ensure that the reduced dynamics thus obtained is physically consistent the semigroup  $\gamma_t$  must be composed of *completely positive* maps[8]. This requirement comes from the possibility of the system of interest,  $S$ , of being coupled to some so-called "ancilla" system,  $A$ . Naturally, every linear map  $L$  describing a physical transformation must preserve the positivity of every state  $\rho$ : if this were not so, then the system density matrix could develop some negative eigenvalues, which would contradict the statistical interpretation of the eigenvalues as probabilities [9]. So, in order for  $L$  to preserve the positivity of the spectrum of every  $\rho$ ,  $L$  must be a positive map. This, however, is not sufficient, as the system  $S$  described by  $\rho$  might be coupled to a so-called "ancilla" system  $A$ . If a physical transformation, represented by the positive map  $L$ , is performed on the system  $S$  that is statistically coupled to the system  $A$  which does not undergo the same transformation, then it is necessary to consider the tensor product of maps  $id_A \otimes L$  on the composite system  $A + S$ , where  $id_A$  is the identity on the state space  $\mathcal{S}_A$  of system  $A$ . Therefore, in order for  $L$  to correctly represent a physical transformation, it is not sufficient for  $L$  to be positive: the whole tensor product  $id_A \otimes L$  must be positive for any ancilla  $A$ , i.e. the map  $L$  must be *completely positive* [8].

The typical effect of noise and dissipation on a system  $S$  immersed in a large environment  $E$  is decoherence; in certain specific situations, however, the environment  $E$  may even create quantum correlations between the subsystems which compose  $S$ . This possibility depends on the form of the Kossakowski matrix that characterizes the dissipative part of the generator  $L$ . In [10] an inequality was found, involving the entries of such a matrix which, if fulfilled, is sufficient to ensure that a specific initial separable pure state of two qubits gets entangled.

Part of this PhD work is dedicated to proving that the above-mentioned condition is also necessary to create entanglement in an initially separable state of two qubits only via the noisy evolution due to the common environment in which they are immersed.

On the other hand, another important issue is to understand the behavior of entanglement in an open quantum system evolving under a dissipative dynamics, and it is of particular interest to see whether it can persist asymptotically. This question is also considered in this work.

The topic of the first chapter is *bipartite entanglement*. Firstly, composite systems are described, focusing in particular on bipartite ones, i.e. systems composed of two subsystems, since these are the systems considered in this PhD work. The definition of entangled and non-entangled (separable) state is given both for pure states and for statistical mixtures. Then some definitions and theorems concerning positivity and complete positivity, which will be useful in the following, are given. Positive and completely positive maps are thus introduced and the use of positive maps as a tool to distinguish entangled states from separable ones is explained. Finally, the issue of quantifying entanglement

in a given state is considered and therefore entanglement measures are defined and described, focusing in particular on two measures which will be used in this thesis, namely on the so-called relative entropy of entanglement and concurrence.

The second chapter is dedicated to *open quantum systems*. Firstly, the mathematical character of their irreversible dynamics is described. Then the reduced dynamics of the system  $S$  immersed in an external bath  $E$  is considered: first the constraints on the form of the generator  $L$  of Lindblad type in order to ensure physical consistency of the dynamical maps are illustrated; then the master equation for  $S$  is derived. Further, the two most commonly used Markovian approximations [4, 5], namely the *weak coupling* and the *singular coupling* limits are described in some detail. Then, since one- and two-qubit systems will be mainly dealt with in this thesis, the form of the reduced dynamics and of its dissipative term is given explicitly for one- and two-qubit systems immersed in an external bath. Finally, the asymptotic states of dynamical semigroups are derived in Section 2.4 for a particular dissipative dynamics of interest for this thesis, again focusing on one- and two-qubit states.

The third chapter concerns the study of the properties of open quantum systems and a way of characterizing the action of the bath in terms of physical quantities of the subsystem immersed within it.

The system considered here consists of an electron that can propagate in a one-dimensional wire in which a spin-1/2 impurity is embedded at a fixed position. The electron and the impurity magnetically interact, and the whole system is immersed in an external bath whose noisy effects act only on the spin-1/2 impurity degrees of freedom. Then, the elements of the Kossakowski matrix describing this dissipative dynamics, i.e. the noise parameters, are written in terms of the electron's transmission and reflection probabilities, which can be measured. Moreover, a particular example of the necessity of complete positivity for physical consistency is given, showing that if the dissipative evolution is described by a positive but not completely positive map, negative transmission probabilities can arise.

In the fourth chapter, entanglement in open quantum systems is considered, in the particular case of two-qubit systems, which are mainly of interest in this thesis. As mentioned above, there are some particular cases when the environment can create quantum correlations between the subsystems composing the system  $S$  immersed within it. In this chapter, firstly a sufficient condition for the bath to generate entanglement in an initially separable state of the two qubits is given [10]. Then the possibility of asymptotic persistence of entanglement in a two-qubit state subject to the dissipative dynamics introduced in Section 2.4 is studied. Interestingly it is found that in some cases the environment-induced entanglement can even persist for long times in the asymptotic state.

The fifth chapter deals with environment-induced bipartite entanglement. Here, the sufficient condition presented in Section 4.1 is proved to be also necessary to guarantee

that entanglement is generated only via the bath in an initially separable state of two qubits. Further, the above-mentioned sufficient condition is generalized to bipartite systems of arbitrary dimension, and explicit examples are given both for the two-qubit and for the arbitrary-dimensional bipartite case.

The sixth chapter concerns the time-behavior of entanglement under dissipative dynamics and the possibility of its asymptotic persistence. In particular, the behavior of the variation in time of entanglement (the so-called *entanglement rate*) is compared to the variation in time of entropy (the so-called *entropy rate*). The idea of this comparison stems from the fact that, on one hand, the formalism of open quantum systems has been used to describe the tendency to thermal equilibrium of a small system in weak interaction with a large heat bath at a certain temperature and the main tool in this thermodynamical picture is the quantum relative entropy [4], while on the other, the entanglement measure called *relative entropy of entanglement* provides a pseudo-distance between a state and the closed convex set of separable states [11]. In a previous paper [12] a conjecture was put forward, and proved in a particular case, namely that for open quantum systems where the interaction is due only to the common bath, the entanglement rate is always bounded by the entropy rate. In this work a more general dissipative dynamics (introduced in Sections 2.4 and 4.2) is considered, the master equation is analytically solved for a particular class of initial states and the explicit form of the asymptotic states of the dynamics is found. Thus the time-behavior of entanglement for various initial states is analyzed and the entanglement and entropy rates are compared. This leads to a new conjecture, namely that the one put forward in [12] holds when the asymptotic state is separable but does not when the latter is entangled.

Then there is a chapter that briefly summarizes the results of this PhD work, drawing some conclusions and providing the outlook for future work.

Finally, there are three Appendices in which some details of the more cumbersome calculations are given: Appendix A pertains to the work presented in Chapter 3, while Appendices B and C pertain to that illustrated in Chapter 6.



# Chapter 1

## Entanglement

In this chapter, the quantum property of *entanglement* will be analyzed. Since entanglement represents *quantum correlations* within a system, compound systems will be described in the first section, focusing mainly on bipartite systems, i.e. systems composed of two subsystems. Then the definition of entangled and non-entangled (separable) state will be given both for pure and for mixed states.

In the second section, the focus will be on ways to *distinguish* entangled states from separable ones, using so-called positive maps as a tool for this.

Finally, in the third section, the question of how to *quantify* the amount of entanglement in a given state will be dealt with, and to this end "entanglement measures" will be defined and analyzed.

### 1.1 Compound systems

In general physical systems of many particles or with many degrees of freedom must be dealt with: these represent compound systems, i.e. systems composed of two or more independent subsystems.

A general quantum system composed of  $N$  subsystems  $S = S_1 + S_2 + \dots + S_N$  is described by the Hilbert space  $\mathcal{H}$  which is the tensor product of the Hilbert spaces of the subsystems:  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$  [9]. The states of such systems can either be pure state projectors  $|\psi\rangle\langle\psi|$  on vector states  $|\psi\rangle \in \mathcal{H}$  or mixed states, i.e. density matrices arising from convex combinations of projectors  $\rho := \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ , with  $0 \leq \lambda_i \leq 1$ ,  $\sum_i \lambda_i = 1$ ,  $|\psi_i\rangle \in \mathcal{H}$ . The space of all states of a system  $S$  will be denoted by  $\mathcal{S}_d$ , with  $d$  the dimension of the Hilbert space  $\mathcal{H}$ , and it is a closed, convex set [9].

### 1.1.1 Bipartite systems

In the following only bipartite systems  $S = S_A + S_B$  with discrete variables will be considered: these are described by the Hilbert space  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ , with  $\mathcal{H}_A \equiv \mathbb{C}^{d_A}$ ,  $\mathcal{H}_B \equiv \mathbb{C}^{d_B}$ , the Hilbert space of the first, respectively second, subsystem. Therefore the total Hilbert space of the bipartite system will be  $\mathcal{H} \equiv \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$  with dimension  $d = d_A \times d_B$ , since  $d_A$  and  $d_B$  are the dimensions of  $\mathcal{H}_A$  and  $\mathcal{H}_B$  respectively. An arbitrary vector  $|\psi\rangle \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$  can be written [9] as follows:

$$|\psi\rangle = \sum_{i,j} c_{ij} |\phi_i^A\rangle \otimes |\phi_j^B\rangle,$$

where  $\{|\phi_i^A\rangle\}$  with  $i = 1, \dots, d_A$  and  $\{|\phi_j^B\rangle\}$  with  $j = 1, \dots, d_B$  are the orthonormal bases of  $\mathbb{C}^{d_A}$  and  $\mathbb{C}^{d_B}$  respectively, and  $c_{ij} \in \mathbb{C}$ . Therefore the total Hilbert space  $\mathcal{H}$  will be generated by the basis  $\{|\phi_i^A\rangle\} \otimes \{|\phi_j^B\rangle\}$ ; moreover, given two operators  $O_A, O_B$  acting on  $S_A$ , respectively  $S_B$ , their tensor product on  $S$  is defined by the way it acts on the total basis:

$$O_A \otimes O_B (|\phi_i^A\rangle \otimes |\phi_j^B\rangle) = O_A |\phi_i^A\rangle \otimes O_B |\phi_j^B\rangle.$$

Formally, a local operator acting only on the subsystem  $S_A$  is written  $O_A \otimes \mathbf{I}_B$ , with  $\mathbf{I}_B$  the identity operator on  $S_B$ , and analogously for a local operator  $O_B$  acting only on  $S_B$ .

The space of states, i.e. the convex set of density matrices, of the bipartite system  $S_A + S_B$  will be indicated as  $\mathcal{S}_{d_A \times d_B}$ , and  $\varrho_A, \varrho_B$  will be the statistical operators pertaining to  $S_A$ , respectively  $S_B$ . The density matrix of only one of the two subsystems, i.e. the *reduced density matrix*, is obtained as the partial trace with respect to the Hilbert space of the other subsystem, namely  $\varrho_A = \text{Tr}_B[\varrho_{AB}]$  and  $\varrho_B = \text{Tr}_A[\varrho_{AB}]$ , with  $\varrho_{AB} \in \mathcal{S}_{d_A \times d_B}$ ; it follows that that the mean values of local operators read  $\text{Tr}_{AB}[\varrho_{AB}(O_A \otimes \mathbf{I}_B)] = \text{Tr}_A[\varrho_A O_A]$ ,  $\text{Tr}_{AB}[\varrho_{AB}(\mathbf{I}_A \otimes O_B)] = \text{Tr}_B[\varrho_B O_B]$ .

In order to study the correlations that can be present in a bipartite system, it is useful to consider the Schmidt decomposition [9, 13] of the bipartite state.

**Proposition 1** *Given a state vector  $|\psi_{AB}\rangle \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$ , its **Schmidt decomposition** is*

$$|\psi_{AB}\rangle = \sum_{i=1}^{\min(d_A, d_B)} \sqrt{\lambda_i^A} |r_i^A\rangle \otimes |r_i^B\rangle,$$

with  $\{|r_i^A\rangle\}$  and  $\{|r_i^B\rangle\}$ ,  $i = 1, \dots, \min(d_A, d_B)$ , orthonormal sets for  $\mathbb{C}^{d_A}, \mathbb{C}^{d_B}$  respectively, and  $\min(d_A, d_B)$  the minimum between  $d_A$  and  $d_B$ .

It is evident from this decomposition that the two partial traces  $\varrho_A = \sum_i \lambda_i^A |r_i^A\rangle \langle r_i^A|$  and  $\varrho_B = \sum_i \lambda_i^A |r_i^B\rangle \langle r_i^B|$  have the same eigenvalues  $\lambda_i^A$ ; moreover, the non-zero eigenvalues have the same multiplicity.

### 1.1.2 Entanglement

Firstly, let the bipartite system  $S = S_A + S_B$  be in a **pure** state described by the state vector  $|\psi\rangle \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$ .

**Definition 1** The state  $|\psi\rangle \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$  is **separable** if and only if there exist two vectors  $|\psi_A\rangle \in \mathbb{C}^{d_A}$  and  $|\psi_B\rangle \in \mathbb{C}^{d_B}$  such that  $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$  [14].

Otherwise the state is said to be *entangled*.

For a pure separable state the partial traces are projectors. Indeed, given  $|\psi_{sep}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$ , it follows:

$$\varrho_A = \text{Tr}^{(B)}(|\psi_{sep}\rangle\langle\psi_{sep}|) = \text{Tr}^{(B)}(|\psi_A\rangle\langle\psi_A| \otimes |\psi_B\rangle\langle\psi_B|) = |\psi_A\rangle\langle\psi_A|$$

and analogously for  $\varrho_B = |\psi_B\rangle\langle\psi_B|$ .

From the Schmidt decomposition it can be easily seen that  $|\psi_{AB}\rangle$  is separable if and only if there exists only one coefficient  $\sqrt{r_j} = 1$ ,  $\sqrt{r_i} = 0 \forall i \neq j$ . If instead there are more coefficients which are non-zero, then the state is entangled. In particular, if the coefficients are all the same, then the state is said to be *maximally entangled*.

Further, the distinction between separable and entangled states can be extended to **statistical mixtures** as follows.

**Definition 2** The density matrix  $\varrho_{AB} \in \mathcal{S}_{d_A \times d_B}$  is said to be **separable (entangled)** if and only if it can (cannot) be written as follows [15]:

$$\varrho_{AB} = \sum_{i=1}^n p_i \varrho_i^A \otimes \varrho_i^B \quad (1.1)$$

for some  $n \in \mathbb{N}$ , with weights  $p_i \geq 0 \forall i$  and such that  $\sum_i p_i = 1$ , where  $\varrho_i^A, \varrho_i^B$  are sets of density matrices in  $\mathcal{S}_{d_A}, \mathcal{S}_{d_B}$  respectively.

## 1.2 Positivity and complete positivity

### 1.2.1 Definitions

In this section some general definitions will be given, which will be useful in the following.

**Definition 3** Let  $M_d(\mathbb{C}) := M_d$  be the algebra of  $d \times d$  complex matrices. A Hermitian operator  $X = X^\dagger \in M_d$  is said to be **positive** ( $X \geq 0$ ) if and only if  $\langle \Psi | X | \Psi \rangle \geq 0 \forall \Psi \in \mathbb{C}^d$  [9, 13].

**Definition 4** A linear map  $L : M_m \rightarrow M_n$  is said to be **positive** if and only if  $L(X) \geq 0 \forall X \geq 0$  [16].

**Definition 5** A linear map  $L : M_m \rightarrow M_n$  is said to be **k-positive** if and only if  $id_k \otimes L : M_k \otimes M_m \rightarrow M_k \otimes M_n$  is positive, where  $id_k$  is the identity on  $M_k$  [17].

**Definition 6** A linear map  $L : M_m \rightarrow M_n$  is said to be **completely positive** if and only if  $L$  is  $k$ -positive  $\forall k \in \mathbb{N}$  [17].

The tensor product of a positive map  $L : M_m \rightarrow M_n$  with the identity  $id_k$  can be performed both as

$$id_k \otimes L : M_k \otimes M_m \rightarrow M_k \otimes M_n$$

and as

$$L \otimes id_k : M_m \otimes M_k \rightarrow M_n \otimes M_k,$$

and the same Definition 6 holds for complete positivity.

The following Theorem follows from [18]:

**Theorem 1** The map  $L : M_m \rightarrow M_n$  is completely positive if and only if the tensor product  $id_n \otimes L$  is positive for any  $n \in \mathbb{N}$ .

**Definition 7** A linear map  $L : M_m \rightarrow M_n$  is said to be **k-copositive** if and only if  $T_k \otimes L : M_k \otimes M_m \rightarrow M_k \otimes M_n$  is positive, where  $T_k$  indicates the transposition on  $M_k$  [17].

**Definition 8** A linear map  $L : M_m \rightarrow M_n$  is said to be **completely copositive** if and only if  $L$  is  $k$ -copositive  $\forall k \in \mathbb{N}$  [17].

Completely positive (CP) maps are fully characterized by the following

**Theorem 2 (Kraus-Stinespring Representation)** [19, 20] The map  $L : M_m \rightarrow M_n$  is completely positive if and only if  $L(\cdot) = \sum_i V_i(\cdot)V_i^\dagger$ , with  $V_i \in M_{n \times m}(\mathbb{C}) := M_{n \times m}$ .

Moreover,  $L$  is such that:

1. the trace is preserved if and only if  $\sum_i V_i^\dagger V_i = I$ ;
2. the trace is non-increasing if and only if  $\sum_i V_i^\dagger V_i \leq I$ ;
3. the identity is preserved if and only if  $\sum_i V_i V_i^\dagger = I$ .

Note that the Kraus-Stinespring representation for a given completely positive map is not unique [19, 20].

While completely positive maps can be fully determined by Theorem 2, there is still no complete characterization for generic positive maps. The following Definition, however, helps in the description of some positive maps.

**Definition 9** From [17, 21] a positive map  $L$  is said to be **decomposable** (not decomposable) if and only if it can (cannot) be written as the sum of a completely positive map and a completely copositive map, i.e.

$$L = \Lambda_{CP}^1 + \Lambda_{CP}^2 \circ T$$

where  $\Lambda_{CP}^1$  and  $\Lambda_{CP}^2$  are completely positive maps and  $T$  is the transposition.

The following characterization of positive maps in low dimensions holds [17, 21]:

**Theorem 3** All positive maps  $L : M_2 \rightarrow M_2, M_2 \rightarrow M_3, M_3 \rightarrow M_2$  are decomposable.

If, instead, one of the subspaces of the bipartite system has higher dimension, then there exist positive maps which are not decomposable [17, 21].

### 1.2.2 Positive maps and separability criteria

In the previous section general linear maps  $L$  acting on positive operators  $0 \leq X \in M_d$ , with  $M_d(\mathbb{C}) := M_d$  the algebra of  $d \times d$  complex matrices, were considered. In the following, linear maps acting on the states  $0 \leq \varrho \in \mathcal{S}_d$ , with  $\mathcal{S}_d$  the state space, will be dealt with. Therefore the following Definition is useful:

**Definition 10** Given a linear map  $L : M_m \rightarrow M_n$ , its **dual map**  $L^* : M_n \rightarrow M_m$  is defined as

$$\mathrm{Tr}^{(n)}(\varrho L[X]) = \mathrm{Tr}^{(m)}(L^*[\varrho]X)$$

$\forall X \in M_m, \varrho \in \mathcal{S}_n$  [22].

Every linear map  $L$  describing a physical transformation must preserve the positivity of every state  $\varrho$ : if this were not so, then the system state could develop some negative eigenvalues, which would contradict the statistical interpretation of its eigenvalues as probabilities [9].

In order for  $L$  to preserve the positivity of the spectrum of every  $\varrho$ ,  $L$  must be a positive map. This, however, is not sufficient, as the system  $S_d$  described by  $\varrho$  might be coupled to a so-called "ancilla" system  $S_n$ . If a physical transformation, represented by the positive map  $L$ , is performed on the system  $S_d$  which is statistically coupled to the system  $S_n$ , then it is necessary to consider the tensor product of maps  $id_n \otimes L$  on the composite system  $S_n + S_d$ , where  $id_n$  is the identity on the state space  $\mathcal{S}_n$  of system  $S_n$ . Therefore, in order for  $L$  to correctly represent a physical transformation, it is not sufficient for  $L$  to be positive: the whole tensor product  $id_n \otimes L$  must be positive for any  $n$ , i.e. the map  $L$  must be *completely positive* [8].

The necessity of complete positivity is due to the existence of *entangled* states of the composite system  $S_n + S_d$  [16]. If all of the physical states of a bipartite system were separable

as in Definition 2, then the positivity of map  $L$  would suffice. Indeed, from Definition 2, we know that if  $\varrho \geq 0$  is separable, then  $\varrho \equiv \varrho_{nd} = \sum_i p_i \varrho_i^n \otimes \varrho_i^d$ , and thus it follows that

$$(id_n \otimes L)[\varrho] = \sum_i p_i (id_n[\varrho_i^n] \otimes L[\varrho_i^d]) = \sum_i p_i (\varrho_i^n \otimes L[\varrho_i^d]) \geq 0.$$

If, instead, the state of the bipartite system is entangled,  $\varrho \equiv \varrho^{ent}$ , then it cannot be written as in (1.1) and therefore, in order to have  $(id_n \otimes L)[\varrho^{ent}] \geq 0$  for all  $n$ , the tensor product  $id_n \otimes L$  must be positive, i.e. the map  $L$  must be completely positive.

However, although positive maps do not describe consistent physical transformations, they represent an important tool in the identification of entangled states [23], as will be shown in the Theorems enunciated in this section.

In the following, to simplify the notation, bipartite states  $\varrho \in \mathcal{S}_{d \times d}$  will be considered, but all the results hold also in the general case of bipartite states  $\varrho_{AB} \in \mathcal{S}_{d_A \times d_B}$ .

**Theorem 4** *A state  $\varrho \in \mathcal{S}_{d \times d}$  is **entangled** if and only if there exists a positive map  $L$  on  $\mathcal{S}_d$  such that  $(id_d \otimes L^*)[\varrho]$  is non-positive.*

The simplest example of positive but not completely positive map is the transposition. The following one-way separability criterion comes from [24]:

**Theorem 5 (Peres criterion)** *If a state  $\varrho \in \mathcal{S}_{d \times d}$  is **separable**, then  $\varrho^{T_B} := (id_d \otimes T_B)[\varrho] \geq 0$ , where  $T_B$  represents the transposition on the second subsystem.*

Therefore, if  $\varrho^{T_B} := (id_d \otimes T_B)[\varrho]$  is not positive, then the state  $\varrho$  is entangled: non-positivity under partial transposition implies entanglement; the opposite, however, is not true in general.

A general two-way separability criterion through positive but not completely positive maps comes from [16]:

**Theorem 6 (Horodecki criterion)** *A state  $\varrho \in \mathcal{S}_{d \times d}$  is **separable** if and only if  $(id_d \otimes L)[\varrho] \geq 0$  for all maps  $L : M_d \rightarrow M_d$  which are positive but not completely positive.*

From a result obtained in [16] it follows:

**Corollary** *A state  $\varrho_{AB} \in \mathcal{S}_{d_A \times d_B}$  with  $d_A \times d_B \leq 6$  (i.e.  $2 \times 2, 2 \times 3, 3 \times 2$ ) is **separable** if and only if*

$$\varrho_{AB}^{T_B} := (id_A \otimes T_B)[\varrho_{AB}] \geq 0.$$

The above Corollary follows from Theorems 3 and 6, i.e. from the fact that for  $d_A \times d_B \leq 6$  all positive maps are decomposable: therefore, in this case, the partial transposition detects all entangled bipartite states and the above Corollary offers a necessary and sufficient criterion for separability. Instead, for  $d_A \times d_B > 6$  not all positive maps are decomposable [17, 21] and this implies that in this case positivity under partial transposition is only a necessary, but not sufficient, condition for the separability of a bipartite state  $\varrho_{AB} \in \mathcal{S}_{d_A \times d_B}$  [16].

## 1.3 Entanglement measures

### 1.3.1 Definitions and properties

So far the focus has been on the question of how to *qualify* an entangled state versus a separable state. Another important, though difficult to answer, question is how to *quantify* the amount of entanglement within a given state.

There are various ways in which an *entanglement measure* can be constructed or defined, and these lead to different "families" of entanglement measures, namely [25]:

- axiomatic measures
- convex-roof measures
- operational measures .

In the following, the different approaches to the construction of entanglement measures will be briefly analyzed, focusing on bipartite systems; then two entanglement measures, which will be of particular interest in the rest of this work, will be considered in more detail.

#### Axiomatic approach

In the axiomatic approach entanglement measures  $E(\varrho)$  are constructed by allowing any function of state to be a measure, provided it satisfies the following postulates [11, 26–28]:

1. For any separable state  $\sigma$  the entanglement measure should be zero, i.e.  $E(\sigma) = 0$ ;
2. For any state  $\varrho$  and any local unitary transformation, i.e. for any unitary transformation of the form  $U_A \otimes U_B$ , the amount of entanglement remains unchanged:  $E(\varrho) = E(U_A \otimes U_B \varrho U_A^\dagger \otimes U_B^\dagger)$ ;
3. Monotonicity under LOCC: entanglement cannot increase under local operations and classical communication. Namely, for any LOCC operation, i.e. for any operation of the form  $\Lambda \equiv \Lambda_A \otimes \Lambda_B$  aided only with classical communication [9], it must hold true that  $E(\Lambda[\varrho]) \leq E(\varrho)$ ;
4. Continuity: in the limit of vanishing distance between two density matrices the difference between their entanglement should tend to zero, i.e.  $E(\varrho_1) - E(\varrho_2) \rightarrow 0$  for  $\|\varrho_1 - \varrho_2\| \rightarrow 0$ , with  $\|\varrho_1 - \varrho_2\| := \text{Tr} \sqrt{(\varrho_1 - \varrho_2)^2}$ ;
5. Additivity: a number  $n$  of identical copies of the state  $\varrho$  should contain  $n$  times the entanglement of one copy, i.e.  $E(\varrho^{\otimes n}) = nE(\varrho)$ ;

6. Subadditivity: the entanglement of the tensor product of two states  $\varrho_1$  and  $\varrho_2$ , with  $\varrho_1 \neq \varrho_2$ , should not be larger than the sum of the entanglement of each of the states, i.e.  $E(\varrho_1 \otimes \varrho_2) \leq E(\varrho_1) + E(\varrho_2)$ ;
7. Convexity: the entanglement measure should be a convex function, i.e.  $E(\lambda\varrho_1 + (1-\lambda)\varrho_2) \leq \lambda E(\varrho_1) + (1-\lambda)E(\varrho_2)$  for  $0 < \lambda < 1$ .

Regarding the first condition, in general it is not possible to impose that  $E(\varrho) = 0$  for a generic state  $\varrho$  imply that the latter is separable: indeed, there exist some entanglement measures which vanish on particular classes of entangled states (see, e.g., the *negativity* defined in the following).

The third condition is the one that really restricts the class of possible entanglement measures and was proposed as the most important postulate for the latter [26], although usually it is also the most difficult one to prove [11]. Most of the known entanglement measures, however, satisfy the monotonicity condition on average [25], namely

$$\sum_i p_i E(\sigma_i) \leq E(\varrho),$$

where  $\{p_i, \sigma_i\}$  is the ensemble obtained from the state  $\varrho$  by means of LOCC.

Finally, it should be noted that the monotonicity condition can also be given in more “coarse grained” terms as “monotonicity under SLOCC (stochastic LOCC)” [25, 29, 30], i.e. in terms of operations that transform a state  $\varrho$  into a new state  $\sigma = \frac{\Lambda[\varrho]}{\text{Tr}(\Lambda[\varrho])}$  with some nonzero probability  $\text{Tr}(\Lambda[\varrho]) < 1$ <sup>1</sup>.

For **pure bipartite states** it is rather simple to find entanglement measures: indeed, since there are no classical probabilistic correlations contained in pure states, any unitarily invariant, concave function of the reduced density matrix defines one. The most important entanglement measure for pure states which satisfies the above conditions is the *entropy of entanglement*, and this was proved to be the unique entanglement measure for pure states [11]. The definition of entropy of entanglement is based on that of von Neumann entropy, which for a generic state  $\varrho$  reads

$$S_{vN}(\varrho) := -\text{Tr}[\varrho \ln \varrho] = -\sum_{i=1}^d r_i \ln r_i,$$

where  $r_i$  are the eigenvalues of  $\varrho$ . The von Neumann entropy measures the amount of uncertainty about the state  $\varrho$  and it is zero if and only if the state is pure.

The entropy of entanglement is defined as the von Neumann entropy of the reduced operator  $\varrho_A := \text{Tr}_B[\varrho_{AB}]$  ( $\varrho_B := \text{Tr}_A[\varrho_{AB}]$ ) of the bipartite state  $\varrho_{AB}$  [11, 27], i.e.

$$E_{vN}(\varrho_{AB}) = S_{vN}(\varrho_A) = -\text{Tr}[\varrho_A \ln \varrho_A] = S_{vN}(\varrho_B) = -\text{Tr}[\varrho_B \ln \varrho_B]. \quad (1.2)$$

<sup>1</sup>The case of LOCC corresponds to  $\text{Tr}(\Lambda[\varrho]) = 1$ .



Therefore the property of a pure bipartite state  $\varrho_{AB}$  of being entangled or not is related to the mixedness of its reduced operator  $\varrho_A(\varrho_B)$ : from (1.2) it turns out that the pure state  $\varrho_{AB}$  is separable if and only if the reduced operator  $\varrho_A(\varrho_B)$  is also pure, since in this case the von Neumann entropy of the latter is zero<sup>2</sup>.

In the case of **mixed states**, however, the entropy of entanglement cannot distinguish between classical and quantum correlations [27] and therefore fails to be a good entanglement measure. For mixed states, a class of axiomatic entanglement measures is defined, based on the natural intuition that the closer the state is to a separable state, the less entangled it is. Therefore, these entanglement measures are built as the minimum distance  $\mathcal{D}$  between the given state  $\varrho$  and the set of separable states  $\mathcal{S}_{sep}$ , i.e.

$$E_{\mathcal{D}, \mathcal{S}_{sep}}(\varrho) = \inf_{\sigma \in \mathcal{S}_{sep}} \mathcal{D}(\varrho, \sigma). \quad (1.3)$$

In [32] it was shown that if one takes as distance  $\mathcal{D}$  in (1.3) the Bures metric<sup>3</sup> or the quantum relative entropy

$$S(\varrho||\sigma) := \text{Tr}[\sigma \log \sigma - \sigma \log \varrho], \quad (1.4)$$

which is well defined if  $\text{Supp}(\sigma) \subseteq \text{Supp}(\varrho)$ , then (1.3) indeed satisfies the conditions of being zero for separable states, unitarily invariant, monotone under LOCC and convex, and is thus a good entanglement measure<sup>4</sup>.

The measure based on the quantum relative entropy (1.4) is the so-called *relative entropy of entanglement*, and it will be considered in more detail in Section 1.3.2. Moreover, the quantum relative entropy is very important also in systems which are in contact with large heat baths since in this case, as shown in Section 6.3, this quantity is related to the free energy of the system. This concept, however, will be discussed more precisely in Chapter 6, after having described the dynamics of systems in contact with external baths in Chapters 2 and 4.

### Convex roof approach

For **mixed states** the situation is much more involved, because there are both classical and quantum correlations that must be distinguished between each other through an entanglement measure. Therefore, the generalization of a pure state entanglement measure to a mixed state entanglement measure is by no means straightforward. A proper

<sup>2</sup>In the case of mixed states, only some partial results exist for the relation between the properties of entanglement of a bipartite state and the mixedness of its reduced operators (see, e.g., [31]).

<sup>3</sup>The Bures metric is defined as  $B^2 := 2 - 2\sqrt{F(\varrho, \sigma)}$ , with  $F(\varrho, \sigma) = [\text{Tr}(\sqrt{\varrho\sigma\varrho})^{1/2}]^2$  the fidelity [33, 34].

<sup>4</sup>There exist some interesting results concerning the possibility of introducing geometric quantifications of entanglement in terms of relative entropies also for particular pure bipartite states (see, e.g., [35] for discrete systems and [36] for continuous variables systems).

method of obtaining entanglement measures for mixed states is the so-called *convex roof approach* [37], in which one starts by imposing a measure  $E$  on pure states and then extends it to mixed states in the following way.

Any mixed state  $\rho$  can be expressed as a convex sum of pure states  $|\psi_i\rangle$ :  $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ , with  $p_i \geq 0$ ,  $\sum_i p_i = 1$ . This decomposition, however, is not unique and different decompositions in general lead to different values for a given entanglement measure. Therefore, a proper, unambiguous generalization of a pure state entanglement measure consists in taking the infimum over all decompositions into pure states, i.e. the so-called *convex roof*:

$$E(\rho) = \inf \sum_i p_i E(\psi_i), \quad p_i \geq 0, \quad \sum_i p_i = 1.$$

The first entanglement measure to be constructed in this way was the so-called *entanglement of formation* [26], which is defined as the averaged von Neumann entropy of the reduced density matrices  $\rho_{i,red}$  of the pure states, minimized over all possible decompositions, i.e.

$$E_F(\rho) = \inf \sum_i p_i S(\rho_{i,red}). \quad (1.5)$$

It can be easily checked that this entanglement measure is convex and it has been proved to be monotone under LOCC [26], but it has recently been shown [38] not to be additive<sup>5</sup>, so it cannot be strictly considered an entanglement measure in the axiomatic sense.

For generic two-qubit states an explicit expression was found which leads to an easily computable formula of the entanglement of formation in this particular case [39, 40]: the entanglement measure thus obtained is the so-called *concurrence*, which will be described in detail in Section 1.3.3.

### Operational approach

This method of constructing entanglement measures is connected to the idea of quantifying entanglement with respect to its "usefulness" in terms of communication [23, 26]. The two main entanglement measures constructed in this way are the following [25, 28]:

- *Distillable entanglement*  $E_D$ , which quantifies the amount of maximal entanglement that can be extracted from a given entangled state, i.e. the ratio of maximally entangled output states  $\Phi_2^+$  over the needed input states  $\rho$ . Namely, starting from  $n$  copies of the given state  $\rho$  and having applied an LOCC operation  $\Lambda$ , one obtains the final state  $\sigma_n$ , which is required to approach the desired maximally entangled state  $(\Phi_2^+)^{\otimes m_n} = \Phi_{2^{m_n}}^+$  for large  $n$ . If this is impossible, then  $E_D = 0$ ; otherwise the rate of distillation is given by  $R_D := \lim_{n \rightarrow \infty} \frac{m_n}{n}$  and the distillable entanglement is

$$E_D(\rho) = \sup \{r : \lim_{n \rightarrow \infty} (\inf_{\Lambda} \|\Lambda(\rho^{\otimes n}) - \Phi_{2^{rn}}^+\|) = 0\},$$

<sup>5</sup>It has been recently proved [38] that the *entanglement of formation*  $E_F$  does not satisfy the additivity request, i.e.  $E_F(\rho \otimes \rho) < 2E_F(\rho)$ .

where  $\|\cdot\|$  is the trace norm.

- *Entanglement cost*  $E_C$ , which is dual to  $E_D$ , i.e. it measures how many maximally entangled states are needed in order to create an entangled state. In other terms, it quantifies the ratio of the number of maximally entangled input states  $\Phi_2^+$  over the produced output states  $\varrho$ , minimized over all LOCC operations, i.e.

$$E_C(\varrho) = \inf\{r : \lim_{n \rightarrow \infty} (\inf_{\Lambda} \|\Lambda(\varrho^{\otimes n}) - \Phi_{2^{rn}}^+\|) = 0\}.$$

### Some other entanglement measures

There exist many more entanglement measures and in this subsection a few of them, which for different reasons present an interest, will be briefly described.

*Negativity*: this simple computable measure was introduced in [41] and is defined as the sum of the negative eigenvalues of the partial transpose of the given state  $\varrho$ , i.e.  $\mathcal{N}(\varrho) = \sum_{\lambda < 0} \lambda$ . Further, the *logarithmic negativity*  $E_N(\varrho) := \log(\frac{\mathcal{N}(\varrho)+1}{2})$  was shown to be an upper bound for distillable entanglement [42].

It must be noted, however, that this entanglement measure vanishes for a particular class of entangled states [41], namely for PPT entangled states (see, e.g., [43]): indeed, these are entangled states which remain positive under the partial transposition operation, and therefore their partial transpose has no negative eigenvalues, leading to a vanishing *negativity*. Nevertheless, this measure and its logarithmic version are very commonly used quantities (see, e.g., [44–46]) since they have the major advantage that they can be computed straightforwardly, while many other entanglement measures cannot.

*Geometric measure of entanglement*: this entanglement measure is based on the idea of quantifying the degree to which a pure quantum state is entangled in terms of its distance or angle to the nearest unentangled state. The geometric measure of entanglement was first introduced in the setting of bipartite pure states [47] and then generalized to the multipartite setting [48]. Note that the geometric measure of entanglement differs from the measures proposed in [27] based on the minimal distance between the entangled mixed state and the set of separable *mixed* states, as the former is first defined as the minimal distance between the entangled *pure* state and the set of separable *pure* states, and then it is extended to mixed states by convex roof construction.

For an  $N$ -partite **pure** state  $|\psi\rangle$  the geometric measure of entanglement as a quantifier of global multi-partite entanglement <sup>6</sup> is defined as [49, 50]:

$$E_G(|\psi\rangle) := 1 - \max_{\phi} |\langle \phi | \psi \rangle|^2,$$

<sup>6</sup>A more detailed and interesting classification of the geometric measure of entanglement as *relative* (i.e. partition-dependent) and *absolute* (i.e. partition-independent) in the multipartite setting, which is a bit beyond this thesis, is given in [49].

where the maximum is taken with respect to all pure states that are fully factorized, i.e.  $|\phi\rangle = |\phi_1\rangle \otimes \cdots \otimes |\phi_N\rangle$ , with  $|\phi_j\rangle, j = 1, \dots, N$ , the single-qubit pure states.

Then the geometric measure of entanglement is extended to an  $N$ -partite **mixed** state  $\varrho$  by convex roof as follows [50]:

$$E(\varrho) := \min_{p_i, \psi_i} \sum_i p_i E_G(|\psi_i\rangle),$$

with the decomposition into pure states  $\varrho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ .

*Rains bound:* Rains [51] combined the two concepts of relative entropy of entanglement and negativity to define this measure as

$$E_R(\varrho) = \inf_{\sigma} (S(\varrho||\sigma) + \|\sigma^\Gamma\|),$$

where the infimum is taken over the set of all states,  $S(\varrho||\sigma)$  is the relative entropy,  $\sigma^\Gamma$  is the partial transpose of state  $\sigma$  and  $\|\cdot\|$  is the trace norm. Apart from being explicitly computable when the relative entropy and the negativity are, this entanglement measure is also the best known upper bound on distillable entanglement.

### 1.3.2 Relative entropy of entanglement

The definition of *relative entropy of entanglement* is based on distinguishability and geometrical distance [11]: the main idea is to compare a given quantum state  $\varrho$  of a bipartite system with separable states  $\sigma \in \mathcal{S}_{sep}$ , and then find the separable state that is closest to  $\varrho$ . Having taken the *relative entropy*  $S(\varrho||\sigma) := \text{Tr}[\sigma \log \sigma - \sigma \log \varrho]$  as the distance in (1.3), the definition of the *relative entropy of entanglement* is

$$E_{\mathcal{D}, \mathcal{S}_{sep}}(\varrho) = \inf_{\sigma \in \mathcal{S}_{sep}} \text{Tr}[\sigma \ln \sigma - \sigma \ln \varrho], \quad (1.6)$$

where  $\mathcal{S}_{sep}$  represents the set of separable states.

Although the relative entropy  $S(\varrho||\sigma)$  is not really a distance in the mathematical sense because it is not symmetric, nevertheless (1.6) defines a good entanglement measure that satisfies all the conditions listed in the previous section<sup>7</sup>. Moreover, for pure states the relative entropy of entanglement reduces to the entropy of entanglement [27], which is a satisfying property.

### 1.3.3 Concurrence

This entanglement measure was defined firstly for all mixed states of two qubits having no more than two non-zero eigenvalues [39] and then generalized to arbitrary states

<sup>7</sup>The additivity has only been confirmed numerically but all other properties have been proved analytically [11, 27]

of two qubits [40]. As mentioned in Section 1.3.1, the advantage of this entanglement measure lies in the fact that it is an explicit formulation of the *entanglement of formation* for two-qubit states and leads to an easily computable formula of the latter, as will be shown here.

This formula for entanglement makes use of the so-called spin-flip transformation, which for a pure state of a single qubit  $|\psi\rangle$  leads to

$$|\tilde{\psi}\rangle := \sigma_2 |\psi^*\rangle,$$

with  $|\psi^*\rangle$  the complex conjugate of  $|\psi\rangle$  and  $\sigma_2 \equiv \sigma_y$  the Pauli matrix, while for a mixed state of two qubits  $\varrho$  it leads to

$$\tilde{\varrho} := (\sigma_2 \otimes \sigma_2) \varrho^* (\sigma_2 \otimes \sigma_2),$$

with  $\varrho^*$  the complex conjugate of  $\varrho$ .

In [39, 40] it was shown that the entanglement of a **pure** two-qubit state can be written as

$$E(\psi) = \mathcal{E}(C(\psi)),$$

where the *concurrence*  $C$  is defined as

$$C(\psi) = |\langle \psi | \tilde{\psi} \rangle|, \quad (1.7)$$

and the function  $\mathcal{E}$  is given by

$$\mathcal{E}(C) = H\left(\frac{1 + \sqrt{1 - C^2}}{2}\right), \quad (1.8)$$

where  $H(x) := -x \log x - (1 - x) \log(1 - x)$  is the binary entropy.

For pure two-qubit states the concurrence can also be written explicitly as

$$C(\psi) = \sqrt{2(1 - \text{Tr}[\varrho_{red}^2])}, \quad (1.9)$$

with  $\varrho_{red}$  the reduced state. For two qubits this leads to  $C(\psi) = 2a_1 a_2$ , where  $a_1, a_2$  are the Schmidt coefficients of state  $|\psi\rangle$ .

Another simple explicit expression for the concurrence of a pure two-qubit state is in terms of the coefficients of the state written in the standard computational basis  $\{|0\rangle, |1\rangle\}$ :

$$C(\psi) = 2|a_{00}a_{11} - a_{01}a_{10}|, \quad (1.10)$$

for  $|\psi\rangle = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle$ .

Further, in [40] it was shown that the entanglement of formation for an arbitrary **mixed** state of two qubits can be written as

$$E(\varrho) = \mathcal{E}(C(\varrho)),$$

where  $\mathcal{E}$  is the function in (1.8) and the *concurrence* is defined as

$$C(\varrho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \quad (1.11)$$

with  $\lambda_i$ ,  $i = 1, \dots, 4$ , the eigenvalues of the Hermitian matrix  $R \equiv \sqrt{\sqrt{\varrho}\tilde{\varrho}\sqrt{\varrho}}$ , taken in decreasing order. Alternatively, the real non-negative numbers  $\lambda_i$  can be seen as the square roots of the eigenvalues of the non-Hermitian matrix  $\varrho\tilde{\varrho}$ , taken in decreasing order.

The importance of this entanglement measure lies not only in the fact that it leads to an explicit and easily computable formula for the entanglement of formation of arbitrary two-qubit states, but also in the fact that expression (1.9) can be generalized to define concurrence in higher dimensions.

## Chapter 2

# Open Quantum Systems

In this Chapter, *open quantum systems*, i.e. systems whose interaction with an external environment cannot be neglected, will be considered, and their dynamics will be described in some detail, following especially [5].

In particular, since in Chapters 3, 5 and 6 one- and two-qubit systems are mainly studied, in Section 2.2.3, the master equation and the dissipative term for one- and two-qubit systems immersed in an external bath will be given explicitly.

Then, in Section 2.3, the derivation of the asymptotic states of a dissipative dynamics will be given, again focusing mainly on particular one- and two-qubit cases of interest in this thesis.

### 2.1 Reversible and irreversible dynamics

In standard quantum mechanics the focus is mainly upon *closed* physical systems, i.e. systems which can be considered isolated from the external environment.

Considering a closed system of finite dimension  $n$  in a pure state  $|\psi_t\rangle$ , its dynamics is determined by a Hamiltonian operator  $H \in M_n(\mathbb{C})$  through the Schrödinger equation (setting  $\hbar = 1$ ):

$$\frac{\partial|\psi_t\rangle}{\partial t} = -iH|\psi_t\rangle. \quad (2.1)$$

For mixtures  $\varrho_t$ , this leads to the so-called Liouville-von Neumann equation on the state space  $\mathcal{S}$

$$\frac{\partial\varrho_t}{\partial t} = -i[H, \varrho_t], \quad (2.2)$$

whose solution, with initial condition  $\varrho_{t=0} = \varrho$ , is

$$\varrho_t = U_t\varrho U_{-t}, \quad U_t = e^{-iHt}. \quad (2.3)$$

Having denoted the dynamical map (2.3) by  $\varrho \mapsto \mathbf{U}_t[\varrho] := \varrho_t$ , and the linear action of

the generator on the left hand side of (2.2) by

$$\varrho \mapsto \mathbf{L}_H[\varrho] := -i[H, \varrho], \quad (2.4)$$

the Schrödinger unitary dynamics amounts to exponentiation of  $\mathbf{L}_H$ :

$$\varrho_t = \mathbf{U}_t[\varrho] = e^{t\mathbf{L}_H}[\varrho] = \sum_k \frac{t^k}{k!} \mathbf{L}_H \circ \mathbf{L}_H \circ \cdots \circ \mathbf{L}_H[\varrho],$$

where  $\circ$  indicates the composition of maps. Therefore, the dynamical maps  $\mathbf{U}_t$  form a one-parameter group of linear maps on the state space  $\mathcal{S}$ :  $\mathbf{U}_t \circ \mathbf{U}_s = \mathbf{U}_{t+s}$  for all  $t, s \in \mathbb{R}$ . This fact mathematically describes the *reversible* character of the Schrödinger dynamics, i.e. the fact that the dynamical maps  $\mathbf{U}_t$  can be inverted. Moreover, these maps preserve the spectrum of all states  $\varrho$ , leave the von Neumann entropy unchanged and transform pure states into pure states.

On the other hand, in this work *open* quantum systems will be considered, i.e. systems  $S$  whose interactions with the external environment  $E$ , in which they are immersed, cannot be neglected. Since, in principle, the environment consists of infinitely many degrees of freedom, the proper approach would be that of statistical mechanics [52, 53]; here, however, for sake of clarity, the environment will be described by density matrices  $\varrho_E$  in an infinite dimensional Hilbert space  $\mathcal{H}_E$ .

The compound system of the subsystem together with the environment,  $S + E$ , is a *closed* system whose Hilbert space is the tensor product  $\mathbb{C}^n \otimes \mathcal{H}_E$ , where  $\mathbb{C}^n$  is the Hilbert space of the  $n$ -dimensional subsystem. Therefore, a state  $\varrho_{S+E}$  belonging to the state space  $\mathcal{S}_{S+E}$  of the compound system will evolve reversibly under the action of a group of dynamical maps  $\mathbf{U}_t^{S+E} \equiv e^{t\mathbf{L}_{S+E}}$ . Formally, this group is generated by the exponentiation of the total generator  $\mathbf{L}_{S+E}[\varrho_{S+E}] := -i[H_{S+E}, \varrho_{S+E}]$ , where the total Hamiltonian is

$$H_{S+E} = H_S \otimes \mathbf{I}_E + \mathbf{I}_S \otimes H_E + \lambda H', \quad (2.5)$$

with  $H_S(\mathbf{I}_S)$ ,  $H_E(\mathbf{I}_E)$  the Hamiltonians (identity operators) pertaining to the subsystem, respectively, environment,  $H'$  the Hamiltonian describing the interaction between the subsystem and the environment, and  $\lambda$  an adimensional coupling constant. The total generator  $\mathbf{L}_{S+E}$  can thus be decomposed in the sum:

$$\mathbf{L} \equiv \mathbf{L}_{S+E} = \mathbf{L}_S + \mathbf{L}_E + \lambda \mathbf{L}'. \quad (2.6)$$

Often, when considering a system  $S$  immersed in an external environment, it is important to study the statistical properties of  $S$  alone, which are described by the state  $\varrho_S \in \mathcal{S}_S$ . As seen in Section 1.1.1, when dealing with compound systems, this can be



done by performing a partial trace over the degrees of freedom of the environment  $E$ , i.e.:

$$\mathcal{S}_{S+E} \ni \varrho_{S+E} \mapsto \varrho_S \equiv \text{Tr}_E[\varrho_{S+E}] = \sum_j \langle \psi_j^E | \varrho_{S+E} | \psi_j^E \rangle,$$

with  $\{|\psi_j^E\rangle\}$  an orthonormal basis in  $\mathcal{H}_E$ .

Analogously, it is often interesting to analyze only the dynamics of the state of the subsystem immersed in the external environment. Again, this can be done, in principle, by calculating the action of the total dynamical map on the total state and then taking the partial trace over the environment's degrees of freedom, i.e., given a state  $\varrho_S$  at time  $t = 0$ , the state of  $S$  at any time  $t$  is

$$\varrho_S(t) = \text{Tr}_E(\mathbf{U}_t^{S+E}[\varrho_{S+E}]).$$

On the other hand, the evolution of  $\varrho_S$  can be rewritten as the action of a family of maps on the initial state of the subsystem alone as:

$$\varrho_S(t) \equiv \mathbf{G}_t[\varrho_S].$$

In general these maps depend on  $\varrho_S$ , and in order for them to preserve the convex structure of the state space of the subsystem  $\mathcal{S}_S$ , i.e. to be such that

$$\mathbf{G}_t\left[\sum_j \lambda_j \varrho_S^j\right] = \sum_j \lambda_j \mathbf{G}_t[\varrho_S^j],$$

the initial state of the compound system must factorize [54]. This means that the subsystem and the environment must be initially uncorrelated and therefore that the initial state of the total system must be of the form  $\varrho_{S+E} = \varrho_S \otimes \varrho_E$ . Although this is not true in general, nevertheless this condition is fully consistent in many interesting physical contexts and gives rise to a family of dynamical maps  $\mathbf{G}_t$  which depend on the environment reference state  $\varrho_E$  but act linearly on the state space of the subsystem  $S$ .

Since  $\mathbf{G}_t[\varrho_S] \equiv \text{Tr}_E(\mathbf{U}_t^{S+E}[\varrho_{S+E}])$  and the partial trace breaks time-reversal symmetry, the family of maps  $\mathbf{G}_t$ ,  $t \geq 0$ , describes an *irreversible* dynamics. In general,  $\mathbf{G}_t \circ \mathbf{G}_s \neq \mathbf{G}_{t+s}$ , for  $t, s \geq 0$ , and therefore this family lacks a semigroup composition law. If, however, the interaction of the open quantum system with the environment is weak or the environment time-correlations decay rapidly with respect to the time-variation of the subsystem, then the equality holds,  $\mathbf{G}_t \circ \mathbf{G}_s = \mathbf{G}_{t+s}$ , for  $t, s \geq 0$ , and this indicates the absence of cumulative memory effects. The technical procedures to eliminate the latter, and thus recover semigroups of dynamical maps as reduced time-evolutions for the subsystem alone, are known as *Markovian approximations* and will be discussed in the next section.

As seen in Chapter 1, in order to have physical consistency, the linear map  $\mathbf{G}_t$  must be completely positive. From Theorem 2 it follows that

$$\varrho_S \mapsto \mathbf{G}_t[\varrho_S] = \sum_i V_i(t) \varrho_S V_i^\dagger(t), \quad (2.7)$$

with  $V_i(t) \in M_n(\mathbb{C})$ . Indeed, the evolved state of the subsystem alone can be obtained by partial trace over the environment degrees of freedom as  $\varrho_S(t) = \text{Tr}_E(\mathbf{U}_t^{S+E}[\varrho_{S+E}])$  and, having taken a factorized initial compound state  $\varrho_{S+E} = \varrho_S \otimes \varrho_E$ , it follows that

$$\begin{aligned} \varrho_S(t) &= \text{Tr}_E(\mathbf{U}_t^{S+E}[\varrho_S \otimes \varrho_E]) = \sum_{j,k} r_k^E \langle r_j^E | U_t^{S+E} | r_k^E \rangle \varrho_S \langle r_k^E | U_t^{S+E} | r_j^E \rangle \\ &= \sum_i V_i(t) \varrho_S V_i^\dagger(t), \end{aligned} \quad (2.8)$$

where  $\{|r_j^E\rangle\}$  form a basis of eigenvectors of  $\varrho_E$  with corresponding eigenvalues  $r_j^E$  and  $V_i(t) := \sqrt{r_k^E} \langle r_j^E | U_t^{S+E} | r_k^E \rangle$ . Therefore the complete positivity of the map  $\mathbf{G}_t$  follows from Theorem 2 in Chapter 1.

## 2.2 Reduced dynamics

The completely positive maps  $\mathbf{G}_t$  give a physically consistent description of the dynamics of a system  $S$  interacting with an environment  $E$ , with the only necessary condition that the total initial state be factorized,  $\varrho_{S+E} = \varrho_S \otimes \varrho_E$ : this description is closed, i.e. it depends linearly on the initial state and can be expressed in terms of operators pertaining to  $S$  alone.

From the definition  $V_i(t) := \sqrt{r_k^E} \langle r_j^E | U_t^{S+E} | r_k^E \rangle$  in (2.8) it is evident that the operators  $V_i(t)$  describe the dissipative and noisy effects due to the environment; therefore, since the family of maps  $\mathbf{G}_t$  can contain memory effects, in general it is not straightforward to obtain the reduced dynamics of the subsystem  $S$  alone. If, however, the interaction between subsystem and environment is sufficiently weak or the environment time-correlations decay rapidly with respect to the time-variation of the subsystem, then not only can the dynamics of  $S$  be considered disentangled from that of the total system, but also approximately described by a one-parameter semigroup of maps  $\gamma_t$  such that  $\gamma_t \circ \gamma_s = \gamma_{t+s}$  for  $t, s \geq 0$ . The fact of the maps  $\gamma_t$  forming a semigroup, and therefore satisfying only a forward-in-time composition law, reflects the *irreversible* character of the subsystem's dynamics.

In order to reveal the memory effects due to the environment and contained in the family of maps  $\mathbf{G}_t$ , it is convenient to write the formal integro-differential evolution equation of which  $\mathbf{G}_t$  are solutions. This equation is derived via the so-called *projection technique* [2, 3] and leads to master equations of the form

$$\frac{\partial \varrho_t}{\partial t} = \mathbf{L}_H[\varrho_t] + \mathbf{D}[\varrho_t]. = -i[H_{eff}, \varrho_t] + \mathbf{D}[\varrho_t] \quad (2.9)$$

Here both operators  $\mathbf{L}_H$  and  $\mathbf{D}$  act on the subsystem's state space  $\mathcal{S}_S$ :  $\mathbf{L}_H$  acts as in (2.4),  $\mathbf{L}_H[\varrho_t] = -i[H_{eff}, \varrho_t]$  with the effective Hamiltonian  $H_{eff} = H_{eff}^\dagger \in M_n(\mathbb{C})$ , whereas  $\mathbf{D}$  is a linear operator which cannot be written in commutator form and contains the dissipative and noisy effects due to the environment. Master equations of the form (2.9) can be derived with several so-called Markovian approximations, as will be seen in Section 2.3. Solving (2.9), the reduced dynamics of the subsystem  $S$  is described in terms of a semigroup of linear maps  $\gamma_t, t \geq 0$ , on  $\mathcal{S}_S$ , obtained by exponentiation of the generator:

$$\gamma_t = e^{t(\mathbf{L}_H + \mathbf{D})}. \quad (2.10)$$

In the next section, the conditions to ensure the physical consistency of the semigroup of linear maps  $\gamma_t$  will be given, focusing in particular on the property of complete positivity. Then, in Section 2.2.2, the detailed derivation of the master equation (2.9) will be described.

### 2.2.1 Abstract form of the generators of dynamical semigroups

In this section some conditions on the semigroups of maps  $\gamma_t$  will be given, in order to guarantee their full physical consistency.

First of all, it must be noted that the existence of a generator and an exponential structure as in (2.10) is due to the time-continuity of the semigroup of maps  $\gamma_t$  [55], i.e.:

$$\lim_{t \rightarrow 0} \|\gamma_t[\varrho] - \varrho\| = 0 \quad \forall \varrho \in \mathcal{S}_S,$$

with  $\|X\| = \text{Tr}\sqrt{X^\dagger X}$ ,  $X \in M_n(\mathbb{C})$ .

Further, the semigroup of maps  $\gamma_t$  must satisfy three constraints in order to be physically consistent.

Firstly, since they map states into states, they must preserve the hermiticity of density matrices.

Secondly, they must preserve the trace: this means that the overall probability is constant, so phenomena with loss of probability, such as particle decays, will not be considered.

This constraint corresponds to the request of *unitality* for the dual map, i.e.  $\gamma_t^*[I_d] = I_d$ , where  $I_d$  is the  $d \times d$  identity matrix and  $\gamma_t^*$  is as in Definition 11.

These first two constraints are sufficient to partially fix the form of the generator [56], as shown in the following theorem.

**Theorem 7** *Let  $\gamma_t : M_d(\mathbb{C}) \mapsto M_d(\mathbb{C})$ ,  $t \geq 0$ , form a time-continuous semigroup of hermiticity-preserving and trace-preserving linear maps. Then the semigroup can be written as  $\gamma_t = e^{t(\mathbf{L}_H + \mathbf{D})}$ , where the action of the two terms of the generator on any density matrix  $\varrho \in \mathcal{S}_S$  is*

$$\mathbf{L}_H[\varrho] = -i[H, \varrho], \quad (2.11)$$

$$\mathbf{D}[\varrho] = \sum_{i,j=1}^{d^2-1} K_{ij} \left( F_j^\dagger \varrho F_i - \frac{1}{2} \{F_i F_j^\dagger, \varrho\} \right). \quad (2.12)$$

The matrix of coefficients  $K \equiv [K_{ij}]$  (the so-called Kossakowski matrix) is Hermitian,  $H = H^\dagger$  is the effective Hamiltonian,  $\{F_j\}_{j=0}^{d^2-1}$  with  $F_0 := I_d/\sqrt{d}$  form an orthonormal set of  $d \times d$  matrices such that  $\text{Tr}[F_i F_j] = \delta_{ij}$ , and  $\{ , \}$  represents anticommutation.

The third constraint is that the  $\gamma_t$ 's be positive maps, i.e. that they transform positive matrices into positive matrices. As seen in the first chapter, this is a necessary condition for physical consistency, in order to preserve the positivity of the spectrum of every density matrix and thus not contradict the statistical interpretation of the eigenvalues as probabilities. As previously seen, though, positivity of the maps  $\gamma_t$  is not sufficient to guarantee their physical consistency in the case of the coupling of system  $S$  to an ancilla: for full physical consistency,  $\gamma_t$  must be completely positive.

Positivity and complete positivity of the maps  $\gamma_t$  both depend on the properties of the Kossakowski matrix  $K \equiv [K_{ij}]$ . On one hand, though, since positivity preservation results in an intricate algebraic problem, there are no necessary conditions, but only sufficient ones, on the coefficients  $K_{ij}$  to give rise to positivity-preserving semigroups  $\gamma_t$  [7, 22, 57, 58]. While on the other hand, the condition for  $\gamma_t$  to be completely positive has been proved both for finite-dimensional [59] and infinite [56] systems, under the assumption of boundedness of the generator, and reads:

**Theorem 8** *The semigroup  $\{\gamma_t\}_{t \geq 0}$  consists of completely positive maps if and only if the Kossakowski matrix is positive semi-definite.*

Generators with positive semi-definite Kossakowski matrix are the so-called Kossakowski-Lindblad generators and the resulting semigroups are known as quantum dynamical semigroups.

The physical meaning of the different terms in the master equation

$$\mathbf{L}[\varrho] = -i[H, \varrho] + \sum_{i,j=1}^{d^2-1} K_{ij} \left( F_j^\dagger \varrho F_i - \frac{1}{2} \{F_i F_j^\dagger, \varrho\} \right) \quad (2.13)$$

can be viewed as follows, distinguishing between the dissipative and the noisy contributions of the environment.

- Having set  $W := \sum_{i,j=1}^{d^2-1} K_{ij} F_i F_j^\dagger$ , the anticommutator in (2.13) together with the Hamiltonian term can be incorporated in a pseudo-commutator:

$$-i[H, \varrho] + \frac{1}{2} \sum_{i,j=1}^{d^2-1} K_{ij} \{F_i F_j^\dagger, \varrho\} = -i \left( H - \frac{i}{2} W \right) \varrho + i \varrho \left( H + \frac{i}{2} W \right).$$

This represents damping and this term alone leads to a decrease of the trace of  $\varrho$ : indeed, this is the typical expression for the generator of a decaying system and  $W$  describes the loss of probability that is irreversibly transferred from the system  $S$  to the decay products.

- The remaining terms in (2.13), in the case of a completely positive map  $\gamma_t$ , can be cast into Kraus-Stinespring form and are the analog of the diffusive effect of white noise in classical Brownian motion [60]. The trace-preserving character of  $\gamma_t$  is guaranteed by the sum of all contributions in the master equation (2.13).

## 2.2.2 Master equation and Markovian approximations

As mentioned in Sections 2.1 and 2.2, master equations of the form (2.9) for the subsystem alone are derived starting from the global time-evolution equation

$$\partial_t \varrho_{S+E}(t) = \mathbf{L}_{S+E}[\varrho_{S+E}(t)], \quad (2.14)$$

applying the so-called *projection technique* [2, 3], which consists in tracing away the environment degrees of freedom, and then performing certain so-called Markovian approximations [4, 61, 62], i.e. studying the evolution on a slow time-scale and neglecting fast decaying memory effects.

The total generator in (2.14) is taken to be as in (2.6) and correspondingly the total Hamiltonian is as in (2.5). In particular, the interaction Hamiltonian is assumed to be of the form

$$H' = \sum_{\alpha} V_{\alpha} \otimes B_{\alpha}, \quad (2.15)$$

where  $V_{\alpha}$  and  $B_{\alpha}$  are Hermitian operators acting on the Hilbert spaces  $\mathbb{C}^d$  of  $S$  and  $\mathcal{H}_E$  of  $E$ , respectively. It is more convenient to define *centered environment operators*  $\tilde{B}_{\alpha} := B_{\alpha} - \text{Tr}_E[B_{\alpha}]$ , which lead to a new Hamiltonian for the subsystem  $S$  and a new interaction term<sup>1</sup>:

$$H_S^{\lambda} = H_S + \underbrace{\sum_{\alpha} V_{\alpha} \text{Tr}_E(B_{\alpha})}_{H_S^{(1)}}, \quad \tilde{H}' = \sum_{\alpha} V_{\alpha} \otimes \tilde{B}_{\alpha}, \quad \text{Tr}_E[\varrho_E \tilde{B}_{\alpha}] = 0. \quad (2.16)$$

Obtaining a physically consistent Markovian approximation for the master equation (2.9) for the state of the subsystem is no easy task [4, 61–63]. This is due to the fact that the dynamics of the system  $S$  alone, generated by  $H_S$ , in general does not commute with the interaction with the bath. Therefore, there exists another time-scale  $\tau_S$  in the problem and, in order to have a clear separation between the dynamics of the subsystem and that of the environment, a hierarchy condition for the time-scales,  $\tau_E \ll \tau_S$ , needs to be satisfied.

Now, following [64], the two most commonly used Markovian approximations, namely the *weak coupling* and the *singular coupling* limits, will be described in some detail. The focus will be mainly on the physical consistency, especially on the property of complete positivity, of the derived reduced dynamics for the subsystem.

<sup>1</sup>The redefinition of the subsystem Hamiltonian  $H_S$  amounts to a Lamb shift of the energy levels due to a mean-field, first order in  $\lambda$  approximation of the interaction with the environment  $E$ .

### Weak coupling limit

The first approximation is based on one of the simplest assumptions that allow to distinguish between the subsystem and the environment, namely the hypothesis of *weak coupling* between the two. This condition translates to a very small coupling constant, i.e.  $\lambda \ll 1$ . Moreover, the environment and subsystem time-scales must be such that their ratio  $\tau_E/\tau_S$  is very small, and in this case this is achieved with  $\tau_S \rightarrow \infty$  while  $\tau_E$  remains finite.

Since the coupling constant  $\lambda$  is assumed to be small, the dissipative character of the dynamics emerges on a slow time-scale  $\tau := \lambda^2 t$ . So, concretely, this Markovian approximation consists in:

1. substituting  $\tau/\lambda^2$  for  $t$  in the integro-differential expression for the master equation (see, e.g., [5]);
2. letting  $\lambda \rightarrow 0$ , which permits to perform the so-called *rotating-wave approximation* [65, 66].

Then, given a system-environment interaction of the form (2.16), the time-evolved operators

$$V_\alpha(t) \equiv e^{-t\mathbf{L}_S}[V_\alpha] = e^{itH_S}V_\alpha e^{-itH_S}, \quad \tilde{B}_\alpha(t) \equiv e^{-t\mathbf{L}_E}[\tilde{B}_\alpha] = e^{itH_E}\tilde{B}_\alpha e^{-itH_E} \quad (2.17)$$

are defined, and then the two-point correlation functions

$$G_{\alpha\beta} \equiv \text{Tr}[\varrho_E \tilde{B}_\alpha(s) \tilde{B}_\beta] = \text{Tr}[\varrho_E \tilde{B}_\alpha \tilde{B}_\beta(-s)]$$

are introduced.

The structure of the environment-induced second order effects in the dissipative term are thus of the form:

$$\mathbf{D}[\varrho_S(t)] = - \sum_{\alpha,\beta} \int_0^\infty ds \left\{ G_{\alpha\beta}(s) [V_\alpha(s), V_\beta \varrho_S(t)] + G_{\beta\alpha}(-s) [\varrho_S(t) V_\beta, V_\alpha(s)] \right\}. \quad (2.18)$$

From standard Fourier analysis it follows that [61]

$$\int_0^\infty dt e^{it\omega} G_{\alpha\beta}(t) = \frac{h_{\alpha\beta}(\omega)}{2} + i s_{\alpha\beta}(\omega),$$

where

$$h_{\alpha\beta}(\omega) := \int_{-\infty}^{+\infty} dt e^{it\omega} G_{\alpha\beta}(t) = h_{\beta\alpha}^*(\omega)$$

is a positive semi-definite matrix for every  $\omega$  [61], while

$$s_{\alpha\beta}(\omega) := \frac{1}{2\pi} \mathcal{P} \int_{-\infty}^{+\infty} dw \frac{h_{\alpha\beta}(w)}{w - \omega} = s_{\beta\alpha}^*(\omega)$$

with  $\mathcal{P}$  indicating the principal value.

The dissipative contribution can thus be written in terms of the Fourier transforms of the environment two-point correlation functions, as follows:

$$\begin{aligned} \tilde{\mathbf{D}}[\varrho_S] &= -i \left[ \underbrace{\sum_{\alpha,\beta} \sum_{\omega} s_{\alpha\beta}(\omega) V_{\alpha}(\omega) V_{\beta}^{\dagger}(\omega)}_{H_E^{(2)}}, \varrho_S \right] \\ &+ \underbrace{\sum_{\alpha,\beta} \sum_{\omega} h_{\alpha\beta}(\omega) \left( V_{\beta}^{\dagger}(\omega) \varrho_S V_{\alpha}(\omega) - \frac{1}{2} \{V_{\alpha}(\omega) V_{\beta}^{\dagger}(\omega), \varrho_S\} \right)}_{\mathbf{D}_2}. \end{aligned}$$

This leads to the explicit form of the generator, which can be written as:

$$\begin{aligned} \partial_t \varrho_S(t) &= \mathbf{L}_S^{\lambda}[\varrho_S(t)] + \lambda^2 \tilde{\mathbf{D}}[\varrho_S(t)] \\ &= -i[H_S + \lambda H_E^{(1)} + \lambda^2 H_E^{(2)}, \varrho_S(t)] + \lambda^2 \mathbf{D}_2[\varrho_S(t)]. \end{aligned} \quad (2.19)$$

From this equation it can be seen that the environment's contributions are present not only in the second-order dissipative term  $\mathbf{D}_2$ , but also in a first-order mean-field term  $H_E^{(1)}$  and a second-order term  $H_E^{(2)}$  which lead to the redefinition of an effective Hamiltonian for the subsystem  $S$ .

Most importantly, the positivity of the Kossakowski matrices  $[h_{\alpha\beta}(\omega)]$  [61] guarantees the complete positivity, and thus the physical consistency, of this Markovian approximation.

### Singular coupling limit

The Markovian approximation obtained in the singular coupling limit also follows from an assumption concerning the time-scales of the subsystem and the environment. Namely, in the singular coupling regime, it is assumed that the decay time of correlations in the environment become small, i.e.  $\tau_E \rightarrow 0$ , while the typical variation time of the subsystem,  $\tau_S$ , remains constant. This translates to two-point correlation functions that tend to Dirac deltas in the dissipative terms [59, 67, 68], i.e.  $G_{\alpha\beta}(t) \rightarrow C_{\alpha\beta} \delta(t)$ , and this physically means that the effects of the environment are felt on time-scales of order  $t$ , while in the weak coupling limit the relevant time-scale is  $t/\lambda^2$ .

In this regime the total Hamiltonian (2.5) is rescaled as follows [4]:

$$H_{S+E} = H_S \otimes \mathbf{I}_E + \epsilon^{-2} \mathbf{I}_S \otimes H_E + \epsilon^{-1} \tilde{H}', \quad (2.20)$$

where the interaction Hamiltonian is as in (2.16),  $\tilde{H}' = \sum_{\alpha} V_{\alpha} \otimes \tilde{B}_{\alpha}$ , with centered environment operators  $\tilde{B}_{\alpha}$ . This leads to a dissipative term of the form

$$\hat{\mathbf{D}}[\varrho_S(t)] = - \sum_{\alpha,\beta} \int_0^{\infty} ds \left\{ G_{\alpha\beta}(s) [V_{\alpha}, V_{\beta} \varrho_S(t)] + G_{\beta\alpha}(-s) [\varrho_S(t) V_{\beta}, V_{\alpha}] \right\}. \quad (2.21)$$

Then, as in the weak coupling regime, the environment two-point correlation functions can be written as

$$\int_0^\infty dt G_{\alpha\beta}(t) = \frac{h_{\alpha\beta}}{2} + is_{\alpha\beta},$$

so that (2.21) can be split into two terms, one for the second-order Hamiltonian contribution with  $H_E^{(2)} = \sum_{\alpha,\beta} s_{\alpha\beta} V_\alpha V_\beta$ , and the other representing the true dissipative contribution:

$$\mathbf{D}[\varrho_S] = \sum_{\alpha,\beta} h_{\alpha\beta} \left( V_\beta \varrho_S V_\alpha - \frac{1}{2} \{V_\alpha V_\beta, \varrho_S\} \right). \quad (2.22)$$

This yields the following master equation for the subsystem:

$$\partial_t \varrho_S(t) = -i[H_S + H_E^{(2)}, \varrho_S(t)] + \mathbf{D}[\varrho_S(t)]. \quad (2.23)$$

As for the weak coupling limit, also the singular coupling limit leads to a generator of the Lindblad form (2.13) with a positive semi-definite Kossakowski matrix and thus to a dissipative semigroup of completely positive maps. It must be noted, however, that unlike the weak coupling regime, in the singular coupling regime:

- the operators in the dissipative term  $\mathbf{D}$  in (2.22) are Hermitian;
- thermal Bose or Fermi heat baths are physically consistent only if their temperature is infinite [62, 67, 68], since the two-point correlation functions tend to Dirac deltas in time only if their Fourier transforms tend to a constant.

Moreover, it can be seen that, by going to the slow time  $\tau := \epsilon^2 t$ , the total Hamiltonian (2.20) becomes

$$H_{S+E} = \epsilon^2 H_S \otimes \mathbf{I}_E + \mathbf{I}_S \otimes H_E + \epsilon \tilde{H}',$$

which shows that the singular coupling limit amounts to a weak coupling limit where the free motion generated by the system Hamiltonian  $H_S$  is of the same order as the dissipative effects [4, 69].

### 2.2.3 One- and two-qubit systems

Since most of this PhD work is dedicated to one- and two-qubit systems, in this section the subsystem  $S$  will firstly be taken to be a qubit, which physically could represent a two-level atom, and then will be taken to consist of two qubits.

#### One-qubit system

In this case the system Hilbert space is two-dimensional  $\mathcal{H}_S \equiv \mathbb{C}^2$ . Since the algebra of observables  $M_2(\mathbb{C})$  is linearly spanned by the  $2 \times 2$  identity matrix  $\sigma_0 := I_2$  and the three Pauli matrices  $\sigma_i$ ,  $i = 1, 2, 3$ , the subsystem operators can be written in the basis



$\{\sigma_\mu\}_{\mu=0}^3$  both for the Hamiltonian term  $H_S$  and for the dissipative contribution; the latter, in particular, can be written as in (2.13) with operators  $F_j \equiv \frac{1}{\sqrt{2}}\sigma_j$ ,  $j = 1, 2, 3$ .

Having performed the *weak coupling limit* techniques, the resulting master equation for the subsystem of one qubit is found to be in Kossakowski-Lindblad form:

$$\frac{\partial \varrho_S(t)}{\partial t} = -i[H_{eff}, \varrho_S(t)] + \mathbf{D}^{(1)}[\varrho_S(t)], \quad (2.24)$$

where  $H_{eff}$  is the subsystem effective Hamiltonian and the dissipative term reads

$$\mathbf{D}^{(1)}[\varrho_S] = \sum_{i,j=1}^3 K_{ij} \left( \sigma_j \varrho_S \sigma_i - \frac{1}{2} \{ \sigma_i \sigma_j, \varrho_S \} \right), \quad (2.25)$$

with  $\sigma_i$ ,  $i = 1, 2, 3$ , the Pauli matrices.

The effective Hamiltonian  $H_{eff}$  and the coefficients  $K_{ij}$  of the  $3 \times 3$  Kossakowski matrix are determined by the Hilbert, respectively Fourier transform of the field correlations, and the Kossakowski matrix  $K \equiv [K_{ij}]$  is proved to be positive semi-definite [5]: therefore, the dynamical semigroup generated by (2.24) consists of completely positive maps and thus leads to a physically consistent evolution.

## Two-qubit system

Here a system of two non-interacting two-level atoms immersed in a common bath consisting of a collection of free, independent, scalar fields will be considered: in particular, the master equation and the explicit expression for the dissipative term will be written in the *weak coupling limit*.

Given the two atoms, the total system Hamiltonian will be the sum of two terms:

$$H_S = H_S^{(1)} + H_S^{(2)}, \quad H_S^{(1)} = \frac{\omega}{2} \sum_{i=1}^3 n_i (\sigma_i \otimes I_2), \quad H_S^{(2)} = \frac{\omega}{2} \sum_{i=1}^3 n_i (I_2 \otimes \sigma_i), \quad (2.26)$$

where  $\omega$  is the system frequency, having taken the frequencies of the two atoms to be the same  $\omega_1 = \omega_2 \equiv \omega$ ,  $n_i$  and  $\sigma_i$ ,  $i = 1, 2, 3$ , are the components of a unit vector and the Pauli matrices, respectively, and  $I_2$  is the  $2 \times 2$  identity matrix.

On the other hand, the atoms-bath interaction is described by the Hamiltonian

$$H' = \sum_{i=0}^3 [(\sigma_i \otimes I_2) \otimes \Phi_i(x) + (I_2 \otimes \sigma_i) \otimes \Psi_i(x)], \quad (2.27)$$

where  $\sigma_0 \equiv I_2$  and  $\Phi_i(x)$ ,  $\Psi_i(x)$  are the field operators. In the expression (2.27) for the interaction Hamiltonian it has been assumed that the two atoms are point-like and taken to be in the same position [5]. Moreover, if the two atoms are supposed to be identical, the field operators can be taken the same, i.e.  $\Phi_i = \Psi_i$ .

Having performed the standard *weak coupling limit* techniques, the two-atom state is represented by a  $4 \times 4$  density matrix  $\varrho_S(t)$  which evolves in time according to a quantum dynamical semigroup of completely positive maps generated by a master equation in Kossakowski-Lindblad form:

$$\frac{\partial \varrho_S(t)}{\partial t} = -i[H_{eff}, \varrho_S(t)] + \mathbf{D}^{(2)}[\varrho_S(t)]. \quad (2.28)$$

In the first, unitary term on the right-hand side the effective Hamiltonian appears, which is the sum of  $H_S$  in (2.26) and suitable Lamb contributions, as seen in (2.16):  $H_{eff} = H_{eff}^{(1)} + H_{eff}^{(2)} + H_{eff}^{(12)}$ . While the first two terms in this sum are single-atom contributions,

$$H_{eff}^{(1)} = \sum_{i=1}^3 H_i^{(1)}(\sigma_i \otimes I_2), \quad H_{eff}^{(2)} = \sum_{i=1}^3 H_i^{(2)}(I_2 \otimes \sigma_i), \quad H_{eff}^{(1,2)} \in \mathbb{R}, \quad (2.29)$$

the third term represents a field-generated direct two-atom coupling, which can be written as

$$H_{eff}^{(12)} = \sum_{i,j=1}^3 H_{ij}^{(12)}(\sigma_i \otimes \sigma_j), \quad H_{ij}^{(12)} \in \mathbb{R}. \quad (2.30)$$

The second term on the right-hand side of (2.28), instead, represents the dissipative contribution and can be written as in (2.13)

$$\mathbf{D}^{(2)}[\varrho_S] = \sum_{\alpha,\beta=1}^6 K_{\alpha\beta} \left[ F_\beta \varrho_S F_\alpha - \frac{1}{2} \{F_\alpha F_\beta, \varrho_S\} \right], \quad (2.31)$$

with the  $4 \times 4$  matrices  $F_\alpha := \sigma_\alpha \otimes I_2$  for  $\alpha = 1, 2, 3$  and  $F_\alpha := I_2 \otimes \sigma_\alpha$  for  $\alpha = 4, 5, 6$ . The Kossakowski matrix is thus a  $6 \times 6$  positive semi-definite matrix which can be written as

$$K = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^\dagger & \mathcal{C} \end{pmatrix}, \quad (2.32)$$

where  $\mathcal{A} = \mathcal{A}^\dagger$ ,  $\mathcal{C} = \mathcal{C}^\dagger$  and  $\mathcal{B}$  are  $3 \times 3$  matrices that can be used to decompose the dissipative term (2.31) explicitly as follows (where  $\varrho := \varrho_S$  to make the notation less cumbersome):

$$\begin{aligned} \mathbf{D}^{(2)}[\varrho] &= \sum_{i,j=1}^3 \left( \mathcal{A}_{ij} \left[ (\sigma_j \otimes I_2) \varrho (\sigma_i \otimes I_2) - \frac{1}{2} \{(\sigma_i \sigma_j \otimes I_2), \varrho\} \right] \right. \\ &+ \mathcal{C}_{ij} \left[ (I_2 \otimes \sigma_j) \varrho (I_2 \otimes \sigma_i) - \frac{1}{2} \{(I_2 \otimes \sigma_i \sigma_j), \varrho\} \right] \\ &+ \mathcal{B}_{ij} \left[ (\sigma_j \otimes I_2) \varrho (I_2 \otimes \sigma_i) - \frac{1}{2} \{(\sigma_j \otimes \sigma_i), \varrho\} \right] \\ &\left. + \mathcal{B}_{ji}^* \left[ (I_2 \otimes \sigma_j) \varrho (\sigma_i \otimes I_2) - \frac{1}{2} \{(\sigma_i \otimes \sigma_j), \varrho\} \right] \right). \end{aligned} \quad (2.33)$$

As in the single-atom case, the environment contributions to the effective Hamiltonian  $H_{eff}$  and the entries of the Kossakowski matrix (2.32) are given by the Hilbert, respectively Fourier transforms of the field correlation functions.

The first two contributions in (2.33) are dissipative terms affecting the first, respectively second, atom in absence of the other; while the last two pieces represent the way in which the noise generated by the external fields may correlate the two, otherwise independent, atoms. In Chapter 4, a sufficient condition for the environment to create entanglement in an initially separable two-qubit state immersed within it will be presented and then, in Chapter 5, this condition will be shown to be also necessary; further, in Chapter 5, the sufficient condition from Chapter 4 will be generalized to higher-dimensional bipartite systems.

### 2.3 Asymptotic states

So far dynamical semigroups  $\gamma_t : \mathcal{S}_d \rightarrow \mathcal{S}_d$  acting on the state space have been analyzed. In the case of a finite dimensional Hilbert space, as those considered in this thesis, there always exists at least one stationary state [5]; indeed, in finite dimension the ergodic average of the action of a completely positive one-parameter semigroup on any initial state always exists and the result is clearly a stationary state:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^\infty \gamma_t[\varrho_{in}] dt := E[\varrho_{in}].$$

The approach to equilibrium of semigroups with Kossakowski-Lindblad generator has been studied in general and some rigorous mathematical results are available [4, 70–72]. Some of these results will be presented here and then adapted to particular one- and two-qubit systems of interest for this thesis.

In order to find the explicit expression for the asymptotic state in the cases when this is possible, it is necessary to give some preliminary definitions from the general theory [70–72].

Firstly, it must be noted that the map  $\gamma_t^* : M_d \rightarrow M_d$ , dual to  $\gamma_t$ , will be considered. It is possible to define a conditional expectation through the ergodic average, as follows:

$$M_d \ni X \mapsto \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^\infty \gamma_t^*[X] dt := E^*[X]. \quad (2.34)$$

It can be proved [72] that  $E^*$  is completely positive and maps  $M_d$  into  $\mathcal{M}(\gamma) := \{X \in M_d \mid \gamma_t^*[X] = X \forall t \geq 0\}$ , where the set of fixed points of  $\gamma_t^*$ ,  $\mathcal{M}(\gamma)$ , is a  $C^*$ -algebra [71–73].

The conditional expectation  $E^*$  has the following two important properties:

1. from duality:  $\text{Tr}(E[\varrho]X) = \text{Tr}(\varrho E^*[X])$ ,  $X \in M_d$ ,  $\varrho \in \mathcal{S}_d$ ;
2.  $E^*[X_1 Y X_2] = X_1 E^*[Y] X_2$ ,  $\forall X_{1,2} \in \mathcal{M}(\gamma)$ ,  $Y \in M_d$ .

Further, the following quantities will be useful: the so-called *dissipation function* defined on  $\mathcal{M} \times \mathcal{M}$  with values in  $\mathcal{M}$  (where  $\mathcal{M}$  is the von Neumann algebra to which  $\gamma_t^*$  belongs)

$$\dot{D}_t(X, X)|_{t=0} = \mathbf{L}^*[X^\dagger X] - \mathbf{L}^*[X^\dagger]X - X^\dagger \mathbf{L}^*[X],$$

and its integrated form

$$D_t(X, Y) := \gamma_t^*[X^\dagger Y] - \gamma_t^*[X^\dagger]\gamma_t^*[Y].$$

In general  $D_t(X, X) \geq 0$  for all  $X \in \mathcal{M}, t \geq 0$ ; denoting by

$$\mathcal{N}(\gamma) := \{X \in \mathcal{M} \mid D_t(X, X) = 0 \forall t \geq 0\}$$

the null space of  $\{D_t \mid t \geq 0\}$  and taking  $\mathbf{L}^*[X] = i[H, X] + \sum_i (V_i^\dagger X V_i - \frac{1}{2}\{V_i^\dagger V_i, X\})$ , with  $V_i \in \mathcal{M}$ , one gets

$$0 = \dot{D}_t(X, X)|_{t=0} = \sum_i [X, V_i]^\dagger [X, V_i],$$

which holds true if and only if  $[X, V_i] = 0 \forall i$ . Therefore the null space of  $\{D_t \mid t \geq 0\}$  consists of all  $X \in \mathcal{M}$  which commute with all operators  $V_i$ . Let this subset be denoted by  $\{V_i\}'$ ; it is a subalgebra of  $\mathcal{M}$  and it satisfies the following inclusions [72]:

$$\mathcal{M}(\gamma) \subseteq \mathcal{N}(\gamma) \subseteq \ker \dot{D}.$$

In particular, if  $X \in \{V_i, H\}'$ , then automatically  $\mathbf{L}^*[X] = 0$ , and this implies that  $X \in \mathcal{M}(\gamma)$ . Moreover, in general,  $\{V_i, H\}' \subseteq \mathcal{M}(\gamma)$ ; thus, if  $\{V_i\}' \subseteq \{V_i, H\}'$ , then the following holds true:

$$\mathcal{M}(\gamma) = \mathcal{N}(\gamma) = \ker \dot{D}. \quad (2.35)$$

### 2.3.1 One-qubit case

Here a particular single-qubit system will be considered, which is of interest because of its analogy to the two-qubit system studied in detail in Chapter 6. Taking a one-qubit state whose evolution is given by the master equation

$$\partial_t \varrho_t = \mathbf{L}[\varrho_t] = -i \frac{\omega}{2} [\sigma_3, \varrho_t] + \sum_{i,j=1}^3 \mathcal{A}_{ij} \left( \sigma_i \varrho_t \sigma_j - \frac{1}{2} \{ \sigma_j \sigma_i, \varrho_t \} \right), \quad (2.36)$$

with matrix

$$\mathcal{A} = [\mathcal{A}_{ij}] = \begin{pmatrix} 1 & i\alpha & 0 \\ -i\alpha & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \alpha \in \mathbb{R}, \alpha^2 \leq 1, \quad (2.37)$$

in order to find the stationary state  $\varrho_0$ , it is sufficient to solve the equation for the stationarity of  $\varrho_0$ , i.e.

$$\mathbf{L}[\varrho_0] = 0. \quad (2.38)$$

The explicit solution of (2.38) yields

$$\varrho_0 = \frac{I_2 - \alpha\sigma_3}{2}.$$

This can be seen simply as follows.

To this end it is convenient to decompose the system density matrix  $\varrho_S$  in terms of the Pauli matrices, i.e.

$$\varrho_S = \frac{1}{2}(I_2 + \vec{\varrho} \cdot \vec{\sigma}) \quad (2.39)$$

with  $I_2$  the  $2 \times 2$  identity matrix and  $\vec{\varrho}$  a vector in  $\mathbb{R}^3$ ; then, the master equation (2.36) can be written as a Schrödinger-like equation for the Bloch vector [74]  $|\varrho(t)\rangle$  of components  $(1, \varrho_1(t), \varrho_2(t), \varrho_3(t))$ :

$$\frac{\partial |\varrho(t)\rangle}{\partial t} = -2(\mathcal{H}_{eff} + \mathcal{D})|\varrho(t)\rangle. \quad (2.40)$$

Here  $\mathcal{H}$  and  $\mathcal{D}$  are  $4 \times 4$  matrices corresponding to the effective Hamiltonian and dissipative contributions, respectively, and they can be expressed explicitly as (see, e.g., [5])

$$\mathcal{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \omega & 0 \\ 0 & -\omega & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{D} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ \alpha & 0 & 0 & 2 \end{pmatrix}.$$

Then the stationarity condition (2.38) can thus be written in vectorial form as

$$\mathcal{L}|\varrho_0\rangle \equiv (\mathcal{H} + \mathcal{D})|\varrho_0\rangle = 0, \quad (2.41)$$

with  $|\varrho_0\rangle = (x, y, w, z)$  and the coefficients  $x, y, w, z$  to be determined.

By explicitly computing equation (2.41) with  $\mathcal{H}$  and  $\mathcal{D}$  as above, it follows that  $|\varrho_0\rangle = (1, 0, 0, -\alpha/2)$ , and the stationary state is thus of the form

$$\varrho_0 = \frac{I_2 - \alpha\sigma_3}{2}.$$

### 2.3.2 Two-qubit case

The two-qubit case is more involved than the one-qubit case and for the former the concepts and definitions introduced at the beginning of Section 2.4 will be necessary.

A particular two-qubit case, which is studied in more detail in Chapter 6, will be considered here, namely with Kossakowski matrix  $K = \begin{pmatrix} \mathcal{A} & \mathcal{A} \\ \mathcal{A} & \mathcal{A} \end{pmatrix}$  and master equation of the

form<sup>2</sup>

$$\partial_t X_t = \mathbf{L}^*[X_t] = -i \frac{\Omega}{2} [\Sigma_3, X_t] + \sum_{i,j=1}^3 \mathcal{A}_{ij} \left( \Sigma_i X_t \Sigma_j - \frac{1}{2} \{ \Sigma_j \Sigma_i, X_t \} \right), \quad (2.42)$$

where  $\Omega$  is the system frequency,  $\Sigma_i := \sigma_i \otimes I_2 + I_2 \otimes \sigma_i$ ,  $I_2$  is the  $2 \times 2$  identity matrix,  $\sigma_i$ ,  $i = 1, 2, 3$  are the Pauli matrices and the matrix  $\mathcal{A} \equiv [\mathcal{A}_{ij}]$  is positive definite.

In this case it can be seen that  $\{V_i\}' = \{\Sigma_i\}'$ , which implies that (2.35) is valid with the operators  $\Sigma_i$  in place of the  $V_i$ 's. Then the following Propositions hold true.

**Proposition 2** *Let the generator  $\mathbf{L}^*[X] \equiv \mathbf{L}_H^*[X] + \mathbf{D}^*[X]$  be as in (2.42). Then the commutant is given by  $\{\Sigma_i\}' = \{P, Q\}$ , where  $P, Q$  are the projectors*

$$P = \frac{1}{4} (I_2 \otimes I_2 - \sum_{i=1}^3 \sigma_i \otimes \sigma_i), \quad Q = I_4 - P.$$

**Proof:** Given (2.42), the proof of the above Proposition simply consists in the explicit calculation of the commutant  $\{\Sigma_i\}'$ , as shown here.

The commutant  $\{\Sigma_i\}'$  with  $\Sigma_i = \sigma_i \otimes I_2 + I_2 \otimes \sigma_i$  is given by the set  $\{X \in M_4 \mid [X, \sigma_i \otimes I_2 + I_2 \otimes \sigma_i] = 0, \forall i = 1, 2, 3\}$ , where the general form of the operators  $X$  is

$$X = \sum_j a_j (\sigma_j \otimes I_2) + \sum_j b_j (I_2 \otimes \sigma_j) + \sum_{l,j} c_{lj} (\sigma_l \otimes \sigma_j).$$

Therefore, in order to find the commutant explicitly, the following must hold true:

$$\begin{aligned} 0 = [X, \sigma_i \otimes I_2 + I_2 \otimes \sigma_i] &= \sum_j a_j ([\sigma_j, \sigma_i] \otimes I_2) + \sum_j b_j (I_2 \otimes [\sigma_j, \sigma_i]) + \sum_{l,j} c_{lj} ([\sigma_l, \sigma_i] \otimes [\sigma_j, \sigma_i]) \\ &= 2i \left\{ \sum_{j,k} a_j \epsilon_{jik} (\sigma_k \otimes I_2) + \sum_{j,k} b_j \epsilon_{jik} (I_2 \otimes \sigma_k) \right. \\ &\quad \left. + \sum_{l,j,k} c_{lj} (\epsilon_{lik} (\sigma_k \otimes \sigma_j) + \epsilon_{jik} (\sigma_l \otimes \sigma_k)) \right\}. \end{aligned}$$

By multiplying both sides of the above equation by  $\sigma_p \otimes I_2$  and taking the trace, it follows from the first term on the right-hand side that  $a_j = 0 \forall j$ ; analogously by multiplying both sides by  $I_2 \otimes \sigma_q$  and taking the trace, from the second term it follows that  $b_j = 0 \forall j$ . Then multiplying the last terms by  $\sigma_p \otimes \sigma_q$  and taking the trace yields

$$\sum_l (c_{lq} \epsilon_{lip} + c_{pl} \epsilon_{liq}) = 0,$$

and by direct computation, varying all  $p, q = 1, 2, 3$ , finally the coefficients are found to be

$$c_{11} = c_{22} = c_{33} \neq 0, \quad c_{12} = c_{21} = c_{13} = c_{31} = c_{23} = c_{32} = 0,$$

<sup>2</sup>In the following the subscript  $t$  in  $X_t$  will be omitted to make the notation less cumbersome.

which implies

$$X = \eta_1(I_2 \otimes I_2) + \eta_2 \sum_i \sigma_i \otimes \sigma_i, \quad i = 1, 2, 3, \quad \eta_{1,2} \in \mathbb{R}.$$

The commutant  $\{\Sigma_i\}' \equiv \{X \in M_4 \mid [X, \sigma_i \otimes I_2 + I_2 \otimes \sigma_i] = 0, \forall i = 1, 2, 3\}$  can thus be written as  $\{\Sigma_i\}' = \{P, Q\}$  with the two projectors  $P, Q$  given by

$$P = \frac{1}{4}(I_2 \otimes I_2 - \sum_{i=1}^3 \sigma_i \otimes \sigma_i), \quad Q = I_4 - P.$$

□

**Proposition 3** *Let the generator  $\mathbf{L}^*[X] \equiv \mathbf{L}_H^*[X] + \mathbf{D}^*[X]$  be as in (2.42) with commutant  $\{\Sigma_i\}' = \{P, Q\}$ , where  $P, Q$  are the projectors given in Proposition 1. Assume the dynamical semigroup  $\{\gamma_t \equiv e^{t\mathbf{L}}, t \geq 0\}$  has a stationary state  $\varrho_0$ ; then for every initial state  $\varrho_{in}$  the dynamical semigroup  $\gamma_t$  has an asymptotic state  $\varrho_\infty \equiv E[\varrho_{in}]$  of the form*

$$E[\varrho_{in}] = \text{Tr}(\varrho_{in}) \frac{P\varrho_0P}{\text{Tr}(\varrho_0P)} + \text{Tr}(\varrho_{in}) \frac{Q\varrho_0Q}{\text{Tr}(\varrho_0Q)}, \quad (2.43)$$

where  $\varrho_0$  is any  $\gamma_t$ -invariant faithful state, i.e. a density matrix with no zero eigenvalues.

**Proof:** Since  $\{\Sigma_i\}' = \{P, Q\}$  with  $P, Q$  projectors, it can be shown [72] that the conditional expectation defined in (2.34) can be explicitly written as  $E^*[X] = c_P(X)P + c_Q(X)Q$ , where  $c_P(X), c_Q(X)$  are real coefficients. Since  $P, Q \in \mathcal{M}(\gamma)$ , from the second property of  $E^*$  seen above it follows that  $PE^*[X]P = E^*[PXP] = c_P(X)P$  and analogously for  $Q$ .

By assumption there exists a stationary state of  $\gamma_t$ , i.e. a state  $\varrho_0$  such that  $\gamma_t[\varrho_0] = \varrho_0$ . Then:

$$c_P(X)\text{Tr}(\varrho_0P) \equiv \text{Tr}(\varrho_0E^*[PXP]) = \text{Tr}(E[\varrho_0]PXP) = \text{Tr}(\varrho_0PXP) = \text{Tr}(P\varrho_0PX),$$

where the second equality comes from duality, the third from the stationarity of  $\varrho_0$  and the last from the cyclicity of the trace. The same can be done for the projector  $Q$  and this leads to the following explicit expression for the coefficients

$$c_P(X) = \frac{\text{Tr}(P\varrho_0PX)}{\text{Tr}(\varrho_0P)}, \quad c_Q(X) = \frac{\text{Tr}(Q\varrho_0QX)}{\text{Tr}(\varrho_0Q)},$$

which yield

$$E^*[X] = \frac{\text{Tr}(P\varrho_0PX)}{\text{Tr}(\varrho_0P)}P + \frac{\text{Tr}(Q\varrho_0QX)}{\text{Tr}(\varrho_0Q)}Q. \quad (2.44)$$

Now, having taken a fixed arbitrary initial state  $\varrho_{in}$ , equation(2.44) leads to the following:

$$\begin{aligned} \text{Tr}(\varrho_{in} E^*[X]) &= \text{Tr}(E[\varrho_{in}]X) \\ &= \frac{\text{Tr}(\varrho_{in}P)}{\text{Tr}(\varrho_0P)} \text{Tr}(P\varrho_0PX) + \frac{\text{Tr}(\varrho_{in}Q)}{\text{Tr}(\varrho_0Q)} \text{Tr}(Q\varrho_0QX) \\ &= \text{Tr}\left[\left(\frac{P\varrho_0P}{\text{Tr}(\varrho_0P)} \text{Tr}(\varrho_{in}P) + \frac{Q\varrho_0Q}{\text{Tr}(\varrho_0Q)} \text{Tr}(\varrho_{in}Q)\right)X\right], \end{aligned}$$

where the first equality comes from the duality of  $E^*$ .

Since this must be true for any  $X \in M_d$ , it follows that the asymptotic state of the dynamics  $\varrho_\infty \equiv E[\varrho_{in}]$  can be explicitly written as

$$\varrho_\infty \equiv E[\varrho_{in}] = \text{Tr}(\varrho_{in}P) \frac{P\varrho_0P}{\text{Tr}(\varrho_0P)} + \text{Tr}(\varrho_{in}Q) \frac{Q\varrho_0Q}{\text{Tr}(\varrho_0Q)}.$$

**Remark 1** In the particular case considered in Chapter 6 with generator as in (2.42) where the matrix  $\mathcal{A} \equiv [\mathcal{A}_{ij}]$  is given by (2.37) the stationary faithful state  $\varrho_0$  is found to be of the form (see also [75])

$$\varrho_0 = \frac{1}{4} \left( I_2 \otimes I_2 + \alpha(I_2 \otimes \sigma_3 + \sigma_3 \otimes I_2) + \alpha^2(\sigma_3 \otimes \sigma_3) \right).$$



## Chapter 3

# Determination of the noise parameters in a one-dimensional open quantum system

### 3.1 Introduction

In this chapter, a method to experimentally determine the elements of the Kossakowski matrix, i.e. the noise parameters, of a bath from physical properties of the subsystem immersed within it is proposed.

The open quantum system considered here consists of an electron that propagates through a one-dimensional wire in which a spin-1/2 impurity is embedded. This system is immersed in an environment whose dissipative and noisy effects act only on the spin-1/2 degree of freedom. In this case, since the spin-1/2 impurity corresponds to a qubit, the dissipative term is as in expression (2.25):

$$\mathbf{D}^{(1)}[\varrho_S] = \sum_{i,j=1}^3 K_{ij} \left( \sigma_j \varrho_S \sigma_i - \frac{1}{2} \{ \sigma_i \sigma_j, \varrho_S \} \right),$$

with  $\sigma_i$ ,  $i = 1, 2, 3$ , the Pauli matrices.

Then, as shown in detail in the next section, the elements of the Kossakowski matrix  $K \equiv [K_{ij}]$  are written in terms of the electron's transmission and reflection probabilities, which can be measured.

Moreover, as discussed in Chapter 2, in order for the Markovian dynamics to be physically consistent, the map  $\Gamma_t$  governing the dissipative evolution must be completely positive [8] and this is equivalent to  $K$  being positive semi-definite [56, 59]. Indeed, in Section 3.3, in the simple case of a diagonal Kossakowski matrix, it is explicitly shown that, if one

takes a positive but not completely positive dissipative map, one obtains negative transmission probabilities for certain entangled states, which proves the necessity of complete positivity for physical consistency.

### 3.2 Determination of the Kossakowski matrix elements

Here a system  $S$  is considered in which an electron propagates in a one-dimensional wire interacting magnetically with a spin-1/2 impurity at  $x = 0$ , and the effects of a noisy environment on such a system are analyzed. This is the first step in a framework analogous to that in [76]. There the authors considered an isolated system in which an electron propagates in a one-dimensional wire interacting magnetically with two spin-1/2 impurities at  $x = 0$  and at  $x = x_0$ , and they analyzed the dependence of the electron's transmittivity on the impurities' states. The main idea in this work is to study the effects of a noisy environment on such a system, starting by considering the simpler system of an electron interacting magnetically with only one spin-1/2 impurity. Therefore, firstly the system  $S$  will be considered in the case when the electron and impurity are isolated; then this system will be studied when it is embedded in an external environment which acts with a noisy term only on the spin degree of freedom of the impurity. This latter case will lead to expressions of the Kossakowski matrix elements in terms of the electron transmission coefficients.

In the first case the eigenvalue equation for the energy is the following:

$$H|E\rangle \equiv \left( \frac{p^2}{2m} + \delta(x)J\vec{\sigma} \cdot \vec{s} \right) |E\rangle = E|E\rangle \quad (3.1)$$

where  $p = -i\hbar\nabla$ ,  $m$  is the electron mass,  $J$  is the magnetic coupling constant between electron and impurity, and  $\vec{\sigma}$ ,  $\vec{s}$  is the electron, respectively impurity, spin operator<sup>1</sup>.

Having defined the total spin  $\vec{S} = \vec{\sigma} + \vec{s}$ , the eigenvalue equation (3.1) can be rewritten as follows:

$$\left( \frac{p^2}{2m} + \delta(x)\frac{J}{2} \left( S^2 - \frac{3}{2} \right) \right) |E\rangle = E|E\rangle. \quad (3.2)$$

$S^2$  and  $S_z$  are the constants of motion with eigenvalues  $s$  e  $m = -s, \dots, s$  respectively. In this case two spin-1/2 systems are considered, so the possible values of the total spin eigenvalues  $s$  are 1 and 0.

Given an energy eigenstate  $|E\rangle$ , it is always possible to expand it in terms of the spatial and total spin eigenfunctions:  $|E\rangle = \sum_{i=1}^4 |\psi_{S_i}\rangle \otimes |S_i\rangle$ , where  $\{|S_i\rangle\}_{i=1}^4 = \{|S_1\rangle := \frac{|01\rangle - |10\rangle}{\sqrt{2}}, |S_2\rangle := |00\rangle, |S_3\rangle := \frac{|01\rangle + |10\rangle}{\sqrt{2}}, |S_4\rangle := |11\rangle\}$  have been taken as the total spin basis. If equation (3.1) is projected onto the electron position eigenstates  $\{|x\rangle\}$ , for a fixed spin

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<sup>1</sup>The spin operators are such that the eigenvalues of  $\sigma_z$  and  $s_z$  are  $\pm 1/2$ .

$S_i$ , the differential equation for the wave function  $\psi_{k;S_i}(x)$  is obtained:

$$-\frac{\hbar^2}{2m}\psi''_{k;S_i}(x) + \delta(x)\frac{J}{2}\left(S_i^2 - \frac{3}{2}\right)\psi_{k;S_i}(x) = E\psi_{k;S_i}(x). \quad (3.3)$$

For positive energies  $E = \frac{\hbar^2 k^2}{2m} > 0$ , the solution of equation (3.3) is

$$\psi_{k;S_i}(x) = \begin{cases} e^{ikx} + r_{S_i}^E e^{-ikx} & \text{if } x < 0 \\ t_{S_i}^E e^{ikx} & \text{if } x > 0 \end{cases}$$

where  $r_{S_i}^E$  and  $t_{S_i}^E$  are the electron reflection and transmission coefficients respectively.

The explicit expressions for these coefficients are found by imposing the continuity condition in  $x = 0$  and integrating the Schrödinger equation around  $x = 0$ :

$$t_{S_i}^E = \frac{1}{1 + \frac{i}{4}\pi J \varrho(E)(S_i^2 - \frac{3}{2})}, \quad r_{S_i}^E = \frac{-\frac{i}{4}\pi J \varrho(E)(S_i^2 - \frac{3}{2})}{1 + \frac{i}{4}\pi J \varrho(E)(S_i^2 - \frac{3}{2})}, \quad (3.4)$$

with  $\varrho(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}$  the linear density of states in the wire.

For the positive energies solutions, the eigenstates can be written as follows:

$$|E\rangle = \int dx \sum_{i=1}^4 \left[ \left( e^{ikx} + r_{S_i}^E e^{-ikx} \right) \chi_{L}(x) + t_{S_i}^E e^{ikx} \chi_{R}(x) \right] |x\rangle \otimes |S_i\rangle, \quad (3.5)$$

where  $|S_i\rangle, i = 1, \dots, 4$ , are the total spin basis elements listed above,  $r_{S_i}^E$  and  $t_{S_i}^E$  are the reflection and transmission coefficients from (3.4), and  $\chi_{R(L)}$  is the characteristic function for  $x \geq 0$  ( $x \leq 0$ ).

Calculating the transmission and reflection coefficients for the spin basis elements  $\{S_i\}_{i=1}^4$  explicitly, it is found that  $t_{S_2}^E = t_{S_3}^E = t_{S_4}^E := t_1^E, t_{S_1}^E := t_0^E$ , and  $r_{S_2}^E = r_{S_3}^E = r_{S_4}^E := r_1^E, r_{S_1}^E := r_0^E$ . Thus, having redefined the spin states as

$$|\phi_0^{spin}\rangle := |S_1\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}, \quad |\phi_1^{spin}\rangle := \frac{1}{\sqrt{3}} \sum_{i=2}^4 |S_i\rangle = \frac{1}{\sqrt{3}} \left( |00\rangle + \frac{|01\rangle + |10\rangle}{\sqrt{2}} + |11\rangle \right), \quad (3.6)$$

the energy eigenstates can be rewritten as  $|E\rangle = |\phi_0^E\rangle \otimes |\phi_0^{spin}\rangle + |\phi_1^E\rangle \otimes |\phi_1^{spin}\rangle$ , where the vectors  $|\phi_0^E\rangle, |\phi_1^E\rangle$  are such that

$$\phi_0^E(x) \equiv \langle x | \phi_0^E \rangle := \left( e^{ikx} + r_0^E e^{-ikx} \right) \chi_L(x) + t_0^E e^{ikx} \chi_R(x), \quad (3.7)$$

$$\phi_1^E(x) \equiv \langle x | \phi_1^E \rangle := \sqrt{3} \left[ \left( e^{ikx} + r_1^E e^{-ikx} \right) \chi_L(x) + t_1^E e^{ikx} \chi_R(x) \right]. \quad (3.8)$$

Finally, considering the basis of maximally entangled Bell states,  $|\psi_0\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, |\psi_1\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, |\psi_2\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}, |\psi_3\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$ , the spin states (3.6) can be rewritten as

$$|\phi_0^{spin}\rangle \equiv |\psi_2\rangle, \quad |\phi_1^{spin}\rangle \equiv \frac{1}{\sqrt{3}} \left( |\psi_1\rangle + \sqrt{2}|\psi_0\rangle \right). \quad (3.9)$$

#### 44 Determination of the noise parameters in a one-dimensional open quantum system

If the system  $S$  is embedded in an external environment to which it is weakly coupled, the evolution of the system eigenstates is described by the master equation (2.9) with solution  $\varrho(t) \equiv \Gamma_t[\varrho] = \exp(t\mathbf{L})[\varrho] = \exp(t(\mathbf{L}_H + \mathbf{D}))[\varrho]$ , where  $\varrho \equiv |E\rangle\langle E|$ . Here a dissipative map  $\Gamma_t$  will be considered whose noisy effects act only on the spin degree of freedom of the impurity and leave the electron spin unchanged: therefore  $\mathbf{D} \equiv \mathbf{I} \otimes \mathbf{D}^{(1)}$ , with  $\mathbf{I}$  the identity operator acting on the space and electron spin degrees of freedom, and  $\mathbf{D}^{(1)}$  the Kossakowski-Lindblad term (2.25) corresponding to the dissipative map  $\gamma_t$  acting on the impurity's spin. The aim of this work is precisely to write the elements of the Kossakowski matrix relative to  $\gamma_t$  in terms of the electron transmission and reflection coefficients, and thus determine them operatively. Since the total evolution of the system eigenstates is governed by the map  $\Gamma_t$  which cannot be factorized between space and spin degrees of freedom, an expansion for small times will be considered, stopping at the first order in  $t$ :

$$\Gamma_t[|E\rangle\langle E|] = \exp(t\mathbf{L})[|E\rangle\langle E|] = (\mathbf{I} + t(\mathbf{L}_H + \mathbf{D}))[|E\rangle\langle E|] + O(t^2). \quad (3.10)$$

Since the aim is to find explicit expressions for the Kossakowski matrix elements, the contributions from the dissipative part of the map  $\Gamma_t$ , due to  $\mathbf{D}$ , will be isolated. In order to do so, the spin state  $|\psi_3\rangle = (I_2 \otimes \sigma_3)|\psi_0\rangle$ , which is orthogonal to the spin states in the eigenstate expansion, will be considered, and then the probability of finding the system at a point  $x = x_0$  with total spin state  $|\psi_3\rangle$  will be calculated. Therefore the mean value of (3.10) will be evaluated with respect to the state  $|x_0\rangle \otimes |\psi_3\rangle \equiv |x_0; \psi_3\rangle$ :

$$P_t(x = x_0; |\psi_3\rangle\langle\psi_3|) = \langle x_0; \psi_3 | (\mathbf{I} + t(\mathbf{L}_H + \mathbf{D})) [|E\rangle\langle E|] |x_0; \psi_3\rangle + O(t^2). \quad (3.11)$$

The zeroth order term in (3.11) vanishes because of the orthogonality of  $|\psi_3\rangle$  to the spin states of the eigenstate  $|E\rangle$ , whereas the Hamiltonian term is always zero on the eigenstates, so the only piece that remains is

$$P_t(x = x_0; |\psi_3\rangle\langle\psi_3|) = t\langle x_0; \psi_3 | \mathbf{D} [|E\rangle\langle E|] |x_0; \psi_3\rangle + O(t^2). \quad (3.12)$$

Making use of (3.7) and (3.8), expression (3.12) can be conveniently rewritten as follows:

$$P_t(x = x_0; |\psi_3\rangle\langle\psi_3|) = t\langle\phi^E(x) | \tilde{D} |\phi^E(x)\rangle + O(t^2), \quad (3.13)$$

where  $|\phi^E(x)\rangle = \begin{pmatrix} \phi_0^E(x) \\ \phi_1^E(x) \end{pmatrix}$

and

$$\tilde{D} = \begin{pmatrix} \langle\psi_3 | \mathbf{D} [|\phi_0^{spin}\rangle\langle\phi_0^{spin}|] |\psi_3\rangle & \langle\psi_3 | \mathbf{D} [|\phi_1^{spin}\rangle\langle\phi_0^{spin}|] |\psi_3\rangle \\ \langle\psi_3 | \mathbf{D} [|\phi_0^{spin}\rangle\langle\phi_1^{spin}|] |\psi_3\rangle & \langle\psi_3 | \mathbf{D} [|\phi_1^{spin}\rangle\langle\phi_1^{spin}|] |\psi_3\rangle \end{pmatrix}. \quad (3.14)$$

The matrix  $\tilde{D}$  has the following explicit expression:

$$\tilde{D} = \begin{pmatrix} K_{11} & \frac{1}{\sqrt{3}}(-iK_{21} + K_{31}) \\ \frac{1}{\sqrt{3}}(iK_{12} + K_{13}) & \frac{1}{3}(K_{22} + 2K_{33} + 2\sqrt{2}Im(K_{23})) \end{pmatrix}, \quad (3.15)$$

where  $K_{ij}$ ,  $i, j = 1, 2, 3$ , are the elements of the Kossakowski matrix  $K$  which corresponds to the map  $\gamma_t$  acting on the spin degree of freedom of the impurity.

In this work only entropy-increasing maps are considered, since they describe many interesting situations in different areas of physics (stochastic magnetic fields, quantum baker's map [77–79], XY spin-1/2 chain with quenching of the transverse field [80]): in this case the Kossakowski matrix  $K$  is symmetric and real [61, 81], and therefore has only six different elements. So, in order to explicitly find the Kossakowski matrix elements, six independent linear equations for the  $K_{ij}$ 's are needed.

The first two linear equations are given by the explicit evaluation of (3.13) for  $x > 0$  and for  $x < 0$ , in which the transmission and reflection coefficients appear respectively; whereas the other four can be obtained by calculating the analog of (3.13) for  $x > 0$  and for  $x < 0$  rotating the spin basis. A simple choice for the rotations is to exchange two Pauli matrices while keeping the third fixed, thus rearranging the elements  $K_{ij}$  in (3.15). For instance, a rotation  $R^{(k)}$  that keeps  $\sigma_k$  ( $k = 1, 2, 3$ ) fixed while changing  $\sigma_l$  in  $\pm\sigma_m$  ( $l, m = 1, 2, 3$ ,  $l, m \neq k$ ) can be taken: this will exchange the elements  $K_{lm}$  and  $K_{ml}$  while leaving those with  $i, j = k$  unchanged. In particular, here the following rotations are chosen:

$$R^{(1)}\left(-\frac{\pi}{4}\right) = \frac{I_2 - i\sigma_1}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \quad (3.16)$$

and

$$R^{(2)}\left(-\frac{\pi}{4}\right) = \frac{I_2 - i\sigma_2}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad (3.17)$$

which lead to the following rotated spin bases respectively:

$$|\tilde{\psi}_i^{spin}\rangle := I_2 \otimes R^{(1)}|\psi_i^{spin}\rangle \quad \text{and} \quad |\hat{\psi}_i^{spin}\rangle := I_2 \otimes R^{(2)}|\psi_i^{spin}\rangle. \quad (3.18)$$

Thus (3.13) is calculated for  $x > 0$  and for  $x < 0$  for the three different spin bases, i.e. the probability of finding the evolved state at a point  $x \equiv x_0$  in the three different spin states  $|\psi_3\rangle, |\tilde{\psi}_3\rangle, |\hat{\psi}_3\rangle$  is evaluated. Then the reflection coefficient is written as  $r_{S_i}^E = 1 - t_{S_i}^E$ , and finally six independent linear equations for the elements  $K_{ij}$  are obtained. This linear system can be written in vector form as follows<sup>2</sup>:

$$|P(t)_\alpha\rangle = M_{\alpha\beta}|K_\beta\rangle, \quad \alpha, \beta = 1, \dots, 6, \quad (3.19)$$

<sup>2</sup>Details are given in Appendix A.

with  $M \equiv [M_{\alpha\beta}]$  a  $6 \times 6$  matrix, and vectors

$$|K_\beta\rangle := \begin{pmatrix} K_{11} \\ K_{12} \\ K_{13} \\ K_{22} \\ K_{23} \\ K_{33} \end{pmatrix}, \quad |P(t)_\alpha\rangle := \begin{pmatrix} P_0^T \\ P_1^T \\ P_2^T \\ P_0^R \\ P_1^R \\ P_2^R \end{pmatrix},$$

where  $P_a^T, P_a^R, a = 0, 1, 2$ , are the transmission, respectively reflection, probabilities for the three different spin bases.

The linear system of equations can be inverted if  $\det(M) \neq 0$ . This is indeed the case, and therefore one can explicitly write the Kossakowski matrix elements in terms of the transmission and reflection probabilities, and thus determine the  $K_{ij}$ 's experimentally. Moreover, the experimental determination of the  $K_{ij}$ 's leads to the possibility of actually verifying whether the Kossakowski matrix is positive semi-definite<sup>3</sup>, and thus whether the evolution is completely positive. Further, this could also be a test for the Markovian approximation used: since, as seen in the previous chapter, physically consistent Markovian approximations for the master equation (2.9) must lead to completely positive dynamical semigroups, if the results obtained for the  $K_{ij}$ 's yield a Kossakowski matrix which is not positive semi-definite, this could imply that the particular Markovian approximation chosen to describe the dynamics is not correct.

**Remark 2** The proposal presented here for an operational determination of the Kossakowski matrix elements through transmission probabilities, which can be measured, could also be viewed in the context of experimental characterization of the dynamical evolution of an open quantum system. A well-studied procedure with this aim is known as *quantum process tomography* (QPT) [82–84], where a quantum system  $A$  is subjected to an unknown quantum process  $\mathcal{E}$ . In order to determine  $\mathcal{E}$ , one prepares a fixed set of states  $\{\varrho_j\}$  that form a basis for the set of operators acting on the state space of  $A$  and applies the process  $\mathcal{E}$  to each input state  $\varrho_j$ ; then  $\mathcal{E}(\varrho_j)$  can be experimentally determined through quantum state tomography [13, 85] on the outputs; finally the process  $\mathcal{E}$  can be fully characterized through the operation elements  $E_k$  in its operator sum representation  $\mathcal{E}(\varrho) = \sum_k E_k \varrho E_k^\dagger$ . The physical systems and detailed procedures used in quantum process tomography (see, for example, [86–88]) differ from those used in this work, and in this case the quantum operation describing the evolution of the system is not supposed to be unknown; nevertheless both methods could be viewed in the context of experimental characterization of a quantum process on an open quantum system. Moreover, the

<sup>3</sup>Notice that, in order for the Kossakowski matrix to be positive semi-definite, the transmission and reflection probabilities must be such that the following positivity conditions for  $K$  are fulfilled:  
 $K_{11} \geq 0, K_{22} \geq 0, K_{33} \geq 0, K_{11}K_{22} - K_{12}^2 \geq 0, K_{11}K_{33} - K_{13}^2 \geq 0, K_{22}K_{33} - K_{23}^2 \geq 0, \det(K) \geq 0$ .

analysis of results in quantum process tomography leading to a non-completely positive evolution may be useful for better understanding the implications, in this case, of experimentally obtaining a Kossakowski matrix which is not positive semi-definite. In [88], for example, it is shown that experimental errors made in the QPT procedure can yield results which lead to a non-completely positive quantum operation and that this unphysical result can be corrected. Therefore, it might be possible also in this case, that experimental results leading to a non-positive semi-definite Kossakowski matrix be due to experimental errors in the measuring procedure. Further discussion about this hypothesis, however, would involve taking into account the exact experimental situation, and is therefore outside the scope of this work.

### 3.3 Complete positivity

As seen in Section 2.2.1, in order to guarantee full physical consistency, namely that  $\gamma_t \otimes \text{id}_A$  be positivity preserving on all states of the compound system  $S + A$  for any inert ancilla  $A$ ,  $\gamma_t$  must be completely positive [8] and this is equivalent to  $K$  being positive semi-definite [56, 59].

The necessity of complete positivity arises from the existence of entanglement, since in general entangled bipartite states may become non-positive under the action of positive but not completely positive transformations [16].

In this section it will be shown that, if a positive but not completely positive dissipative map  $\gamma_t$  acting on the impurity's spin is taken and the probability (3.13) is calculated for certain entangled states, negative values for the transmission probability arise.

In order to give an explicit example of this fact, a specific dissipative map  $\gamma_t$  will be used and for simplicity a diagonal Kossakowski matrix will be considered. In this case the matrix  $\tilde{D}$  from (3.15) reduces to

$$\tilde{D} = \begin{pmatrix} K_{11} & 0 \\ 0 & \frac{1}{3}(K_{22} + 2K_{33}) \end{pmatrix} \quad (3.20)$$

and the probability (3.13), to first order in  $t$ , is therefore

$$\begin{aligned} P_t(x = x_0; |\psi_3\rangle\langle\psi_3|) &= t (K_{11}|t_0^E|^2 + (K_{22} + 2K_{33})|t_1^E|^2) \\ &= t \left( K_{11} \frac{16}{16 + 9(\frac{\pi}{2}J\rho(E))^2} + (K_{22} + 2K_{33}) \frac{16}{16 + (\frac{\pi}{2}J\rho(E))^2} \right) \end{aligned} \quad (3.21)$$

having inserted the explicit expressions for the transmission coefficients in the second line.

In particular, a positive but not completely positive map  $\gamma_t$  is considered, acting on

the impurity's spin with Kossakowski matrix  $K = \text{diag}(1,1,-1)$ . Thus the Kosskowski-Lindblad term (2.25) explicitly reads

$$\mathbf{D}^{(1)}[\varrho^{spin}] = \sigma_1 \varrho^{spin} \sigma_1 + \sigma_2 \varrho^{spin} \sigma_2 - \sigma_3 \varrho^{spin} \sigma_3 - \varrho^{spin}$$

with  $\varrho^{spin}$  the impurity's spin state. Since the spin-1/2 impurity consists of a qubit, its state can be written in Bloch vector form:  $\varrho^{spin} = \frac{I_2 + \vec{\varrho} \cdot \vec{\sigma}}{2}$ , where  $I_2$  is the identity in  $\mathbb{C}^2$ ,  $\vec{\varrho} = (\varrho_1, \varrho_2, \varrho_3)$  and  $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ , with  $\sigma_i$ ,  $i = 1, 2, 3$ , the Pauli matrices. Thus the evolved state will be

$$\varrho^{spin}(t) \equiv \gamma_t[\varrho^{spin}] = \frac{1 + \varrho_1 \sigma_1 + \varrho_2 \sigma_2 + e^{-4t} \varrho_3 \sigma_3}{2}.$$

$\varrho^{spin}(t)$  is such that  $\|\varrho^{spin}(t)\|^2 < \|\varrho^{spin}\|^2 \leq 1$  and therefore the map  $\gamma_t$  gives rise to a positive evolution. On the other hand, though, the Kossakowski matrix  $K = \text{diag}(1,1,-1)$  is not positive semi-definite, thus the corresponding dissipative map  $\gamma_t$  is not completely positive, and evaluating (3.21) explicitly it is straightforward to see that we obtain a *negative* transmission probability.

Notice that this physical inconsistency arises from dealing with a positive but not completely positive map and an *entangled* state. Indeed, using duality, the matrix  $\tilde{D}$  that appears in expression (3.13) for the transmission probability can be rewritten as

$$\tilde{D} = \begin{pmatrix} \langle \phi_0^{spin} | \mathbf{D} [|\psi_3\rangle\langle\psi_3|] | \phi_0^{spin} \rangle & \langle \phi_1^{spin} | \mathbf{D} [|\psi_3\rangle\langle\psi_3|] | \phi_0^{spin} \rangle \\ \langle \phi_0^{spin} | \mathbf{D} [|\psi_3\rangle\langle\psi_3|] | \phi_1^{spin} \rangle & \langle \phi_1^{spin} | \mathbf{D} [|\psi_3\rangle\langle\psi_3|] | \phi_1^{spin} \rangle \end{pmatrix},$$

where the spin state  $|\psi_3\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$  is maximally entangled for the electron and impurity spins. Therefore, evaluating the probability (3.21) of finding the system at a point  $x = x_0$  with total spin state  $|\psi_3\rangle$  is equivalent to applying the generator  $\mathbf{D} \equiv \mathbf{I} \otimes \mathbf{D}^{(1)}$ , relative to the positive but not completely positive map  $\gamma_t$ , to the entangled state  $|\psi_3\rangle$ , and this leads to the physical inconsistency of a negative transmission probability.

**Remark 3** If, instead, the map  $\gamma_t$  is completely positive, expression (3.13) is always positive. Indeed, from the choice of the spin state  $|\psi_3\rangle$ , the only contribution to (3.12) is given by the noise term  $\mathbf{N}[\cdot]$ , which can be written as follows:

$$\begin{aligned} \mathbf{N}[\varrho] &= \sum_{i,j} K_{ij} \sigma_j \varrho \sigma_i^\dagger = \sum_l c_l \left( \sum_j \bar{\psi}_l^{(j)} \sigma_j \right) \varrho \left( \sum_i \psi_l^{(i)} \sigma_i^\dagger \right) \\ &= \sum_l c_l \left( \sum_j \bar{\psi}_l^{(j)} \sigma_j \right) \varrho \left( \sum_i \bar{\psi}_l^{(i)} \sigma_i \right)^\dagger = \sum_l \sqrt{c_l} \tilde{W}_l \varrho \sqrt{c_l} \tilde{W}_l^\dagger \equiv \sum_l W_l \varrho W_l^\dagger, \end{aligned}$$

where  $\{|\psi_l\rangle\}$  is a basis of eigenstates of the Kossakowski matrix  $K \equiv \sum_l c_l |\psi_l\rangle\langle\psi_l|$  such that  $K_{ij} = \sum_l c_l \psi_l^{(i)} \bar{\psi}_l^{(j)}$ .  $\mathbf{N}[\varrho]$  is in Kraus-Stinespring form and thus completely positive. Therefore, rewriting the action of the dissipative generator  $\mathbf{D}$  in (3.12), we have:

$$P_t(x = x_0; |\psi_3\rangle\langle\psi_3|) = t \langle x_0; \psi_3 | \mathbf{I} \otimes \mathbf{N}^{spin} [ |E\rangle\langle E | ] | x_0; \psi_3 \rangle + O(t^2),$$



where  $\mathbf{I}$  is the identity operator for the position and electron spin degrees of freedom, while  $\mathbf{N}^{spin}$  is the noise term acting on the impurity's spin.

The complete positivity of the latter guarantees the positivity of  $\mathbf{I} \otimes \mathbf{N}^{spin}$ , and thus  $P_t(x = x_0; |\psi_3\rangle\langle\psi_3|)$  is always positive.

### 3.4 Conclusions

The main idea in this chapter is to propose a way of experimentally determining the elements  $K_{ij}$  of a Kossakowski matrix, i.e. the noise parameters, in terms of the transmission and reflection probabilities of an electron, which can be measured. The system considered is a one-dimensional wire in which an electron propagates interacting magnetically with a spin-1/2 impurity fixed in the same wire; this system is then embedded in an external environment which acts with a noisy term only on the spin degree of freedom of the impurity. The electron's transmission and reflection coefficients are calculated, and expressions for the transmission and reflection probabilities are found in terms of the Kossakowski matrix elements. This leads to the possibility of having experimental access to the noise parameters and of actually verifying whether the Kossakowski matrix is positive semi-definite, and thus whether the evolution is completely positive. Further, it could also be a test for the Markovian approximation used: if the results obtained for the  $K_{ij}$ 's lead to a Kossakowski matrix which is not positive semi-definite, this could imply that the particular Markovian approximation used to describe the dynamics is not appropriate.

Moreover, a concrete example of the necessity of complete positivity for physical consistency is given: indeed, it is shown that a positive but not completely positive dissipative map acting on the impurity's spin can yield negative transmission probabilities when considering, for instance, an entangled state with maximal entanglement between the electron spin and the impurity spin.

## 50 Determination of the noise parameters in a one-dimensional open quantum system

## Chapter 4

# Open quantum systems and entanglement

As seen in Chapter 2, the effect of the environment on a subsystem immersed within it is of dissipative and thermal nature. Since the main effect of the environment on systems immersed within it is decoherence, it would seem natural, therefore, to assume that any entanglement present in a subsystem immersed within an external bath would also be dissipated. Nonetheless, this natural intuition not always holds true: there are, indeed, some cases in which the environment can create and even enhance entanglement within the subsystem (see e.g. [44, 89–92])<sup>1</sup>. In order to study the behavior of entanglement in open quantum systems it is necessary, first of all, to consider composite systems. Coherently with Chapter 1, only bipartite systems will be considered here and, as a straightforward generalization of the case analyzed in Section 2.4, a two-qubit system will be considered. These two two-level atoms will be immersed in the same set of free fields and will be taken to be non-interacting between each other: this means that any interaction or correlations between the two atoms are due to the common bath within which they are immersed.

In the first section, having written the master equation for the two-qubit system in the *weak coupling limit*, it will be seen under which conditions entanglement can be generated between the two atoms just via the bath-mediated coupling, following [5].

Then, in the second section, the possibility of asymptotic persistence of entanglement in a two-qubit state subject to the particular dissipative dynamics considered in section 2.4.2 is studied.

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<sup>1</sup>Recently this has been shown to be the case also in systems of biological interest, such as light-harvesting complexes (see, e.g., [45], [46]).

## 4.1 Entanglement generation in a two-qubit system

Here a system of two non-interacting two-level atoms immersed in a common bath consisting of a collection of free, independent, scalar fields will be considered, and a sufficient condition for the environment to create entanglement in an initially separable two-qubit state immersed within it will be presented.

Given the two atoms, the total system Hamiltonian will be the sum of the two terms in (2.26) and (2.27), i.e. of a system Hamiltonian  $H_S = H_S^{(1)} + H_S^{(2)}$  and an atoms-bath interaction Hamiltonian  $H'$ .

In the *weak coupling limit* the master equation is in Kossakowski-Lindblad form

$$\frac{\partial \varrho_S(t)}{\partial t} = -i[H_{eff}, \varrho_S(t)] + \mathbf{D}^{(2)}[\varrho_S(t)],$$

with the explicit expressions for the effective Hamiltonian and the dissipative term given in (2.29)-(2.31) and (2.33), and Kossakowski matrix as in (2.32).

The first two contributions in (2.33) are dissipative terms affecting the first, respectively second, atom in absence of the other; while the last two pieces represent the way in which the noise generated by the external fields may correlate the two, otherwise independent, atoms.

As mentioned in Chapter 2, the environment contributions to the effective Hamiltonian  $H_{eff}$  and the entries of the Kossakowski matrix (2.32) are given by the Hilbert, respectively Fourier transforms of the field correlation functions. In particular, the matrices  $[H_{ij}^{(12)}]$  in (2.30) and  $\mathcal{B} \equiv [\mathcal{B}_{ij}]$  in (2.33) do not vanish only if the bath state  $\varrho_\beta$  correlates bath-operators coupled to different atoms, i.e. if the expectations  $\text{Tr}[\varrho_\beta \Phi_i(t) \Psi_i(0)]$  are nonzero, with  $\Phi_i(x), \Psi_i(x)$  the field operators. This is of importance in the study of entanglement generation between the two atoms via the bath-mediated interaction: indeed, only in this case is there a possibility of environment-induced entanglement generation; while, if both  $H_{ij}^{(12)} = 0$  and  $\mathcal{B}_{ij} = 0$ , the two atoms evolve independently and initially separable states certainly will not get entangled (although they will probably become more mixed).

Now the conditions under which the common bath may generate entanglement in an initially separable state of the two atoms immersed within it will be found. In order to do so, since the system consists of two two-level atoms, the partial transposition criterion (see Section 1.2) will be used to detect entanglement. More precisely, the environment is not able to generate entanglement if and only if the operation of partial transposition preserves the positivity of the system state  $\varrho(t)$  for all times. Here, in four main steps, the conditions for this not to hold, and thus for entanglement to be generated through the environment, will be derived.

Firstly, the two-atom system is prepared in a separable state, which, without loss of generality, can be taken to be pure<sup>2</sup>:

$$\varrho(0) = |\varphi\rangle\langle\varphi| \otimes |\psi\rangle\langle\psi|. \quad (4.1)$$

Then, the partial transposition operation (over, say, the second factor) is performed on both sides of the master equation (2.28), yielding an evolution equation for the matrix  $\tilde{\varrho}(t)$ , which is the partially transposed state of  $\varrho(t)$ :

$$\frac{\partial \tilde{\varrho}(t)}{\partial t} = -i[\tilde{H}_{eff}, \tilde{\varrho}(t)] + \tilde{\mathbf{D}}^{(2)}[\tilde{\varrho}(t)]. \quad (4.2)$$

It must be noted that the original Hamiltonian and dissipative terms in (2.28) are mixed together in the new "Hamiltonian" and "dissipative" pieces, i.e. both  $\tilde{H}_{eff}$  and  $\tilde{\mathbf{D}}^{(2)}$  contain contributions both from the unitary and from the dissipative terms in (2.28). On one hand, the new "Hamiltonian"  $\tilde{H}_{eff}$  can be written explicitly as

$$\tilde{H}_{eff} = \sum_{i=1}^3 H_i^{(1)}(\sigma_i \otimes I_2) + \sum_{i,j=1}^3 H_i^{(2)} E_{ij}(I_2 \otimes \sigma_j) + \sum_{i,j=1}^3 \text{Im}(B \cdot E)_{ij}(\sigma_i \otimes \sigma_j), \quad (4.3)$$

where  $\text{Im}$  indicates the imaginary part, while  $E$  is the diagonal  $3 \times 3$  matrix  $E = \text{diag}(-1, 1, -1)$  and does not appear in the term pertaining only to the first atom because the partial transposition operation is performed on the second atom. On the other hand, the new "dissipative" contribution can be written as in (2.31) but with a new "Kossakowski" matrix  $K \rightarrow \mathcal{E} \cdot \tilde{K} \cdot \mathcal{E}$ , with

$$\tilde{K} = \begin{pmatrix} \mathcal{A} & \text{Re}(\mathcal{B}) + i(H^{(12)}) \\ \text{Re}(\mathcal{B}^T) - i(H^{(12)})^T & \mathcal{C}^T \end{pmatrix}, \quad (4.4)$$

$$\mathcal{E} = \begin{pmatrix} I_3 & 0 \\ 0 & E \end{pmatrix},$$

where  $\text{Re}$  indicates the real part and  $T$  denotes full matrix transposition, while  $h^{(12)}$  is the coefficient matrix in (2.30).

Although the partially transposed master equation (4.2) is in Kossakowski-Lindblad form, nonetheless the time-evolution it generates could result to be neither completely positive nor positive, and it need not preserve the positivity of the initial state  $\tilde{\varrho}(0) \equiv \varrho(0)$ : this is due to the fact that the new coefficient matrix  $\tilde{K}$  is not necessarily positive semi-definite.

Then, in order to see if entanglement has been generated by the environment in the initially separable state (4.1), the presence of negative eigenvalues of  $\tilde{\varrho}(t)$  must be

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<sup>2</sup>Indeed, if the environment cannot generate entanglement in pure states, it certainly cannot do so in mixed states, since any of the latter can be written as a convex sum of the former.

checked. To this end, instead of examining the full equation (4.2), it is convenient to study the quantity

$$Q(t) := \langle \chi | \tilde{\rho}(t) | \chi \rangle,$$

where  $\chi$  is an arbitrary four-dimensional vector [10]. Now, if an initially separable state  $\tilde{\rho}$  has indeed developed a negative eigenvalue, then at some time  $t^*$  its spectrum must have crossed the zero value, because of continuity. This means there exists a vector  $|\chi\rangle$  such that  $Q(t^*) = 0$ ,  $Q(t) > 0$  for  $t < t^*$  and  $Q(t) < 0$  for  $t > t^*$ . Therefore, entanglement creation can be detected by the presence of a negative first derivative of  $Q(t)$  at  $t = t^*$ . Moreover, since by assumption  $\rho(t^*)$  is separable, it is not restrictive to set  $t^* = 0$ . Formally, an initially separable state of the two atoms,  $\rho(0) = \tilde{\rho}(0)$  as in (4.1), becomes entangled via the nosy dynamics of the common bath within which they are immersed if there exists a vector  $|\chi\rangle^3$  such that:

1.  $Q(0) = 0$  and
2.  $\partial_t Q(0) < 0$ .

**Remark 4** The above-stated criterion is only sufficient for entanglement generation, but not necessary. The proof of its necessity is part of this PhD work and will be given in detail in Chapter 5.

Moreover, when  $\partial_t Q(0) = 0$ , special attention is required: in this case, higher order derivatives of  $Q(t)$  need to be examined in order to check entanglement creation.

Finally, now it will be shown how the above-stated criterion can be used concretely as a test for entanglement creation by a suitable manipulation of the expression for  $\partial_t Q(0)$ . First of all, in the two-dimensional Hilbert spaces pertaining to the two atoms the orthonormal bases  $\{|\varphi\rangle, |\tilde{\varphi}\rangle\}$  and  $\{|\psi\rangle, |\tilde{\psi}\rangle\}$  are introduced, where  $|\varphi\rangle, |\psi\rangle$  are the vectors defining  $\rho(0)$  in (4.1) and  $|\varphi\rangle, |\psi\rangle, |\tilde{\varphi}\rangle, |\tilde{\psi}\rangle$  can all be obtained from unitary rotations applied to the standard basis  $\{|0\rangle, |1\rangle\}$  of eigenstates of  $\sigma_3$  ( $\sigma_3|0\rangle = |0\rangle, \sigma_3|1\rangle = -|1\rangle$ ), i.e.:

$$|\varphi\rangle = U|0\rangle \quad |\tilde{\varphi}\rangle = U|1\rangle, \quad (4.5)$$

$$|\psi\rangle = V|0\rangle \quad |\tilde{\psi}\rangle = V|1\rangle. \quad (4.6)$$

Then, by using the orthogonal transformations  $\mathcal{U}$  and  $\mathcal{V}$  that  $U$  and  $V$  respectively induce on the Pauli matrices,

$$U^\dagger \sigma_i U = \sum_{j=1}^3 \mathcal{U}_{ij} \sigma_j, \quad V^\dagger \sigma_i V = \sum_{j=1}^3 \mathcal{V}_{ij} \sigma_j, \quad (4.7)$$

$\partial_t Q(0)$  can be written as a quadratic form in the components of the probe vector  $|\chi\rangle$ . This yields the following condition for entanglement generation:

<sup>3</sup>The vector  $|\chi\rangle$  must be chosen entangled, otherwise the quantity  $Q(t)$  can never be negative.

**Lemma 1** *There exists a vector  $|\chi\rangle$  such that  $\partial_t \mathcal{Q}(0) < 0$  if and only if its corresponding discriminant is negative, i.e. explicitly if and only if*

$$\langle u | \mathcal{A} | u \rangle \langle v | \mathcal{C}^T | v \rangle - |\langle v | (Re(\mathcal{B}) + i(H^{(12)})^T) | u \rangle|^2 < 0. \quad (4.8)$$

The three-dimensional vectors  $|u\rangle$  and  $|v\rangle$  contain the information about the initial factorized state (4.1) and their components can be expressed as follows:

$$u_i = \sum_{j=1}^3 \mathcal{U}_{ij} \langle 0 | \sigma_j | 1 \rangle, \quad v_i = \sum_{j=1}^3 \mathcal{V}_{ij} \langle 1 | \sigma_j | 0 \rangle. \quad (4.9)$$

An explicit operational sufficient condition for environment-induced entanglement to be generated between two atoms immersed in common bath and initially in a separable state has thus been found: the external quantum fields can create entanglement between two atoms evolving with the Markovian dynamics generated by (2.28) and characterized by the Kossakowski matrix (2.32), if there exist orthogonal transformations  $\mathcal{U}$  and  $\mathcal{V}$  such that the inequality (4.8) is satisfied. From a physical point of view, this means that, in order for the bath to create entanglement, the contributions coming from the interaction Hamiltonian,  $H_{eff}^{(12)}$ , and from the part of the dissipative term involving both atoms together,  $\mathcal{B}$ , must be sufficiently strong compared to the pieces of the Kossakowski matrix pertaining to the two atoms separately,  $\mathcal{A}$  and  $\mathcal{C}$ .

The entanglement test in (4.8) is very general and can be applied to all situations in which a bipartite system is undergoing a dissipative Markovian evolution in an external environment.

If, in particular, the two atoms composing the subsystem interact with the same set of external fields, then the field operators can be taken to be the same in (2.27), i.e.  $\Psi_i = \Phi_i$ . This implies that all three submatrices appearing in the Kossakowski matrix (2.32) are identical,  $[\mathcal{A}_{ij}] = [\mathcal{B}_{ij}] = [\mathcal{C}_{ij}]$ , and they all become equal to the Kossakowski matrix for a single atom [5]

$$\mathcal{A}_{ij} = \mathcal{B}_{ij} = \mathcal{C}_{ij} = A\delta_{ij} - iB\epsilon_{ijk}n_k + Cn_in_j, \quad (4.10)$$

where the quantities  $A, B, C$  depend on the system frequency  $\omega$  and on the inverse temperature  $\beta$  [5]

$$A = \frac{\omega}{4\pi} \left[ \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}} \right], \quad B = \frac{\omega}{4\pi}, \quad (4.11)$$

$$C = \frac{\omega}{4\pi} \left[ \frac{2}{\beta\omega} - \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}} \right]. \quad (4.12)$$

In this case, the Hamiltonian pieces (2.29) and (2.30) are also simplified: the single-atom terms  $H_{eff}^{(1)}$  and  $H_{eff}^{(2)}$  can be written exactly as in the original system Hamiltonian (2.26) with a renormalized frequency  $\tilde{\omega}$  replacing the system frequency  $\omega$  [5], while the direct

two-atom coupling term can be expressed as

$$H_{eff}^{(12)} = -\frac{i}{2} \sum_{i,j=1}^3 \{[\mathcal{K}_\beta(\omega) + \mathcal{K}_\beta(-\omega)]\delta_{ij} + [2\mathcal{K}_\beta(0) - \mathcal{K}_\beta(\omega) - \mathcal{K}_\beta(-\omega)]n_i n_j\}(\sigma_i \otimes \sigma_j),$$

where  $n_i, i = 1, 2, 3$ , are the components of a unit vector and  $\mathcal{K}_\beta(\omega) := \frac{\mathcal{P}}{i\pi} \int_{-\infty}^{+\infty} dz \frac{\mathcal{G}_\beta(z)}{z-\omega}$  is the scalar Wightmann function ( $\mathcal{P}$  indicates the principal value) [5].

The function  $\mathcal{K}_\beta(\omega)$  can be split into a vacuum term and a temperature-dependent piece [5]; the latter contribution, however, is odd in  $\omega$ , so it follows that  $H_{eff}^{(12)}$  does not actually involve  $T = \beta^{-1}$ , because it is the same Lamb shift that would have been generated in the case of a two-atom system in the vacuum. Since the focus here is on temperature-induced phenomena, this vacuum-related term will not be considered in the following and the attention will be concentrated just on the effects of the dissipative contribution  $\mathbf{D}^{(2)}[\rho]$  in (2.31).

Now, in this simplified scenario, condition (4.8) for entanglement generation can also be written in a compacter form, since it only involves the one Hermitian  $3 \times 3$  matrix  $\mathcal{A} \equiv [\mathcal{A}_{ij}]$ . Indeed, by taking  $u_i = v_i$  in (4.9), from (4.7) it follows that  $|\psi\rangle = |\tilde{\varphi}\rangle$  in (4.5), and the entanglement condition (4.8) thus reduces to:

$$|\langle u | \text{Im}(\mathcal{A}) | u \rangle|^2 > 0. \quad (4.13)$$

Therefore, as long as  $\mathcal{A}$  is not real, i.e. the parameter  $B$  in (4.10) is nonzero, entanglement between the two atoms can be generated through their weak coupling to the common bath in which they are immersed.

It must be noted, however, that this happens only for small times: neither (4.13) nor the more general condition (4.10) can say anything about asymptotic entanglement. In order to study the latter, the structure of the dynamics generated by the master equation (2.28) must be analyzed directly, as was seen in Chapter 2.

## 4.2 Asymptotic entanglement

In this section, the possibility of asymptotic persistence of entanglement in a system composed of two qubits immersed in a common bath will be studied. This will be done in the simplified scenario considered in Section 2.4.2, i.e. in the case of a Kossakowski

matrix of the form  $K = \begin{pmatrix} \mathcal{A} & \mathcal{A} \\ \mathcal{A} & \mathcal{A} \end{pmatrix}$  and master equation

$$\partial_t \varrho_t = \mathbf{L}[\varrho_t] = -i \frac{\Omega}{2} [\Sigma_3, \varrho_t] + \sum_{i,j=1}^3 \mathcal{A}_{ij} \left( \Sigma_i \varrho_t \Sigma_j - \frac{1}{2} \{ \Sigma_j \Sigma_i, \varrho_t \} \right), \quad (4.14)$$

where  $\Omega$  is the system frequency,  $\Sigma_i := \sigma_i \otimes I_2 + I_2 \otimes \sigma_i$ ,  $I_2$  is the  $2 \times 2$  identity matrix,  $\sigma_i, i = 1, 2, 3$  are the Pauli matrices.



This master equation is dual to the one in (2.42) and from Propositions 2 and 3 in Chapter 2 it follows that in this case the asymptotic states can be written as

$$\varrho_\infty \equiv E[\varrho_{in}] = \frac{1}{4} \left[ I_2 \otimes I_2 + \sum_{i=1}^3 \hat{\varrho}_i \Sigma_i + \sum_{i,j=1}^3 \hat{\varrho}_{ij} S_{ij} \right], \quad (4.15)$$

where the coefficients  $\hat{\varrho}_{ij} = \hat{\varrho}_{ji}$  depend on the initial state, as will be shown in the following, and  $S_{ij} := \sigma_i \otimes \sigma_j + \sigma_j \otimes \sigma_i$  ( $i = 1, 2, 3$ ). Further, from explicit computation (see, e.g., [5]) it can be seen that for a dynamical generator as in (4.14) the stationary faithful state is of the form

$$\varrho_0 = \frac{1}{2} (I_2 - R\vec{n} \cdot \vec{\sigma}) \otimes \frac{1}{2} (I_2 - R\vec{n} \cdot \vec{\sigma}), \quad (4.16)$$

with  $R$  the temperature ratio <sup>4</sup>  $R := B/A = \frac{1-e^{-\beta\omega}}{1+e^{-\beta\omega}}$  (where  $A, B$  are the quantities defined in (4.11) and  $\beta \equiv T^{-1}$ ).

In order to explicitly find the components  $\hat{\varrho}_i$  and  $\hat{\varrho}_{ij}$  of (4.15), it proves convenient to decompose the  $4 \times 4$  density matrix  $\varrho(t)$  describing the state of the two atoms along the Pauli matrices, in analogy to the Bloch decomposition for one atom:

$$\varrho(t) = \frac{1}{4} \left[ I_2 \otimes I_2 + \sum_{i=1}^3 \varrho_{0i}(t) I_2 \otimes \sigma_i + \sum_{i=1}^3 \varrho_{i0}(t) \sigma_i \otimes I_2 + \sum_{i,j=1}^3 \varrho_{ij}(t) \sigma_i \otimes \sigma_j \right], \quad (4.17)$$

where the components  $\varrho_{0i}(t)$ ,  $\varrho_{i0}(t)$ ,  $\varrho_{ij}(t)$  are all real.

Then, inserting the expression (4.16) into (2.43) and (4.17) into (4.14), the explicit form of the set of all equilibrium states of the dynamics (4.14) can be derived and yields:

$$\begin{aligned} \hat{\varrho}_i &= -\frac{R}{3+R^2} (\tau+3) n_i \\ \hat{\varrho}_{ij} &= \frac{1}{2(3+R^2)} [(\tau-R^2) \delta_{ij} + R^2 (\tau+3) n_i n_j], \end{aligned} \quad (4.18)$$

where  $\tau := \sum_{i=1}^3 \varrho_{ii}$  represents the trace of  $\varrho_{ij}$  from (4.17) and is a constant of motion. Further, the requirement of positivity of the initial density matrix  $\varrho(0)$  implies that  $-3 \leq \tau \leq 1$ . From (4.18) it can be seen that the stationary density matrices depend on the initial condition  $\varrho(0)$  only through the value of  $\tau$ .

As seen in the previous section, in some conditions the external bath within which the two atoms are immersed is able to generate entanglement for small times in an initially separable state of the two atoms via the noisy dynamics. On the other hand, though, the effect of the environment on a subsystem immersed within it, in general, is decoherence and thermalization. Therefore, it could seem remarkable that any entanglement initially generated between the two atoms by the external fields might persist even in the asymptotic state.

<sup>4</sup>Notice that  $0 \leq R \leq 1$  and the two boundary values correspond to the infinite and zero temperature limits, respectively.

Now, in order to see whether there is any entanglement in the asymptotic state of the dynamics (4.14) of the two atoms, one could simply use condition (4.13). Since the system considered consists of two two-level subsystems, however, it is more convenient to use the *concurrence* (see Section 1.3.3) to see whether the asymptotic state is entangled or not: indeed, the concurrence is an entanglement measure, so it would not only reveal the presence of entanglement in the asymptotic state, but it would also *quantify* it.

In the case of the asymptotic state given in (4.18), the concurrence explicitly reads:

$$C[\hat{\rho}] = \max \left\{ 0, \frac{(3 - R^2)}{2(3 + R^2)} \left[ \frac{5R^2 - 3}{3 - R^2} - \tau \right] \right\}. \quad (4.19)$$

The concurrence (4.19) is a decreasing function of  $\tau$ , with maximum value  $C[\hat{\rho}] = 1$  for  $\tau = -3$  and minimum  $C[\hat{\rho}] = 0$  for  $\tau = (5R^2 - 3)/(3 - R^2)$ . Therefore the asymptotic state (4.18) can indeed be entangled, provided the initial state  $\rho(0)$  is such that

$$\tau < \frac{5R^2 - 3}{3 - R^2}.$$

This is a very interesting result, since it implies that the dissipative dynamics given by the master equation (4.14) not only can generate entanglement for small times, but it can also enhance it in the asymptotic long-time regime.

With this in mind, in the next two chapters, entanglement in open quantum systems is analyzed from both perspectives: in the first one, the necessity of condition (4.8) is proved, thus studying entanglement generation for small times; while in the second one, given a dissipative evolution that satisfies (4.13) and is thus known to be able to create entanglement, the asymptotic behavior of entanglement is analyzed in detail for a particular class of states.

## Chapter 5

# Environment-Induced Bipartite Entanglement

### 5.1 Introduction

In this chapter, bipartite systems, consisting first of two qubits and then of two subsystems of arbitrary dimension, immersed in a common bath are considered.

As seen in Chapter 2, the typical effect of noise and dissipation on a system  $S$  immersed in a large environment  $E$  is decoherence; as shown in Chapter 4, however, in certain specific situations, the environment  $E$  may even build quantum correlations between the subsystems which compose  $S$ . This possibility depends on the form of the Kossakowski matrix that characterizes the dissipative part  $\mathbf{D}$  of the generator  $\mathbf{L}$ . As shown in Section 4.1, in [10] an inequality was found, involving the entries of such a matrix which, if fulfilled, is sufficient to ensure that a specific initial separable pure state of two qubits gets entangled.

This inequality is basically derived by looking at first derivatives of evolving mean values that involve the generator only and not its powers. In this chapter it is proved that, apart from marginal cases whose control needs second or higher powers of the generator, this inequality is also necessary for entangling two qubits via immersion within a common environment.

Further, higher dimensional bipartite systems are considered, composed of two  $d$ -level subsystems embedded in a common environment, and sets of inequalities involving the entries of a higher rank Kossakowski matrix are provided. It turns out that if at least one of these inequalities is fulfilled, the two parties get entangled by their reduced dynamics.

## 5.2 Entanglement generation between two qubits

In this section a system  $S$  will be considered that is composed of two initially separable qubits immersed in a common external bath  $E$  with which they weakly interact, but not directly interacting between each other ([5], pages 3124-3126); thus the total Hamiltonian is  $H_T = H_1 + H_2 + H_B + \lambda H_I$ , where  $H_1, H_2$  and  $H_B$  are Hamiltonians pertaining to the first and second qubit, respectively the bath within which they are immersed, while the interaction Hamiltonian is given by  $H_I = \sum_{i=1}^3 ((\sigma_i \otimes I_2) \otimes B_i^{(1)} + (I_2 \otimes \sigma_i) \otimes B_i^{(2)})$  with  $I_2$  the identity  $2 \times 2$  matrix and  $B_i^{(a)}$ ,  $a = 1, 2$ ,  $i = 1, 2, 3$ , bath operators that describe the interaction with the two qubits. In the following, the convenient notation  $\sigma_i^{(1)} := \sigma_i \otimes I_2$  and  $\sigma_i^{(2)} := I_2 \otimes \sigma_i$  will be used, and the explicit expressions for the two-qubit master equation (2.28), the effective Hamiltonian (2.29)-(2.30) and the dissipative term (2.33) given in Chapter 2 will be repeated here for the benefit of the reader. As seen in Chapters 2 and 4, by means of standard *weak coupling limit* techniques, the reduced dynamics of  $S$  is given by the Master equation [5, 59, 64]

$$\frac{\partial \varrho_t}{\partial t} = \mathbf{L}_H[\varrho_t] + \mathbf{D}[\varrho_t] = -i[H_{eff}, \varrho_t] + \mathbf{D}[\varrho_t] \quad (5.1)$$

where  $H_{eff} = H_{eff}^{(1)} + H_{eff}^{(2)} + H_{eff}^{(12)}$ , with  $H_{eff}^{(a)} = \sum_{i=1}^3 H_i^{(a)} \sigma_i^{(a)}$ ,  $H_i^{(a)} \in \mathbb{R}$ ,  $a = 1, 2$ , Hamiltonians of the two qubits independently,

$$H_{eff}^{(12)} = \sum_{i,j=1}^3 H_{ij}^{(12)} (\sigma_i \otimes \sigma_j), \quad H_{ij}^{(12)} \in \mathbb{R}, \quad (5.2)$$

a Hamiltonian term describing a bath-mediated interaction between the qubits, while

$$\begin{aligned} \mathbf{D}[\varrho(t)] = & \sum_{i,j=1}^3 \left( \mathcal{A}_{ij} \left[ \sigma_j^{(1)} \varrho \sigma_i^{(1)} - \frac{1}{2} \{ \sigma_i^{(1)} \sigma_j^{(1)}, \varrho \} \right] \right. \\ & + \mathcal{C}_{ij} \left[ \sigma_j^{(2)} \varrho \sigma_i^{(2)} - \frac{1}{2} \{ \sigma_i^{(2)} \sigma_j^{(2)}, \varrho \} \right] \\ & + \mathcal{B}_{ij} \left[ \sigma_j^{(1)} \varrho \sigma_i^{(2)} - \frac{1}{2} \{ \sigma_j^{(1)} \sigma_i^{(2)}, \varrho \} \right] \\ & \left. + \mathcal{B}_{ji}^* \left[ \sigma_j^{(2)} \varrho \sigma_i^{(1)} - \frac{1}{2} \{ \sigma_i^{(1)} \sigma_j^{(2)}, \varrho \} \right] \right) \end{aligned} \quad (5.3)$$

is a Kossakowski-Lindblad contribution describing dissipation and noise<sup>1</sup>. The  $3 \times 3$  matrices  $\mathcal{A} = \mathcal{A}^\dagger$ ,  $\mathcal{C} = \mathcal{C}^\dagger$  and  $\mathcal{B}$  form the so-called Kossakowski matrix

$$K = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^\dagger & \mathcal{C} \end{pmatrix}, \quad (5.4)$$

<sup>1</sup>In the following the dissipative term will be denoted simply as  $\mathbf{D}$ , instead of  $\mathbf{D}^{(2)}$ , to make the notation less cumbersome.

which must be positive semi-definite to ensure the physical consistency of the reduced dynamics of  $S$  [56, 59].

It is natural to call the generated semigroup entangling if there exist at least two vector states  $|\psi\rangle$  and  $|\varphi\rangle$  of the two parties such that  $\gamma_t[Q]$  is entangled for some  $t > 0$ , where  $Q := |\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi|^2$ .

Because of the Peres-Horodecki criterion [16], in the case of two qubits the semigroup  $\gamma_t$  is entangling if and only if there exist such a  $Q$  and  $t > 0$  such that  $T^{(2)} \circ \gamma_t[Q]$  is not positive definite, where  $T^{(2)} \equiv (\text{id} \otimes T) : M_4(\mathbb{C}) \mapsto M_4(\mathbb{C})$  is the partial transposition on the second qubit with  $\text{id} : M_2(\mathbb{C}) \mapsto M_2(\mathbb{C})$  the identity operation on the first qubit and  $T : M_2(\mathbb{C}) \mapsto M_2(\mathbb{C})$  is the transposition with respect to the basis of eigenvectors of the Pauli matrix  $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ .

Since  $T \circ T = \text{id}$ , the maps  $\tilde{\gamma}_t := T^{(2)} \circ \gamma_t \circ T^{(2)}$  form a semigroup, namely

$$\tilde{\gamma}_s \circ \tilde{\gamma}_t = \tilde{\gamma}_t \circ \tilde{\gamma}_s = \tilde{\gamma}_{s+t}, \quad \forall s, t \geq 0, \quad (5.5)$$

with generator  $\tilde{\mathbf{L}} := T^{(2)} \circ \mathbf{L} \circ T^{(2)}$ . Setting  $\tilde{Q} := T^{(2)}[Q] = |\psi\rangle\langle\psi| \otimes |\varphi^*\rangle\langle\varphi^*|$ , where  $|\varphi^*\rangle$  denotes the vector state whose components in the chosen basis are the conjugates of those of  $|\varphi\rangle$ ,  $\gamma_t$  results entangling if and only if there exist a  $Q$  and  $t > 0$  such that  $\tilde{\gamma}_t[\tilde{Q}] \not\geq 0$ .

**Proposition 4** *The semigroup  $\gamma_t : M_4(\mathbb{C}) \mapsto M_4(\mathbb{C})$  is entangling if there exist a separable initial projector  $Q \in M_4(\mathbb{C})$  and a vector  $\Phi \in \mathbb{C}^4$  such that:*

$$\langle \Phi | \tilde{Q} | \Phi \rangle = 0 \quad \text{and} \quad \langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle < 0. \quad (5.6)$$

*Vice versa, the semigroup  $\gamma_t$  cannot be entangling if*

$$\langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle > 0 \quad (5.7)$$

*for all initial separable projectors  $Q \in M_4(\mathbb{C})$  and vectors  $\Phi \in \mathbb{C}^4$  such that  $\langle \Phi | \tilde{Q} | \Phi \rangle = 0$ .*

**Remark 5** Notice that in case of an equality, the argument of Proposition 4 cannot be used to conclude that entanglement is or is not generated by the semigroup  $\gamma_t$ . A concrete instance of this fact will be given in Example 1.

**Proof:** As stated above,  $\gamma_t$  results entangling if and only if there exist  $Q$  and  $t > 0$  such that  $\tilde{\gamma}_t[\tilde{Q}] \not\geq 0$ , i.e. if and only if there exist  $Q, t > 0$  and  $\Phi \in \mathbb{C}^4$  such that  $\langle \Phi | \tilde{\gamma}_t[\tilde{Q}] | \Phi \rangle < 0$ . Since  $\langle \Phi | \tilde{Q} | \Phi \rangle \geq 0$ , the latter condition is equivalent to the existence of a smallest  $t^* \geq 0$  and  $\epsilon_0 > 0$  such that

$$\langle \Phi | \tilde{\gamma}_{t^*}[\tilde{Q}] | \Phi \rangle = 0 \quad (a) \quad \text{and} \quad \langle \Phi | \tilde{\gamma}_{t^*+\epsilon}[\tilde{Q}] | \Phi \rangle < 0 \quad \forall \epsilon_0 \geq \epsilon > 0 \quad (b).$$

<sup>2</sup>Notice that if  $\gamma_t$  cannot entangle initially separable pure states then it cannot entangle separable mixed states.

The assumption on  $t^*$  means that  $\tilde{\gamma}_{t^*}[\tilde{Q}]$  is still separable, whence it can be decomposed in a convex sum of pure separable projectors,  $\tilde{\gamma}_{t^*}[\tilde{Q}] = \sum_{i,j} \lambda_{ij} Q_{ij}$ ,  $0 \leq \lambda_{ij} \leq 1$ . Then, condition (a) implies  $\langle \Phi | Q_{ij} | \Phi \rangle = 0$  for all  $Q_{ij}$ , while, from the semigroup composition law (5.5) and condition (b) it follows that there exist  $i$  and  $j$  such that  $\langle \Phi | \tilde{\gamma}_\epsilon[Q_{ij}] | \Phi \rangle < 0$  for all  $0 < \epsilon \leq \epsilon_0$ . The continuity of the semigroup formed by the  $\tilde{\gamma}_t$  implies that (see for instance [52])

$$\lim_{\epsilon \rightarrow 0^+} \langle \Phi | \frac{\tilde{\gamma}_\epsilon[Q_{ij}] - Q_{ij}}{\epsilon} | \Phi \rangle = \langle \Phi | \tilde{\mathbf{L}}[Q_{ij}] | \Phi \rangle = \lim_{\epsilon \rightarrow 0^+} \frac{\langle \Phi | \tilde{\gamma}_\epsilon[Q_{ij}] | \Phi \rangle}{\epsilon}.$$

If  $\gamma_t$  is entangling, then for at least one of the  $Q_{ij}$  it must be true that  $\langle \Phi | Q_{ij} | \Phi \rangle = 0$  and  $\langle \Phi | \tilde{\mathbf{L}}[Q_{ij}] | \Phi \rangle < 0$ , so that if (5.7) holds as stated,  $\gamma_t$  cannot be entangling. Vice versa, if (5.6) holds then  $\tilde{\gamma}_t[\tilde{Q}] \not\geq 0$  in a right neighborhood of  $t = 0$  and the semigroup  $\gamma_t$  is entangling. □

In order to concretely apply the previous result, the following notations will be introduced. For given  $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^2$ , let  $|u\rangle, |v\rangle$  denote the vectors in  $\mathbb{C}^3$  with components

$$u_i := \langle \psi | \sigma_i | \psi_\perp \rangle, \quad v_i := \epsilon_i \langle \varphi^* | \sigma_i | \varphi^* \rangle = \langle \varphi_\perp | \sigma_i | \varphi \rangle, \quad (5.8)$$

where  $\sigma_i, i = 1, 2, 3$  are the Pauli matrices in the chosen standard representation, whence, under transposition,  $\sigma_i^T = \epsilon_i \sigma_i$ , with  $\epsilon_i = +1$  when  $i = 1, 3$  and  $\epsilon_i = -1$  when  $i = 2$ . Moreover,  $\{\psi, \psi_\perp\}, \{\varphi, \varphi_\perp\}$  are the orthonormal bases in  $\mathbb{C}^2$  corresponding to  $\psi$  and  $\varphi$ . Let  $\mathcal{C}^T$  denote the transposition of the  $3 \times 3$  matrix  $\mathcal{C}$  in (5.4),  $Re(\mathcal{B})$  the  $3 \times 3$  matrix whose entries are  $Re(\mathcal{B})_{ij} := \frac{\mathcal{B}_{ij} + \mathcal{B}_{ij}^*}{2}$  and  $H^{(12)}$  is the  $3 \times 3$  real matrix formed by the coefficients  $H_{ij}^{(12)}$  of  $H_{eff}^{(12)}$  in (5.2).

From Proposition 4, it follows that we have to focus on  $\tilde{\mathbf{L}}[\tilde{Q}]$ . When  $\mathbf{L} = \mathbf{L}_H + \mathbf{D}$  as

in (5.2) and in (5.3), the action of the new generator explicitly reads

$$\begin{aligned}
\tilde{\mathbf{L}}[\varrho] &:= T^{(2)} \circ \mathbf{L} \circ T^{(2)}[\varrho] = -i \sum_{i=1}^3 \left[ H_i^{(1)} \sigma_i^{(1)} + H_i^{(2)} \epsilon_i \sigma_i^{(2)}, \varrho \right] \\
&+ \sum_{i,j=1}^3 \left( i H_{ij}^{(12)} \epsilon_j \sigma_j^{(2)} \varrho \sigma_i^{(1)} - i H_{ij}^{(12)} \epsilon_j \sigma_i^{(1)} \varrho \sigma_j^{(2)} \right) \\
&+ \sum_{i,j=1}^3 \mathcal{A}_{ij} \left( \sigma_j^{(1)} \varrho \sigma_i^{(1)} - \frac{1}{2} \left\{ \sigma_i^{(1)} \sigma_j^{(1)}, \varrho \right\} \right) \\
&+ \sum_{i,j=1}^3 \mathcal{C}_{ji} \epsilon_i \epsilon_j \left( \sigma_j^{(2)} \varrho \sigma_i^{(2)} - \frac{1}{2} \left\{ \sigma_i^{(2)} \sigma_j^{(2)}, \varrho \right\} \right) \\
&+ \sum_{i,j=1}^3 \mathcal{B}_{ij} \epsilon_i \left( \sigma_j^{(1)} \sigma_i^{(2)} \varrho - \frac{1}{2} \sigma_j^{(1)} \varrho \sigma_i^{(2)} - \frac{1}{2} \sigma_i^{(2)} \varrho \sigma_j^{(1)} \right) \\
&+ \sum_{i,j=1}^3 \mathcal{B}_{ji}^* \epsilon_j \left( \varrho \sigma_i^{(1)} \sigma_j^{(2)} - \frac{1}{2} \sigma_i^{(1)} \varrho \sigma_j^{(2)} - \frac{1}{2} \sigma_j^{(2)} \varrho \sigma_i^{(1)} \right). \tag{5.9}
\end{aligned}$$

By regrouping the terms in (5.9) as in (5.3), it can be seen that, with respect to (5.4), the Kossakowski matrix associated with  $\tilde{\mathbf{L}}$  is now

$$\tilde{K} = \begin{pmatrix} \mathcal{A} & \tilde{\mathcal{B}} \\ \tilde{\mathcal{B}}^\dagger & \tilde{\mathcal{C}} \end{pmatrix}, \quad \tilde{\mathcal{B}}_{ij} := -\epsilon_i \left( \frac{\mathcal{B}_{ij} + \mathcal{B}_{ij}^*}{2} + i H_{ji}^{(12)} \right), \quad \tilde{\mathcal{C}}_{ij} = \epsilon_i \epsilon_j \mathcal{C}_{ji}. \tag{5.10}$$

Notice that, in spite of the fact that (5.4) is positive semi-definite,  $\tilde{K}$  need not be so and therefore  $\tilde{\gamma}_t$  is not necessarily completely positive or even positive; this allows for the possibility that  $\tilde{\gamma}_t[\tilde{Q}]$  be not positive semi-definite.

From Proposition 4 it follows that the focus can be limited to the mean values of  $\tilde{\mathbf{L}}[\tilde{Q}]$  with respect to vectors  $\Phi \in \mathbb{C}^4$  that belong to the subspace orthogonal to  $\tilde{Q}$ . Therefore, the attention can be restricted upon the matrix  $\tilde{Q}^\perp \tilde{\mathbf{L}}[\tilde{Q}] \tilde{Q}^\perp$ ,  $\tilde{Q}^\perp := I_2 - \tilde{Q}$ , that will be represented with respect to the following orthonormal basis

$$\begin{aligned}
|\Psi_1\rangle &:= |\psi\rangle \otimes |\varphi^*\rangle, & |\Psi_2\rangle &:= |\psi\rangle \otimes |\varphi_\perp^*\rangle, \\
|\Psi_3\rangle &:= |\psi_\perp\rangle \otimes |\varphi^*\rangle, & |\Psi_4\rangle &:= |\psi_\perp\rangle \otimes |\varphi_\perp^*\rangle,
\end{aligned} \tag{5.11}$$

where  $|\psi\rangle, |\varphi\rangle$  are the 2-dimensional vectors which define  $Q$ , and  $\tilde{Q} = |\Psi_1\rangle\langle\Psi_1|$ .

In calculating the matrix elements  $\langle\Psi_i|\tilde{\mathbf{L}}[\tilde{Q}]\Psi_j\rangle$ , it can be seen that only two scalar products contribute to them, either of the form  $\langle\Psi_i|I_2 \otimes \sigma_j|\Psi_1\rangle$  or of the form  $\langle\Psi_i|\sigma_j \otimes I_2|\Psi_1\rangle$ .

So  $\mathbf{L}^\perp := \tilde{Q}^\perp \tilde{\mathbf{L}}[\tilde{Q}] \tilde{Q}^\perp = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & M_{22} & M_{23} & 0 \\ 0 & M_{23}^* & M_{33} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ , where  $M_{ij} := \langle \Psi_i | \tilde{\mathbf{L}}[\tilde{Q}] | \Psi_j \rangle$ ; explicitly,

$$M_{22} = \sum_{i,j} \mathcal{C}_{ji} \epsilon_i \epsilon_j \langle \varphi_\perp^* | \sigma_j | \varphi^* \rangle \langle \varphi^* | \sigma_i | \varphi_\perp^* \rangle = \langle v | \mathcal{C}^T | v \rangle \quad (5.12)$$

$$M_{33} = \sum_{i,j} \mathcal{A}_{ij} \langle \psi_\perp | \sigma_j | \psi \rangle \langle \psi | \sigma_i | \psi_\perp \rangle = \langle u | \mathcal{A} | u \rangle \quad (5.13)$$

$$\begin{aligned} M_{23} &= - \sum_{i,j} \left( i H_{ij}^{(12)} + \frac{\mathcal{B}_{ji} + \mathcal{B}_{ji}^*}{2} \right) \epsilon_j \langle \varphi_\perp^* | \sigma_j | \varphi^* \rangle \langle \psi | \sigma_i | \psi_\perp \rangle \\ &= - \langle v | \left( i(H^{(12)})^T + \text{Re}(\mathcal{B}) \right) | u \rangle. \end{aligned} \quad (5.14)$$

**Proposition 5** Given an initial projector  $M_4(\mathbb{C}) \ni Q = |\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi|$ , with  $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^2$ , consider the matrix  $M = \begin{pmatrix} M_{22} & M_{23} \\ M_{23}^* & M_{33} \end{pmatrix}$  with entries as in (5.12)–(5.14). Then,

1. if  $\det(M) \equiv \langle u | \mathcal{A} | u \rangle \langle v | \mathcal{C}^T | v \rangle - |\langle v | \left( \text{Re}(\mathcal{B}) + i(H^{(12)})^T \right) | u \rangle|^2 < 0$ , for at least one pair  $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^2$ , the semigroup  $\gamma_t$  with generator as in (5.1), (5.2), (5.3) entangles  $Q$ ;
2. if  $\det(M) \equiv \langle u | \mathcal{A} | u \rangle \langle v | \mathcal{C}^T | v \rangle - |\langle v | \left( \text{Re}(\mathcal{B}) + i(H^{(12)})^T \right) | u \rangle|^2 > 0$ , for all choices of  $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^2$ , the semigroup  $\gamma_t$  is not entangling.

**Proof:** The proof of the first statement is a simple application of Proposition 4.

If  $\det(M) < 0$ , there exists a vector  $|\Phi\rangle$  such that  $\tilde{Q}|\Phi\rangle = 0$  and  $\langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle < 0$ . Then a first order expansion in  $t \geq 0$  gives  $\langle \Phi | \tilde{\gamma}_t[\tilde{Q}] | \Phi \rangle \simeq t \langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle < 0$ . This implies that  $\tilde{\gamma}_t[\tilde{Q}]$  is not positive semi-definite in a right neighborhood of  $t = 0$ , whence  $\gamma_t[Q]$  is entangled<sup>3</sup>.

If  $\det(M) > 0$ , then (5.7) holds so, if  $\tilde{Q}|\Phi\rangle = 0$  and  $\Phi \neq \Psi_4$  (and  $\Phi \neq \Psi_1$  since only the subspace orthogonal to  $\tilde{Q} = |\Psi_1\rangle\langle\Psi_1|$  needs to be considered), a first order expansion in  $t \geq 0$  gives  $\langle \Phi | \tilde{\gamma}_t[\tilde{Q}] | \Phi \rangle \simeq t \langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle = t \langle \Phi | \mathbf{L}^\perp | \Phi \rangle > 0$ .

If  $\Phi = \Psi_4$ , then  $\langle \Phi | \mathbf{L}^\perp | \Phi \rangle = 0$  and the argument based on the first derivative seems to be not conclusive; however,  $\Psi_4$  is separable and therefore  $\langle \Psi_4 | \tilde{\gamma}_t[\tilde{Q}] | \Psi_4 \rangle \geq 0$  for all  $t \geq 0$ . Hence, if  $\det(M) > 0$  for all choices of  $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^2$ ,  $\gamma_t$  cannot be entangling.  $\square$

Unlike the last part of the previous proof, when  $M$  has an eigenvalue equal to zero, namely if  $\langle u | \mathcal{A} | u \rangle \langle v | \mathcal{C}^T | v \rangle = |\langle v | \left( \text{Re}(\mathcal{B}) + i(H^{(12)})^T \right) | u \rangle|^2$ , then, in order to check whether the semigroup  $\gamma_t$  is entangling or not, it is necessary to go to the second or higher order terms in the small  $t \geq 0$  expansion of  $\langle \Psi | \tilde{\gamma}_t[\tilde{Q}] | \Psi \rangle$ . In fact, if  $\det(M) = 0$ , there exists  $|\Psi_\perp^\perp\rangle$  such that  $\mathbf{L}^\perp |\Psi_\perp^\perp\rangle = 0$  so that  $\langle \Psi_\perp^\perp | \tilde{\gamma}_t[\tilde{Q}] | \Psi_\perp^\perp \rangle \simeq t^2/2 \langle \Psi_\perp^\perp | \tilde{\mathbf{L}}^2[\tilde{Q}] | \Psi_\perp^\perp \rangle$ . As the following example shows, the non-negativity of the matrix  $M$  does not fix the non-entangling

<sup>3</sup>This is essentially what was proved in [10].



character of  $\gamma_t$ : strict positivity as in point 2. of Proposition 5 is necessary for this to be true.

**Example 1** For sake of simplicity, the Hamiltonian terms in (5.1) will be set to zero and the following Kossakowski matrix will be considered:

$$K = \begin{pmatrix} \mathcal{A} & \mathcal{A} \\ \mathcal{A} & \mathcal{A} \end{pmatrix} \quad \text{with} \quad \mathcal{A} = \begin{pmatrix} 1 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & x \end{pmatrix},$$

with  $x \geq 1$  so that  $K \geq 0$ . Using the notation  $\sigma_i^{(1)} \equiv \sigma_i \otimes I_2$ ,  $\sigma_i^{(2)} \equiv I_2 \otimes \sigma_i$ , the purely dissipative generator can be written as [5]

$$\mathbf{L}^{(2)}[\rho] \equiv \mathbf{D}^{(2)}[\rho] = \sum_{i,j=1}^3 \sum_{p,q=1}^2 \mathcal{A}_{ij} \left( \sigma_j^{(p)} \rho \sigma_i^{(q)} - \frac{1}{2} \left\{ \sigma_i^{(q)} \sigma_j^{(p)}, \rho \right\} \right), \quad (5.15)$$

and it generates a continuous one-parameter semigroup of completely positive maps  $\gamma_t = e^{t\mathbf{L}}$ . The Kossakowski matrix (5.10) associated with the generator  $\tilde{\mathbf{L}}$  of  $\tilde{\gamma}_t := T^{(2)} \circ \gamma_t \circ T^{(2)}$  reads

$$\tilde{K} = \begin{pmatrix} \mathcal{A} & -Re(\mathcal{A}) \\ -Re(\mathcal{A})^\dagger & \mathcal{A}^T \end{pmatrix} = \begin{pmatrix} 1 & 0 & i & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -i & 0 & x & 0 & 0 & -x \\ -1 & 0 & 0 & 1 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -x & i & 0 & x \end{pmatrix}$$

and is not positive definite, its non-zero eigenvalues being  $1 \pm \sqrt{2}$  and  $x \pm \sqrt{1+x^2}$ . This ensures that  $\tilde{\gamma}_t$  is not completely positive; moreover, it turns out that, for some values of  $x$ , it is not even positivity preserving, leaving a chance that for some initial separable projector  $Q$  there exists  $t > 0$  such that  $\tilde{\gamma}_t[\tilde{Q}]$  might not be positive semi-definite.

Indeed, let  $Q = |0\rangle\langle 0| \otimes |0\rangle\langle 0| = \tilde{Q}$  where  $\sigma_3|0\rangle = |0\rangle$  and  $\sigma_3|1\rangle = -|1\rangle$ ; then,  $|u\rangle = |v\rangle = (1, -i, 0)$ , and  $\langle u|\mathcal{A}|u\rangle = \langle u|\mathcal{A}^T|u\rangle = \langle u|Re(\mathcal{A})|u\rangle = 1$ . Therefore,  $\det(M) = 0$

and the vector  $|\Psi_1^\perp\rangle = |\Psi_2\rangle + |\Psi_3\rangle$  is eigenvector of  $\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$  with eigenvalue

0. Considering the second order term in the expansion of  $\langle \Psi_1^\perp | \tilde{\gamma}_t[\tilde{Q}] | \Psi_1^\perp \rangle$ , explicit calculations give  $\langle \Psi_1^\perp | \tilde{\mathbf{L}}^2[\tilde{Q}] | \Psi_1^\perp \rangle = 16x - 24$ . Thus, the semigroup  $\tilde{\gamma}_t$  is not positivity preserving and  $\gamma_t = e^{t\mathbf{L}}$  has different entangling properties depending on the value of parameter  $x$ :  $\gamma_t = e^{t\mathbf{L}}$  entangles  $Q$  for  $1 \leq x < 3/2$ ; it does not do so for  $x > 3/2$ ; while if  $x = 3/2$ , the third order term of the expansion in  $t \geq 0$  has to be considered.

**Remark 6** If  $\mathcal{A} = \mathcal{B} = \mathcal{C} = 0$  in (5.4) and  $H_{eff}^{(a)} = 0$  in (5.1), the time-evolution is purely reversible and governed by the interaction Hamiltonian  $H_{eff}^{(12)} = \sum_{i,j=1}^3 H_{ij}^{(12)} (\sigma_i \otimes \sigma_j)$  in (5.2); then the sufficient condition for entanglement in Proposition 5 reduces to (see in particular (5.14))

$$|\langle u | H^{(12)} | v \rangle|^2 > 0 \quad (5.16)$$

for some  $|u\rangle, |v\rangle \in \mathbb{C}^3$  of the form (5.8).

In [93] it is shown that there can be found local unitary transformations

$$\sigma_i^A := U_A^\dagger \sigma_i U_A = \sum_{k=1}^3 O_{ik}^A \sigma_k, \quad \sigma_j^B := U_B^\dagger \sigma_j U_B = \sum_{l=1}^3 O_{lj}^B \sigma_l, \quad (5.17)$$

such that  $H_{eff}^{(12)} = \sum_{i,j=1}^3 H_{ij}^{(12)} (\sigma_i \otimes \sigma_j)$  can always be recast as

$$(U_A \otimes U_B) H^{(12)} (U_A^\dagger \otimes U_B^\dagger) := \hat{H}^\pm = \mu_1 \sigma_1^A \otimes \sigma_1^B \pm \mu_2 \sigma_2^A \otimes \sigma_2^B + \mu_3 \sigma_3^A \otimes \sigma_3^B$$

( $\hat{H}^+$  if  $\det(H^{(12)}) \geq 0$ ,  $\hat{H}^-$  if  $\det(H^{(12)}) < 0$ ), where  $\mu_1 \geq \mu_2 \geq \mu_3 \geq 0$  are the sorted eigenvalues of  $\sqrt{(H^{(12)})^\dagger H^{(12)}}$ . Further, the maximal entangling capability  $\eta_{max}$  of an interaction Hamiltonian  $H_{eff}^{(12)}$  is defined as

$$\eta_{max} := \max |\langle \chi^1 \otimes \chi^2 | H_{eff}^{(12)} | \chi_\perp^1 \otimes \chi_\perp^2 \rangle| = \max |\langle \tilde{\chi}^1 \otimes \tilde{\chi}^2 | \hat{H}^\pm | \tilde{\chi}_\perp^1 \otimes \tilde{\chi}_\perp^2 \rangle| = (\mu_1 + \mu_2)^2,$$

with  $|\tilde{\chi}^1\rangle := U_A |\chi^1\rangle$  and  $|\tilde{\chi}^2\rangle := U_B |\chi^2\rangle$ , the maximum value being attained at  $|\tilde{\chi}^1\rangle = |0\rangle_A$  eigenstate of  $\sigma_3^A$  and  $|\tilde{\chi}^2\rangle = |1\rangle_B$  eigenstate of  $\sigma_3^B$ . Now consider (5.16) and observe that

$$|\langle u | H^{(12)} | v \rangle|^2 = \left| \sum_{i,j} H_{ij}^{(12)} \epsilon_j \langle \psi_\perp | \sigma_i | \psi \rangle \langle \varphi^* | \sigma_j | \varphi_\perp^* \rangle \right|^2 = (\mu_1 + \mu_2)^2$$

for  $|\psi\rangle = U_A |0\rangle_A$  and  $|\varphi^*\rangle = U_B |0\rangle_B$ . Therefore, the maximal entanglement capability of a two-qubit Hamiltonian coincides with the the largest possible value that fulfils the sufficient condition (5.16).

**Remark 7** Since partial transposition provides an exhaustive entanglement witness also in the case of a two-level system coupled to a three-level system [16], similar arguments as those developed above can be applied to derive necessary and sufficient conditions for entanglement generation even in this case. The proofs both of necessity and of sufficiency would be the direct generalization of that of the two-qubit case with Pauli matrices acting on the first subsystem and, for instance, Gell-Mann matrices acting on the second, as will be explained at the beginning of the next subsection. A concrete physical example of entanglement conditions for a spin-1/2 coupled to a spin-1 can be found in [94]. In the following, bipartite systems consisting of two  $d$ -level systems will be discussed; this includes, for instance, bipartite systems of  $n$  qubits each, which are a natural generalization of the system previously considered, although positivity under partial transposition is not sufficient to exclude entanglement.

### 5.3 Entanglement generation in higher dimensional bipartite systems

The argument of the proof of sufficiency in Proposition 5 can be extended to higher dimensional bipartite systems consisting of two  $d$ -dimensional subsystems. It must be noticed that when  $d \geq 3$ , no extension of condition (5.7) is possible for there can be entangled states which remain positive under partial transposition [95], that is,  $\gamma_t$  might result entangling despite  $\tilde{\gamma}_t$  being positive on initially separable states. On the other hand, though, the larger  $d$  gets, the more sufficient conditions can be obtained for the generation of entanglement.

Let  $\{F_k\}_{k=0}^{d^2-1}$ ,  $F_0 := I_d/\sqrt{d}$ , be an orthonormal set of  $d \times d$  Hermitian matrices such that  $\text{Tr}(F_i F_j) = \delta_{ij}$  and, under transposition,  $F_k^T = \eta_k F_k$ , where  $\eta_k = \pm 1$ . For instance, as  $F_k$ 's the generalized Gell-Mann matrices [96] can be taken, since they satisfy this request. For a bipartite system where the two parties consist of  $n$  qubits, the matrices  $F_k$  can be chosen as tensor products of  $n$  Pauli matrices, whence  $\eta_k$  is the product of  $n$   $\varepsilon_i$ , where  $\sigma_i^T = \varepsilon_i \sigma_i$  as in the previous section.

If a system  $S$  is considered, composed of two subsystems each of finite dimension  $d$  immersed in a common external bath  $E$  with which they weakly interact, but not directly interacting between each other, the 2-dimensional Master equation (5.1) can be generalized with the  $F_k$  matrices defined above. Thus the total Hamiltonian is  $H_T = H_1 + H_2 + H_B + \lambda H_I$ , where  $H_1$ ,  $H_2$  and  $H_B$  are Hamiltonians pertaining to the first and second subsystem, respectively to the bath, while the interaction Hamiltonian is given by

$$H_I = \sum_{i=1}^{d^2-1} \sum_{a=1}^2 F_i^{(a)} \otimes B_i^{(a)}, \quad F_i^{(1)} := F_i \otimes I_d, \quad F_i^{(2)} := I_d \otimes F_i,$$

with  $I_d$  the  $d \times d$  identity matrix and  $B_i^{(a)}$  bath operators. Again by means of standard *weak coupling limit* techniques, the reduced dynamics of  $S$  is given by the Master equation

$$\frac{\partial \varrho_t}{\partial t} = \mathbf{L}_H[\varrho_t] + \mathbf{D}[\varrho_t] = -i[H_{eff}, \varrho_t] + \mathbf{D}[\varrho_t] \quad (5.18)$$

where  $H_{eff} = H_{eff}^{(1)} + H_{eff}^{(2)} + H_{eff}^{(12)}$ , with  $H_{eff}^{(a)} = \sum_{i=1}^{d^2-1} H_i^{(a)} F_i^{(a)}$ ,  $H_i^{(a)} \in \mathbb{R}$ ,  $a = 1, 2$ , Hamiltonians of the two subsystems independently,

$$H_{eff}^{(12)} = \sum_{i,j=1}^{d^2-1} H_{ij}^{(12)} (F_i \otimes F_j), \quad H_{ij}^{(12)} \in \mathbb{R}, \quad (5.19)$$

a Hamiltonian term describing a bath-mediated interaction between the subsystems,

while

$$\begin{aligned}
\mathbf{D}[\varrho(t)] = \sum_{i,j=1}^{d^2-1} & \left( \mathcal{A}_{ij} \left[ F_j^{(1)} \varrho F_i^{(1)} - \frac{1}{2} \{ F_i^{(1)} F_j^{(1)}, \varrho \} \right] \right. \\
& + \mathcal{C}_{ij} \left[ F_j^{(2)} \varrho F_i^{(2)} - \frac{1}{2} \{ F_i^{(2)} F_j^{(2)}, \varrho \} \right] \\
& + \mathcal{B}_{ij} \left[ F_j^{(1)} \varrho F_i^{(2)} - \frac{1}{2} \{ F_j^{(1)} F_i^{(2)}, \varrho \} \right] \\
& \left. + \mathcal{B}_{ji}^* \left[ F_j^{(2)} \varrho F_i^{(1)} - \frac{1}{2} \{ F_i^{(1)} F_j^{(2)}, \varrho \} \right] \right), \quad (5.20)
\end{aligned}$$

is a Kossakowski-Lindblad contribution describing dissipation and noise.  $\mathcal{A} = \mathcal{A}^\dagger, \mathcal{C} = \mathcal{C}^\dagger$  and  $\mathcal{B}$  are  $(d^2 - 1) \times (d^2 - 1)$  matrices which define a  $2(d^2 - 1) \times 2(d^2 - 1)$  Kossakowski matrix  $K = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^\dagger & \mathcal{C} \end{pmatrix}$ . As in the  $d = 2$  case, in order to guarantee the complete positivity of the dynamical map  $\gamma_t = e^{t\mathbf{L}}$  and thus its full physical consistency against coupling with generic ancillas and the existence of entangled states, the Kossakowski matrix must be positive semi-definite,  $K \geq 0$  [56, 59].

As in Propositions 4 and 5, let  $Q = |\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi|$ , with  $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^d$ , be an initial separable projector of the two  $d$ -level systems. Then the semigroup  $\tilde{\gamma}_t = e^{t\tilde{\mathbf{L}}}$  and its generator  $\tilde{\mathbf{L}} = T^{(2)} \circ \mathbf{L} \circ T^{(2)}$  will be considered, where  $T^{(2)}$  is the partial transposition operated on the second factor. The form of  $\tilde{\mathbf{L}}$  is the same as in (5.9) and (5.10) with the  $F_k$  matrices instead of the Pauli matrices and  $\eta_i$  in place of  $\varepsilon_i$ .

According to Proposition 4 and the proof of point 1 in Proposition 5, in order to find sufficient conditions for  $\gamma_t$  to be entangling, it is sufficient to study the case when  $\tilde{Q}^\perp \tilde{\mathbf{L}}[\tilde{Q}] \tilde{Q}^\perp$  has a negative eigenvalue, where  $\tilde{Q} = T^{(2)}[Q] = |\psi\rangle\langle\psi| \otimes |\varphi^*\rangle\langle\varphi^*|$ ,  $\tilde{Q}^\perp = I_d - \tilde{Q}$ .

Let  $\{|\psi_i\rangle\}_{i=1}^d$  and  $\{|\varphi_i\rangle\}_{i=1}^d$  be two orthonormal bases for the two parties, with  $|\psi_1\rangle = |\psi\rangle$  and  $|\varphi_1\rangle = |\varphi^*\rangle$ . A convenient enumeration for the corresponding basis of the composite system is as follows:  $|\Psi_{d(k-1)+\ell}\rangle := |\psi_k \otimes \varphi_\ell\rangle$  for  $k, \ell = 1, 2, \dots, d$ . Set  $i = d(k-1)+\ell$ ,  $i = 1, 2, \dots, d^2$ ; then,  $\tilde{Q} := |\Psi_1\rangle\langle\Psi_1|$  and  $\tilde{Q}^\perp := \sum_{i=2}^{d^2} |\Psi_i\rangle\langle\Psi_i|$ .

Since  $F_i^{(1)} = F_i \otimes I_d$  and  $F_i^{(2)} = I_d \otimes F_i$ , with respect to the chosen basis, only the entries  $M_{ij} := \langle\Psi_i|\tilde{Q}^\perp \tilde{\mathbf{L}}[\tilde{Q}] \tilde{Q}^\perp|\Psi_j\rangle$  with either  $k = 1$  or  $\ell = 1$  in  $i = \ell + d(k-1)$  survive, while all those with  $k \neq 1$  and  $\ell \neq 1$  vanish. There are  $2(d-1)$  basis vectors with either  $k = 1$  or  $\ell = 1$ :

$$|\Psi_2\rangle = |\psi_1 \otimes \varphi_2\rangle, |\Psi_3\rangle = |\psi_1 \otimes \varphi_3\rangle, \dots, |\Psi_d\rangle = |\psi_1 \otimes \varphi_d\rangle \quad (5.21)$$

$$|\Psi_{d+1}\rangle = |\psi_2 \otimes \varphi_1\rangle, |\Psi_{2d+1}\rangle = |\psi_3 \otimes \varphi_1\rangle, \dots, |\Psi_{(d-1)d+1}\rangle = |\psi_d \otimes \varphi_1\rangle,$$

and  $(d-1)^2$  vectors with  $k \neq 1$  and  $\ell \neq 1$ . Therefore the focus can be limited to  $\tilde{Q}^\perp \tilde{\mathbf{L}}[\tilde{Q}] \tilde{Q}^\perp$  restricted to the subspace spanned by the vectors in (5.21), i.e. on a  $2(d-1) \times 2(d-1)$  non-zero submatrix that will be called  $M$ . This matrix is composed of four  $(d-1)$ -dimensional

square blocks and its entries can be written in analogy to the  $d = 2$  case generalizing the vectors  $|u\rangle, |v\rangle$  in (5.8). Explicitly,  $(d - 1)$  vectors  $|u^{(n)}\rangle$  and  $(d - 1)$  vectors  $|v^{(m)}\rangle$  are defined, with  $(d^2 - 1)$  components each, given by

$$u_i^{(n)} := \langle \psi_1 | F_i | \psi_n \rangle, \quad n = d + 1, d + 2, \dots, 2d - 1, \quad i = 1, \dots, d^2 - 1, \quad (5.22)$$

$$v_i^{(m)} := \eta_i \langle \varphi_1 | F_i | \varphi_m \rangle, \quad m = 2, \dots, d, \quad i = 1, \dots, d^2 - 1. \quad (5.23)$$

Further, a Hermitian  $2(d - 1) \times 2(d - 1)$  matrix  $M = [M_{\alpha, \beta}]$  is introduced, with entries

$$M_{\alpha, \beta} := \langle v^{(\alpha+1)} | \mathcal{C}^T | v^{(\beta+1)} \rangle, \quad \alpha, \beta = 1, 2, \dots, d - 1$$

$$M_{\alpha, \beta} := \langle u^{(\alpha+1)} | \mathcal{A} | u^{(\beta+1)} \rangle, \quad \alpha, \beta = d, d + 1, \dots, 2(d - 1)$$

$$M_{\alpha, \beta} := -\langle v^{(\alpha+1)} | \left( i(H^{(12)})^T + \text{Re}(\mathcal{B}) \right) | u^{(\beta+1)} \rangle, \quad \alpha = 1, \dots, d - 1, \quad \beta = d, \dots, 2(d - 1)$$

$$M_{\alpha, \beta} := -\overline{\langle v^{(\beta+1)} | \left( i(H^{(12)})^T + \text{Re}(\mathcal{B}) \right) | u^{(\alpha+1)} \rangle}, \quad \alpha = d, \dots, 2(d - 1), \quad \beta = 1, \dots, d - 1.$$

In Proposition 5, it was seen that the negativity of the determinant of the matrix  $M = [M_{\alpha, \beta}]$  with  $d = 2$  is a sufficient condition for a bath-mediated entanglement of an initial separable projector. For a bipartite system composed of two  $d$ -level subsystems, the argument generalizes as follows.

**Proposition 6** *If at least one of the principal minors of the  $2(d - 1) \times 2(d - 1)$  matrix  $M = [M_{\alpha, \beta}]$  is negative, then the semigroup  $\gamma_t$  is entangling: there are  $2^d(2^{d-2} - 1) + 1$  conditions at the most, each one of them ensuring bipartite entanglement generation through immersion in a common environment.*

**Proof:** Let  $R$  be one of  $M$ 's principal sub-matrices. If  $\det(R) < 0$ , then there exists a vector  $|\Phi\rangle$  in the support of  $\tilde{Q}^\perp \tilde{\mathbf{L}}[\tilde{Q}] \tilde{Q}^\perp$  such that  $\langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle < 0$  and  $\langle \Phi | \tilde{Q} | \Phi \rangle = 0$ . Thus, an expansion at small times  $t \geq 0$  yields

$$\langle \Phi | \tilde{\gamma}_t[\tilde{Q}] | \Phi \rangle \simeq t \langle \Phi | \tilde{\mathbf{L}}[\tilde{Q}] | \Phi \rangle < 0,$$

which implies that  $\tilde{\gamma}_t[\tilde{Q}]$  is not positive semi-definite in a right neighborhood of  $t = 0$  and  $\gamma_t[Q]$  becomes entangled in that time-interval.

Being a  $2(d - 1) \times 2(d - 1)$  matrix,  $M$  has  $2^{2(d-1)} - 1$  principal sub-matrices; however, since  $\mathcal{A}$  and  $\mathcal{C}$  in (5.20) are positive matrices, all their  $2(2^{d-1} - 1)$  principal minors cannot be negative: therefore, all the diagonal elements of  $M$  are surely non-negative. Thus at most  $(2^{2(d-1)} - 1) - 2(2^{d-1} - 1) = 4^{d-1} - 2^d + 1$  principal minors are left that are not necessarily positive <sup>4</sup>.  $\square$

<sup>4</sup>In the two-qubit case,  $d = 2$ , which implies  $4 - 2^2 + 1 = 1$  sufficient condition for entanglement, as found in Proposition 5.

**Example 2** A state of four qubits (1, 2, 3, 4) will be considered, immersed in a dissipative environment such that their states evolve in time according to a Master equation (5.18) with a purely dissipative generator of the form

$$\begin{aligned} \mathbf{L}[\varrho] &= \sum_{p=1}^4 \sum_{i,j=1}^3 K_{ij}^{(1)} \left( \sigma_j^{(p)} \varrho \sigma_i^{(p)} - \frac{1}{2} \{ \sigma_i^{(p)} \sigma_j^{(p)}, \varrho \} \right) \\ &+ \sum_{p \neq q=1}^4 \sum_{i,j=1}^3 K_{ij}^{(2)} \left( \sigma_j^{(p)} \varrho \sigma_i^{(q)} - \frac{1}{2} \{ \sigma_i^{(p)} \sigma_j^{(q)}, \varrho \} \right). \end{aligned} \quad (5.24)$$

In terms of the matrices  $F_k$  in (5.20), one has  $F_k := F_{i+3(p-1)} = \frac{1}{\sqrt{2}} \sigma_i^{(p)}$ ,  $i = 1, 2, 3$ ,  $p = 1, 2$  and a Kossakowski matrix

$$K_4 = \begin{pmatrix} K^{(1)} & K^{(2)} & K^{(2)} & K^{(2)} \\ K^{(2)} & K^{(1)} & K^{(2)} & K^{(2)} \\ K^{(2)} & K^{(2)} & K^{(1)} & K^{(2)} \\ K^{(2)} & K^{(2)} & K^{(2)} & K^{(1)} \end{pmatrix}.$$

Taking  $K^{(1)} = \begin{pmatrix} 1 & iz & 0 \\ -iz & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$  and  $K^{(2)} = \begin{pmatrix} x & 0 & 0 \\ 0 & -x & 0 \\ 0 & 0 & 0 \end{pmatrix}$  with  $z, x$  real numbers, in order

for the semigroup generated by (5.24) to be completely positive, the Kossakowski matrix  $K_4$  must be positive semi-definite; this implies  $z^2 + 9x^2 \leq 1$  as its non-zero eigenvalues are  $1 \pm \sqrt{x^2 + z^2}$  and  $1 \pm \sqrt{9x^2 + z^2}$ .

Consider the fully separable state  $Q_4 := (|0\rangle\langle 0| \otimes |0\rangle\langle 0|) \otimes (|0\rangle\langle 0| \otimes |0\rangle\langle 0|)$ ,  $\sigma_3|0\rangle = |0\rangle$ ; then the vectors defined in (5.22) are

$$|u^{(5)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ -i \\ 0 \end{pmatrix}, \quad |v^{(2)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ i \\ 0 \end{pmatrix}, \quad |u^{(6)}\rangle = \begin{pmatrix} 1 \\ -i \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |v^{(3)}\rangle = \begin{pmatrix} 1 \\ i \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

while  $|u^{(7)}\rangle$  and  $|v^{(4)}\rangle$  are the null vector. Therefore, the  $2(d-1) \times 2(d-1) = 6 \times 6$  matrix  $M = [M_{\alpha\beta}]$  reduces to a  $4 \times 4$  matrix of the form

$$M = 2 \begin{pmatrix} 1+z & 0 & x & x \\ 0 & 1+z & x & x \\ x & x & 1+z & 0 \\ x & x & 0 & 1+z \end{pmatrix}.$$

Since  $z^2 \leq z^2 + 9x^2 \leq 1$ , its principal minors of order 1, equal to  $2(1+z)$ , are all positive; those of order 2 are the determinants of  $2 \begin{pmatrix} 1+z & 0 \\ 0 & 1+z \end{pmatrix}$ ,  $2 \begin{pmatrix} 1+z & x \\ x & 1+z \end{pmatrix}$ , and are

also positive if  $(1+z)^2 > x^2$ . Those of order 3,  $D(x, z) := 8(1+z)((1+z)^2 - 2x^2)$ , namely the determinants of the matrices

$$2 \begin{pmatrix} 1+z & 0 & x \\ 0 & 1+z & x \\ x & x & 1+z \end{pmatrix}, \quad 2 \begin{pmatrix} 1+z & x & x \\ x & 1+z & 0 \\ x & 0 & 1+z \end{pmatrix},$$

can nevertheless be negative. In fact, there is a region in the plane  $(x, z)$  where  $z^2 + 9x^2 \leq 1$  and  $(1+z)^2 > x^2$ , while  $(1+z)^2 < 2x^2$ . The corresponding values  $(x, z)$  ensure that  $K_4$  is positive semi-definite, whereas  $M$  is not; correspondingly, the four-qubit dissipative dynamics entangles the two pairs  $(1, 2)$  and  $(3, 4)$  initially in the pure separable state  $Q_4$ .

The fact that the principal minors of order 2 are non-negative has the following physical interpretation. The form of the generator of the dissipative dynamics of the two pairs of qubits is such that if any pair of qubits is eliminated by taking the trace of (5.24) over their Hilbert spaces, the resulting generator for the remaining pair  $(i, j)$  of qubits amounts to keeping only the  $i$ -th and  $j$ -th row and column of  $K_4$ , thereby leading to a same dissipative time-evolution associated with the Kossakowski matrix  $K_2 = \begin{pmatrix} K^{(1)} & K^{(2)} \\ K^{(2)} & K^{(1)} \end{pmatrix}$  for any pair  $(i, j)$  of qubits. Moreover, given  $Q_4$ , any pair of qubits is in the same state  $Q_2 = |0\rangle\langle 0| \otimes |0\rangle\langle 0|$  with the vectors  $|u\rangle$  and  $|v\rangle$  defined in (5.8) that read  $|u\rangle = (1, -i, 0)$ ,  $|v\rangle = (1, i, 0)$  and yield a matrix  $M_2 = 2 \begin{pmatrix} 1+z & x \\ x & 1+z \end{pmatrix}$ . By assumption  $\det(M_2) > 0$ , thus, according to Proposition 5, the two-qubit semigroup associated with the Kossakowski matrix  $K_2$  cannot entangle  $Q_2$ ; nonetheless, the four-qubit semigroup associated with  $K_4$  entangles  $Q_4$ . This means that the dissipative map relative to the generator (5.24) governing the time-evolution of this four-qubit state  $Q_4$  cannot entangle any two qubits, as, say, qubit 1 and qubit 2, but it can nevertheless entangle a *pair* of qubits with another *pair*, as, say, qubits  $(1, 2)$  and qubits  $(3, 4)$ . This leads to a vaster scenario for entanglement generation: indeed, given the symmetry of the dynamics in (5.24), the four-qubit state  $Q_4$  can be viewed both as a bipartite state where each subsystem has dimension  $d = 4$  or as a multipartite system composed of four separate qubits. From the former point of view, from Proposition 6 it follows that for larger systems there could be more possibilities of environment-induced entanglement generation; while from the latter, genuine multipartite entanglement could be considered with different partitionings.

## 5.4 Conclusions

In this chapter it has been shown that the sufficient condition found in [10] for the creation of entanglement between two qubits immersed in a common environment by means of their reduced dissipative dynamics is, apart from marginal cases, also necessary. Moreover, the basic argument in [10] has been extended to higher dimensional

bipartite open quantum systems, thereby obtaining sufficient conditions for entangling a separable pure state in terms of the negativity of the principal minors of certain matrices that depend on the generator of the dynamics and on the given state to get entangled. Since the number of principal minors increases with the dimension of the parties, for more than two qubits a richer variety of noise-induced entanglement is available. An explicit example is provided, in which a purely dissipative time evolution can entangle two subsystems, each consisting of two qubits, without entangling any two single qubits.



## Chapter 6

# Entanglement and entropy rates in open quantum systems

### 6.1 Introduction

In this chapter, an open quantum system consisting of two qubits immersed in a common bath will be considered: first its reduced dynamics will be derived and then the behavior of entanglement and entropy in such a system will be compared.

The formalism of open quantum systems has been introduced to describe the tendency to thermal equilibrium of a small system in weak interaction with a large heat bath at a certain temperature. The main tool in this thermodynamical picture is the quantum relative entropy [4]; it is related to the difference between the free energy of the irreversibly evolving open quantum system and that of its equilibrium asymptotic state: this difference monotonically decreases in time because so does the quantum relative entropy with respect to completely positive maps [97], as quantum dynamical semigroups are. Namely, the time derivative of the quantum relative entropy, called *entropy rate*, has a definite sign.

As seen in Chapter 1, the quantum relative entropy has also been used as a possible measure of the entanglement content of a quantum state: the so-called *relative entropy of entanglement* provides a pseudo-distance between a state and the closed convex set of separable states [11].

In [12] the natural question was raised whether the entropy production due to thermodynamical tendency to equilibrium is somewhat related to the *entanglement rate*, that is to the speed of variation of the relative entropy of entanglement. A conjecture was put forward that for systems immersed in an external bath without a direct source of entanglement due to Hamiltonian interactions, the absolute value of the entanglement production is always smaller than the entropy production.

As seen in Chapter 2, typically, a system  $S$  immersed in a large environment  $E$  is subjected to decoherence; therefore, one expects quantum entanglement to be generically depleted by a dissipative and noisy time-evolution. The conjecture mentioned above is motivated by the fact that, if a quantum open system tends to a separable equilibrium state, then, in a suitable neighborhood of the latter, the entanglement production is zero while the entropy production is not. Indeed, in [12] a concrete example that validates the conjecture is offered of a two-qubit system in which only one of them evolves as a quantum open system. In such a case an initial maximally entangled state evolves towards a separable steady state with an entropy production always larger than the speed with which entanglement is dissipated.

However, as shown in Chapter 4, in certain specific situations, an environment affecting both parties of a bipartite system may even build quantum correlations between the subsystems which compose  $S$  (see, e.g., [5, 44, 89–92]). In particular, in [5] this possibility is shown to depend on the specific form of the generator of the reduced dynamics. In [10] an inequality was found, involving the entries of such a matrix which, if fulfilled, is sufficient to ensure that a specific initial separable pure state of two qubits gets entangled. Further, as shown in Chapter 5, in [98] this inequality was proven to be a necessary and sufficient condition for environment-induced entanglement in an initially separable pure state of two qubits. Even more interestingly, starting from an initially separable state, the entanglement generated at small times can persist asymptotically; also, starting from an initially entangled state, its entanglement content can asymptotically increase.

This chapter is organized as follows: in Section 2, the open dynamics of two qubits is considered with a generator that depends on a parameter which allows to range over all the above mentioned cases, analytically solving the master equation; then, in Section 3, the notions of entropy and entanglement rates and the conjecture from [12] are introduced; finally, in Section 4, numerically studying the time-behavior of the entanglement and entropy rates for various initial states, it is shown that, whenever there is asymptotic entanglement the conjecture in [12] is violated, while it holds if there is no asymptotic entanglement.

## 6.2 The Reduced Dynamics

Let a bipartite system composed of two qubits be immersed in an external environment in such a way that, via standard weak-coupling limit techniques [61], their reduced, irreversible dynamics can be described by means of the master equation

$$\partial_t \varrho_t = \mathbf{L}[\varrho_t] = -i \frac{\Omega}{2} [\Sigma_3, \varrho_t] + \sum_{i,j=1}^3 \mathcal{A}_{ij} \left( \Sigma_i \varrho_t \Sigma_j - \frac{1}{2} \{ \Sigma_j \Sigma_i, \varrho_t \} \right), \quad (6.1)$$

where  $\Omega$  is the system frequency,  $\Sigma_i := \sigma_i \otimes I_2 + I_2 \otimes \sigma_i$ ,  $I_2$  is the  $2 \times 2$  identity matrix,  $\sigma_i$ ,  $i = 1, 2, 3$  are the Pauli matrices and the matrix

$$\mathcal{A} = [\mathcal{A}_{ij}] = \begin{pmatrix} 1 & i\alpha & 0 \\ -i\alpha & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \alpha \in \mathbb{R}, \alpha^2 \leq 1, \quad (6.2)$$

is positive semi-definite. This latter request ensures that the semigroup generated by (6.1) consist of completely positive maps  $\gamma_t$  for all  $t \geq 0$ , as explained in Chapter 2.

The master equation (6.1) with matrix  $\mathcal{A}$  as in (6.2) describes precisely the two-qubit case studied in Chapters 2 (Section 2.3) and 4 (Section 4.2), and these formulas have been repeated here for the benefit of the reader.

**Remark 8** As seen in the previous chapter, by means of the single qubit Pauli matrices  $\sigma_i^{(1)} = \sigma_i \otimes I_2$  and  $\sigma_i^{(2)} = I_2 \otimes \sigma_i$  the purely dissipative contribution to the generator can be written as [5]

$$\mathbf{D}[\rho_t] = \sum_{i,j=1}^3 \mathcal{A}_{ij} \sum_{p,q=1}^2 \left( \sigma_i^{(p)} \rho_t \sigma_j^{(q)} - \frac{1}{2} \left\{ \sigma_j^{(q)} \sigma_i^{(p)}, \rho_t \right\} \right). \quad (6.3)$$

In this way there are six Kraus operators  $\sigma_i^{(p)}$ ,  $p = 1, 2$ ,  $i = 1, 2, 3$  and the  $6 \times 6$  Kossakowski matrix reads

$$K = [K_{ij}^{(pq)}] = \begin{pmatrix} K^{(11)} & K^{(12)} \\ K^{(21)} & K^{(22)} \end{pmatrix} = \begin{pmatrix} \mathcal{A} & \mathcal{A} \\ \mathcal{A} & \mathcal{A} \end{pmatrix}. \quad (6.4)$$

From the theory of open quantum systems (see Chapter 2) it is known that the coefficients  $K_{ij}^{(pq)}$  in the Kossakowski matrix relative to the  $i$ -th Pauli matrix of the  $p$ -th qubit, respectively the  $j$ -th Pauli matrix of the  $q$ -th qubit,  $p, q = 1, 2$ ,  $i, j = 1, 2, 3$ , are determined by the Fourier transforms of the two-point time-correlation functions with respect to an environment equilibrium state  $\omega$ ,  $\omega(B_i^{(p)} B_j^{(q)}(t))$ , of the environment operators  $B_i^{(p)}$  appearing in the system-environment interaction  $H_I = \sum_{i=1}^3 (\sigma_i^{(1)} \otimes B_i^{(1)} + \sigma_i^{(2)} \otimes B_i^{(2)})$ . The symmetric form of (6.3) thus results when both qubits are linearly coupled to bath operators such that:  $B_{1,2,3}^{(1)} = B_{1,2,3}^{(2)} = B_{1,2,3}$  and  $\omega(B_{1,2} B_3(t)) = 0$ .

**Remark 9** Considering two qubits weakly interacting with a thermal bath modeled as a collection of spinless, massless scalar fields (see, e.g., [5]) at very high temperature  $T = 1/\beta$ , the parameter  $\alpha$  in the Kossakowski matrix is related to  $\beta$ , i.e.  $\alpha = -\beta\Omega$ , where  $\Omega$  is the system frequency when isolated from the environment. Correspondingly, in the case of one qubit immersed in such a thermal bath at high temperature ( $\beta \ll 1$ ), any initial state is driven to the thermal asymptotic state

$$\rho_\infty = \frac{\exp(-\beta\Omega\sigma_3)}{2 \cosh \beta\Omega} \simeq \frac{1}{2} (1 - \beta\Omega\sigma_3).$$

The master equation (6.1) is explicitly integrated in Appendix B; in the following the focus will be mainly upon the time-evolution of initial states of the form

$$\varrho = a |1\rangle\langle 1| + d |2\rangle\langle 2| + b |3\rangle\langle 3| + c |4\rangle\langle 4|, \quad a, b, c, d \in \mathbb{R}^+, \quad a + b + c + d = 1, \quad (6.5)$$

diagonal with respect to the orthonormal vectors

$$|1\rangle = |00\rangle, \quad |2\rangle = |11\rangle, \quad |3\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \quad |4\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}, \quad (6.6)$$

where  $\sigma_3|0\rangle = |0\rangle$ ,  $\sigma_3|1\rangle = -|1\rangle$ , and  $|00\rangle, |01\rangle, |10\rangle, |11\rangle$  form the so-called standard basis in  $\mathbb{C}^2 \otimes \mathbb{C}^2$ , with respect to which the states (6.5) are represented by

$$\varrho = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & \frac{b+c}{2} & \frac{b-c}{2} & 0 \\ 0 & \frac{b-c}{2} & \frac{b+c}{2} & 0 \\ 0 & 0 & 0 & d \end{pmatrix}. \quad (6.7)$$

From equations (B.4)–(B.9) and (B.11) in Appendix B, it turns out that these initial states evolve at time  $t \geq 0$  into states of the same form

$$\varrho_t = a_t |1\rangle\langle 1| + d_t |2\rangle\langle 2| + b_t |3\rangle\langle 3| + c_t |4\rangle\langle 4|, \quad (6.8)$$

where  $c_t = c$  and

$$\begin{aligned} a_t &= \frac{(1-\alpha)^2}{3+\alpha^2} R + \sqrt{1-\alpha^2} \frac{(1+\alpha)^2 a - 2(1-\alpha)d + (1+\alpha)^2 b}{(1+\alpha)(3+\alpha^2)} E_-(t) \\ &+ \frac{2(1+\alpha)a - (1-\alpha)^2(b+d)}{3+\alpha^2} E_+(t) \end{aligned} \quad (6.9)$$

$$\begin{aligned} d_t &= \frac{(1+\alpha)^2}{3+\alpha^2} R - \sqrt{1-\alpha^2} \frac{2(1+\alpha)a - (1-\alpha)^2(b+d)}{(1-\alpha)(3+\alpha^2)} E_-(t) \\ &- \frac{(1+\alpha)^2 a - 2(1+\alpha)d + (1+\alpha)^2 b}{3+\alpha^2} E_+(t) \end{aligned} \quad (6.10)$$

$$\begin{aligned} b_t &= \frac{(1-\alpha^2)}{3+\alpha^2} R + \sqrt{1-\alpha^2} \frac{(1+\alpha)^3 a + (1-\alpha)^3 d - 2(1-\alpha^2)b}{(3+\alpha^2)(1-\alpha^2)} E_-(t) \\ &+ \frac{2(1+\alpha^2)b - (1-\alpha^2)(a+d)}{3+\alpha^2} E_+(t), \end{aligned} \quad (6.11)$$

with  $R = a + b + d = 1 - c$  and

$$E_+(t) = e^{-8t} \cosh 4t \sqrt{1-\alpha^2}, \quad E_-(t) = e^{-8t} \sinh 4t \sqrt{1-\alpha^2}.$$

Since  $\lim_{t \rightarrow +\infty} E_{\pm}(t) = 0$ , the asymptotic states resulting from the initial states (6.5) are

$$\varrho_{\infty}(c) = \frac{(1-\alpha)^2}{3+\alpha^2} (1-c) |1\rangle\langle 1| + \frac{(1+\alpha)^2}{3+\alpha^2} (1-c) |2\rangle\langle 2| + \frac{(1-\alpha^2)}{3+\alpha^2} (1-c) |3\rangle\langle 3| + c |4\rangle\langle 4|. \quad (6.12)$$

There is thus a one-parameter family  $\{\varrho_\infty(c)\}_{0 \leq c \leq 1}$  of asymptotic states such that all initial states of the form (6.5) with the same  $c$  go into the same  $\varrho_\infty(c)$ .

In order to study the asymptotic entanglement generation capability of the present model, the entanglement of two-qubit states  $\rho$  will be measured by the concurrence (see Chapter 1):

$$C(\varrho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\},$$

where  $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0$  are the square roots of the positive eigenvalues of  $\varrho\tilde{\varrho}$  with  $\tilde{\varrho} = \sigma_2 \otimes \sigma_2 \varrho^* \sigma_2 \otimes \sigma_2$ ,  $\varrho^*$  denoting the complex conjugated matrix. For two-qubit states of the form (6.7),  $\rho = \rho^*$  and one easily computes

$$\tilde{\varrho} = \begin{pmatrix} d & 0 & 0 & 0 \\ 0 & \frac{b+c}{2} & \frac{b-c}{2} & 0 \\ 0 & \frac{b-c}{2} & \frac{b+c}{2} & 0 \\ 0 & 0 & 0 & a \end{pmatrix}, \quad \varrho\tilde{\varrho} = \begin{pmatrix} ad & 0 & 0 & 0 \\ 0 & \frac{b^2+c^2}{2} & \frac{b^2-c^2}{2} & 0 \\ 0 & \frac{b^2-c^2}{2} & \frac{b^2+c^2}{2} & 0 \\ 0 & 0 & 0 & ad \end{pmatrix}.$$

This latter matrix has positive eigenvalues  $ad$  (twice degenerate),  $b^2, c^2$ ; then, their square roots  $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$  in decreasing order yield

$$C(\varrho) = \max\left\{0, 2\left(\frac{|b-c|}{2} - \sqrt{ad}\right)\right\} \quad (6.13)$$

$$C(\varrho_\infty) = \max\left\{0, \frac{|1 - \alpha^2 - 4c| - 2(1 - \alpha^2)(1 - c)}{3 + \alpha^2}\right\}. \quad (6.14)$$

**Remark 10** As already emphasized in the introduction, despite decoherence, the presence of an environment need not have only destructive effects in relation to entanglement: entanglement can even be asymptotically increased with respect to the initial amount. This can happen in the present case and the entanglement generation capability of the environment is entirely due to the non-Hamiltonian contribution (6.3) to the generator in (6.1). Indeed, the two-qubit Hamiltonian does not contain coupling terms and cannot be a source of entanglement; instead, this can be true for (6.3) because the off-diagonal contributions in the Kossakowski matrix (6.4) couple the two qubits. Of course, this is only necessary, but not sufficient to ensure entanglement generation and its asymptotic persistence. They indeed depend on a trade-off between the off-diagonal couplings and the purely decohering diagonal terms in (6.4).

### 6.3 Entropy and Entanglement Rates

In this section the notions of entropy and entanglement rates will be introduced; for sake of simplicity, finite  $d$ -level systems will be considered, whose states are described by normalized, positive,  $d \times d$  density matrices  $\varrho \in M_d(\mathbb{C})$ . Given two such density matrices,

their quantum relative entropy is defined in Section 1.3.2 in (1.4).

Consider a quantum system with Hamiltonian  $H$ ; if in contact with a heat bath at temperature  $T = 1/\beta$  (with the Boltzmann constant  $\kappa = 1$ ), it is expected to be driven asymptotically into the thermal (Gibbs) state  $\varrho_T = e^{-\beta H}/Z_\beta$ , where  $Z_\beta = \text{Tr}[e^{-\beta H}]$ . Suppose that under an irreversible time-evolution  $\varrho \mapsto \varrho_t$ , an initial state  $\varrho$  is driven into thermal equilibrium, that is  $\lim_{t \rightarrow +\infty} \varrho_t = \varrho_T$ ; then,

$$\frac{1}{\beta} S(\varrho_t || \varrho_T) = \frac{1}{\beta} \text{Tr} \left( \varrho_t (\log \varrho_t + \log Z_\beta + \beta H) \right) = -T S(\varrho_t) + \text{Tr}(\varrho_t H) + T \log Z_\beta,$$

where  $S(\varrho) = -\text{Tr} \varrho \log \varrho$  is the von Neumann entropy of the state  $\varrho$ . Since the second term corresponds to the system's internal energy, the first two contributions give the system's free energy corresponding to the time-evolving state  $\varrho_t$  [4]:

$$F(\varrho_t) = U(\varrho_t) - T S(\varrho_t), \quad U(\varrho_t) = \text{Tr}(\varrho_t H).$$

Finally,  $F(\varrho_T) = -\log Z_\beta$  implies that the quantum relative entropy is related to the difference of free energies

$$S(\varrho_t || \varrho_T) = \beta \left( F(\varrho_t) - F(\varrho_T) \right).$$

Because of the second law of thermodynamics, the above quantity should be positive and its time-derivative non-positive. The first property is guaranteed by the properties of the quantum relative entropy [97], while the second one holds true when the irreversible time-evolution is given by a Markovian semigroup, that is when  $\varrho_t = \gamma_t[\varrho]$  and  $\gamma_t \circ \gamma_s = \gamma_{s+t}$  for all  $s, t \geq 0$ . Indeed, since  $\gamma_t[\varrho_T] = \varrho_T$ , it follows that

$$\begin{aligned} S(\varrho_t || \varrho_T) &= S(\gamma_t[\varrho] || \gamma_t[\varrho_T]) = S(\gamma_{t-s} \circ \gamma_s[\varrho] || \gamma_{t-s} \circ \gamma_s[\varrho_T]) \\ &\leq S(\gamma_s[\varrho] || \gamma_s[\varrho_T]) = S(\varrho_s || \varrho_T) \quad \forall 0 \leq s \leq t, \end{aligned}$$

where the last inequality comes from the fact that the quantum relative entropy decreases under the action of completely positive trace-preserving maps [97].

Based on the previous thermodynamical arguments, it is possible to consider generic open quantum dynamics  $\varrho \mapsto \gamma_t[\varrho] = \varrho_t$  with asymptotic states  $\lim_{t \rightarrow +\infty} \varrho_t = \varrho_\infty$ , that are not necessarily thermal ones. The speed of convergence to such stationary states starting from an initial state  $\varrho$  will then be measured by the *entropy rate*

$$\sigma[\varrho_t] = -\frac{d}{dt} S(\varrho_t || \varrho_\infty) = \text{Tr} \left( \dot{\varrho}_t (\log \varrho_\infty - \log \varrho_t) \right). \quad (6.15)$$

The entropy production that accompanies the tendency to equilibrium of the states of the form (6.8) is easily computed; indeed, since the states  $\varrho_t$  and  $\varrho_\infty$  are diagonal with respect to the same orthonormal basis, the entropy rate (6.15) has the analytic expression

$$\sigma[\varrho_t] = \dot{a}_t \log \frac{(1-\alpha)^2(1-c)}{a_t(3+\alpha^2)} + \dot{b}_t \log \frac{(1-\alpha^2)(1-c)}{b_t(3+\alpha^2)} + \dot{d}_t \log \frac{(1+\alpha)^2(1-c)}{d_t(3+\alpha^2)}. \quad (6.16)$$

When the density matrix  $\rho$  is the state of, say, a bipartite quantum system, it makes sense to introduce the *relative entropy of entanglement* (1.6) as a measure of the entanglement content of  $\rho$ . Indeed, the above quantity vanishes if and only if  $\rho$  is separable and can be used to measure the distance of  $\rho$ <sup>1</sup> from the convex set of separable states; furthermore, it cannot increase, but at most remain constant, under the action of local operations, described by trace-preserving completely positive maps acting independently on the two parties [27, 32].

Analogously to what was done for the entropy production, one may look at the *entanglement rate* when the system evolves, i.e. at the time-derivative of the pseudo-distance

$$\sigma_E[\varrho_t] = \frac{d}{dt} E[\varrho_t]. \quad (6.17)$$

In [12] it was argued that

$$\left| \sigma_E[\varrho_t] \right| \leq \sigma[\varrho_t] \quad (6.18)$$

always holds in absence of direct entangling interactions between the parties. The argument on which the conjecture is based is that decoherence is expected to deplete entanglement before reaching the asymptotic state and thus before the entropy production vanishes. Such asymptotic intuition is then extrapolated at all times.

Now the various possibilities offered by the reduced dynamics discussed in the previous section will be illustrated; in particular, the entropy and entanglement rates will be compared, thus checking the validity of the conjecture (6.18).

Firstly an explicit expression for the relative entropy of entanglement (1.6) will be derived in the case of states of the form (6.8) and then the behavior of its time-derivative will be computed numerically (6.17).

It is convenient to rewrite the relative entropy of entanglement (1.6) as follows:

$$E(\varrho_t) = -S(\varrho_t) - \sup_{\varrho_{sep}} \text{Tr} \left( \varrho_t \log \varrho_{sep} \right), \quad (6.19)$$

where  $S(\varrho_t)$  is the von Neumann entropy of the time-evolving state. The following result, which is proved in Appendix C, helps to explicitly solve the above maximization problem.

**Proposition 7** *In the case of states as in (6.8), the supremum in (6.19) is achieved for separable states of the form*

$$\varrho_{sep} = x|1\rangle\langle 1| + u|3\rangle\langle 3| + v|4\rangle\langle 4| + y|2\rangle\langle 2|, \quad (6.20)$$

where the parameters  $x, y, u, v$  are real and such that

$$x + u + v + y = 1, \quad \frac{|u - v|}{2} \leq \sqrt{xy}. \quad (6.21)$$

<sup>1</sup>The relative entropy of entanglement is not exactly a distance since it is not symmetric.

This leads to the following maximization problem

$$E(\varrho_t) = -S(\varrho_t) - \sup_{\varrho \in \mathcal{S}_{sep}^{diag}} \left( a_t \log x + d_t \log y + b_t \log u + c_t \log v \right), \quad (6.22)$$

which can be analytically solved.

## 6.4 Results

The above maximization problem is explicitly solved in Appendix C thus permitting to calculate numerically the entanglement rate (6.17), to compare it with the entropy rate (6.15) and to check the conjecture (6.18). This will be done in a number of cases that cover all possible initial and asymptotic entanglement properties: for each one the behaviors of the relative entropy and of the relative entropy of entanglement will be plotted separately, while the entropy rate and the entanglement rate are plotted together for direct comparison.

In the following, the choice of the range of values for the plots' axes was made only for graphic reasons to make the plots clearer. Moreover, in the first four cases, the parameter in the matrix  $\mathcal{A}$  is taken to be  $\alpha = 0.5$  as it makes the plots easier to read; changing  $\alpha$  does not alter the results. In the last example, instead, two different behaviors of the entanglement of the initial state are shown, depending on the choice of the parameter  $\alpha$ .

**Case 1.** An initial pure separable state (6.23) goes into a mixed separable state; the dissipative time-evolution is not able to generate entanglement at any time, as shown by the second and the third plot below where the entropy of entanglement and the entanglement rate are both zero. In this case the conjecture (6.18) holds.

$$\begin{aligned} \varrho &= |1\rangle\langle 1| \\ \varrho_\infty &= \frac{(1-\alpha)^2}{3+\alpha^2} |1\rangle\langle 1| + \frac{(1+\alpha)^2}{3+\alpha^2} |2\rangle\langle 2| + \frac{(1-\alpha^2)}{3+\alpha^2} |3\rangle\langle 3| \\ C(\varrho) &= C(\varrho_\infty) = 0 \end{aligned} \quad (6.23)$$

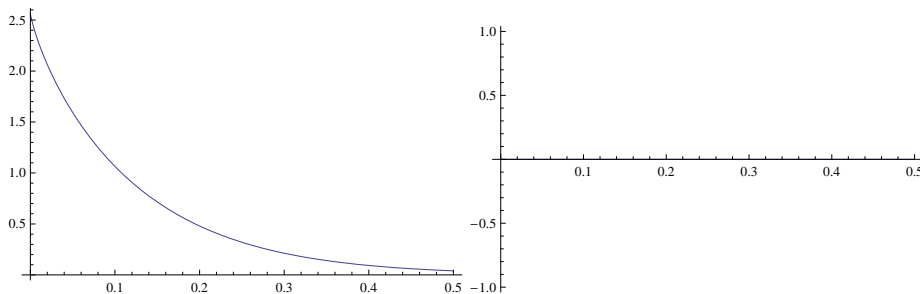


Figure 6.1: Case 1:  $\alpha = 0.5$ ; Left:  $S(\varrho_t)$ ; Right:  $E(\varrho_t)$



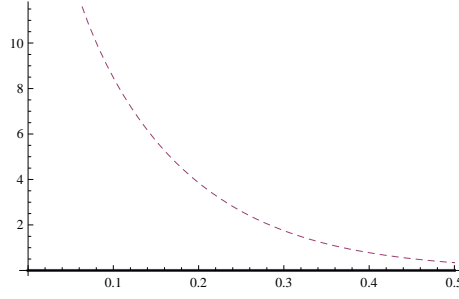


Figure 6.2: Case 1:  $\alpha = 0.5$ ;  $\sigma[\varrho_t]$  dashed line,  $|\sigma_E[\varrho_t]|$  continuous line

**Case 2.** An initial mixed separable state (6.24) goes into a mixed entangled state and the conjecture (6.18) is violated after some time.

$$\begin{aligned} \varrho &= \frac{1}{2} |3\rangle\langle 3| + \frac{1}{2} |4\rangle\langle 4| & (6.24) \\ \varrho_\infty &= \frac{(1-\alpha)^2}{2(3+\alpha^2)} |1\rangle\langle 1| + \frac{(1+\alpha)^2}{2(3+\alpha^2)} |2\rangle\langle 2| + \frac{(1-\alpha^2)}{2(3+\alpha^2)} |3\rangle\langle 3| + \frac{1}{2} |4\rangle\langle 4| \\ C(\varrho) &= 0, \quad C(\varrho_\infty) = \frac{2\alpha^2}{3+\alpha^2} \geq 0 \quad \forall \alpha \in [-1, 1]. \end{aligned}$$

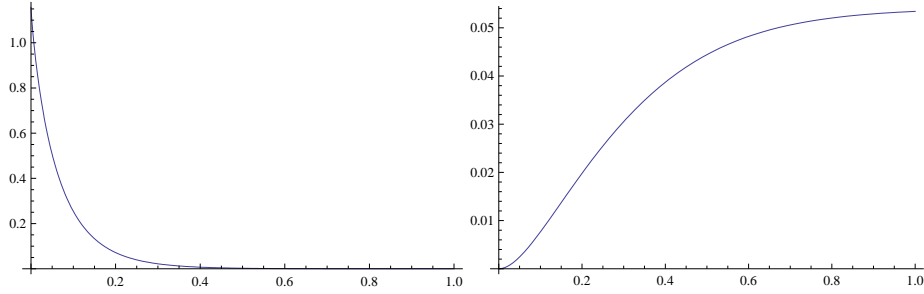


Figure 6.3: Case 2:  $\alpha = 0.5$ ; Left:  $S(\varrho_t || \varrho_\infty)$ ; Right:  $E[\varrho_t]$

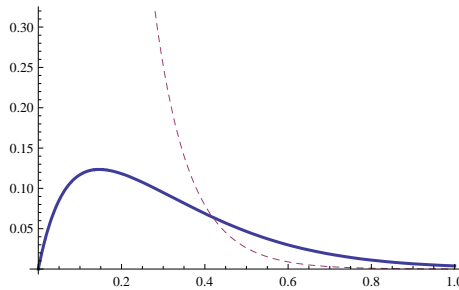


Figure 6.4: Case 2:  $\alpha = 0.5$ ;  $\sigma[\varrho_t]$  dashed line,  $|\sigma_E[\varrho_t]|$  continuous line

**Case 3.** An initial mixed entangled state (6.25) goes into an asymptotic mixed state

which is more or equally entangled and the conjecture (6.18) is violated after some time.

$$\begin{aligned} \varrho &= \frac{1}{10} |1\rangle\langle 1| + \frac{1}{10} |2\rangle\langle 2| + \frac{1}{10} |3\rangle\langle 3| + \frac{7}{10} |4\rangle\langle 4| \\ \varrho_\infty &= \frac{3(1-\alpha)^2}{10(3+\alpha^2)} |1\rangle\langle 1| + \frac{3(1+\alpha)^2}{10(3+\alpha^2)} |2\rangle\langle 2| + \frac{3(1-\alpha^2)}{10(3+\alpha^2)} |3\rangle\langle 3| + \frac{7}{10} |4\rangle\langle 4| \\ C(\varrho) &= \frac{2}{5}, \quad C(\varrho_\infty) = \frac{2}{5} \frac{3+4\alpha^2}{3+\alpha^2} \geq \frac{2}{5} \quad \forall \alpha \in [-1, 1]. \end{aligned} \quad (6.25)$$

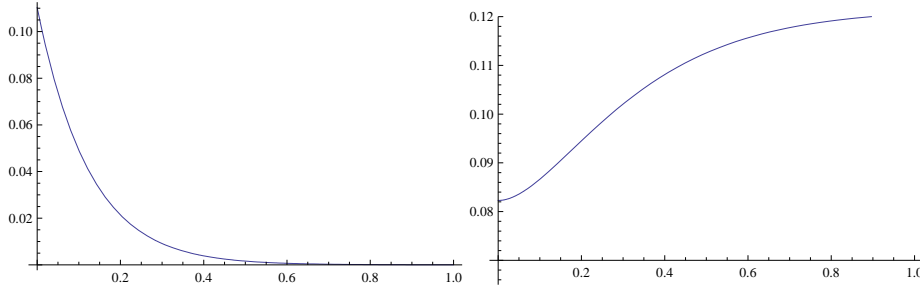


Figure 6.5: Case 3:  $\alpha = 0.5$ ; Left:  $S(\varrho_t || \varrho_\infty)$ ; Right:  $E[\varrho_t]$

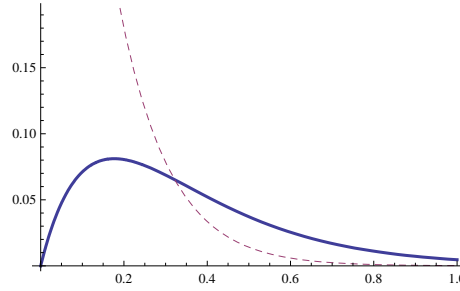


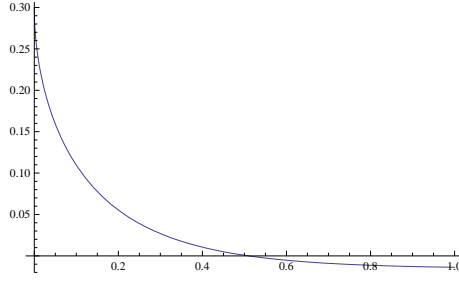
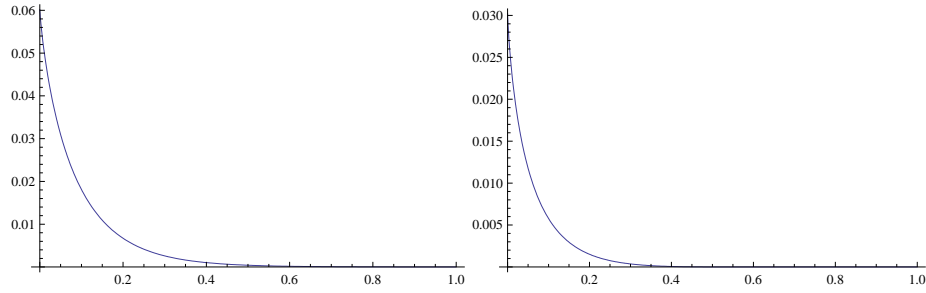
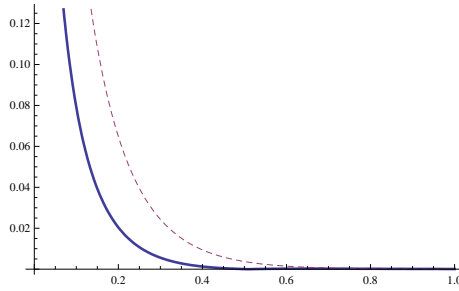
Figure 6.6: Case 3:  $\alpha = 0.5$ ;  $\sigma[\varrho_t]$  dashed line,  $|\sigma_E[\varrho_t]|$  continuous line

**Case 4.** An initial mixed entangled state (6.26) goes into a state with less entanglement

$$\begin{aligned} \varrho &= \frac{1}{2} |2\rangle\langle 2| + \frac{1}{10} |3\rangle\langle 3| + \frac{2}{5} |4\rangle\langle 4| \\ \varrho_\infty &= \frac{3(1-\alpha)^2}{5(3+\alpha^2)} |1\rangle\langle 1| + \frac{3(1+\alpha)^2}{5(3+\alpha^2)} |2\rangle\langle 2| + \frac{3(1-\alpha^2)}{5(3+\alpha^2)} |3\rangle\langle 3| + \frac{2}{5} |4\rangle\langle 4| \\ C(\varrho) &= \frac{3}{5}, \quad \begin{cases} C(\varrho_\infty) = 0 & \text{for } \alpha^2 \leq \frac{3}{11} \\ C(\varrho_\infty) = \frac{11\alpha^2-3}{5(3+\alpha^2)} < \frac{3}{5} & \text{for } \frac{3}{11} < \alpha^2 \leq 1 \end{cases} \end{aligned} \quad (6.26)$$

With the choice  $\alpha = 0.5$ , the dissipative time-evolution shows a sudden death of entanglement, that is the concurrence<sup>2</sup> (6.13) vanishes at finite time. The conjecture (6.18) always holds.

<sup>2</sup>In Figure 7, instead of plotting the concurrence as defined in (6.13), the difference  $|b-c| - 2\sqrt{ad}$  is plotted: this simply means that, as soon as this difference becomes negative, the state is separable.

Figure 6.7: Case 4:  $\alpha = 0.5$ ;  $C(\varrho_t)$ Figure 6.8: Case 4:  $\alpha = 0.5$ ; Left:  $S(\varrho_t || \varrho_\infty)$ ; Right:  $E[\varrho_t]$ Figure 6.9: Case 4:  $\alpha = 0.5$ ;  $\sigma[\varrho_t]$  dashed line,  $|\sigma_E[\varrho_t]|$  continuous line

**Case 5.** An initial mixed entangled state (6.27) goes into a mixed entangled state with more or less entanglement depending on the choice of the parameter  $\alpha$ .

$$\begin{aligned} \varrho &= \frac{3}{10} |2\rangle\langle 2| + \frac{1}{10} |3\rangle\langle 3| + \frac{3}{5} |4\rangle\langle 4| & (6.27) \\ \varrho_\infty &= \frac{2(1-\alpha)^2}{5(3+\alpha^2)} |1\rangle\langle 1| + \frac{2(1+\alpha)^2}{5(3+\alpha^2)} |2\rangle\langle 2| + \frac{2(1-\alpha^2)}{5(3+\alpha^2)} |3\rangle\langle 3| + \frac{3}{5} |4\rangle\langle 4| \\ C(\varrho) &= \frac{1}{2}, \quad C(\varrho_\infty) = \frac{3(1+3\alpha^2)}{5(3+\alpha^2)} \end{aligned}$$

The concurrence of the asymptotic state  $C(\varrho_\infty)$  can be larger or smaller than  $C(\varrho) = \frac{1}{2}$  depending on the value of the parameter  $\alpha$ .

If, for instance,  $\alpha = 0.5$ , then  $C(\varrho_\infty) < \frac{1}{2}$ , i.e. the asymptotic state has less entanglement than the initial state, and from the plot of the entanglement rate vs. the entropy rate

(Figure 11) it can be seen that the conjecture (6.18) is always violated.

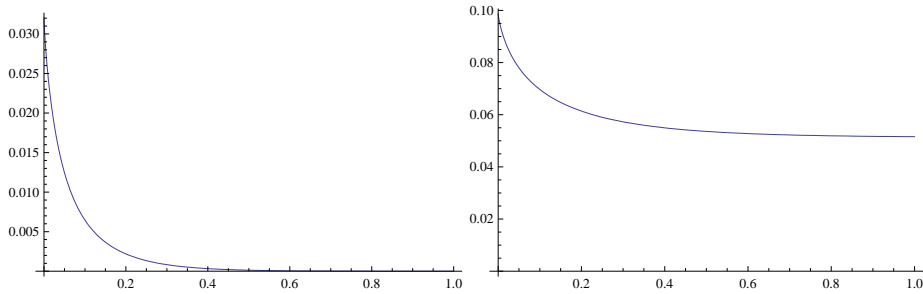


Figure 6.10: Case 5:  $\alpha = 0.5$ ; Left:  $S(\rho_t || \rho_t)$ ; Right:  $E[\rho_t]$

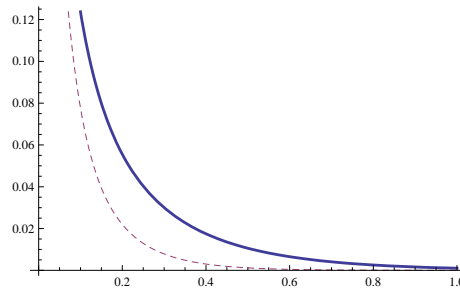


Figure 6.11: Case 5:  $\alpha = 0.5$ ;  $\sigma[\rho_t]$  dashed line,  $|\sigma_E[\rho_t]|$  continuous line

If, instead, the value e.g.  $\alpha = 0.8$  is taken, then the initial entanglement first diminishes and then increases again, leading to an asymptotic state with more entanglement than the initial one, as can be seen from the plot of the entropy of entanglement as a function of time (Figure 12). From the corresponding plot of the entanglement rate vs. the entropy rate (Figure 13) it can be seen that in this case the conjecture (6.18) is violated after some time.

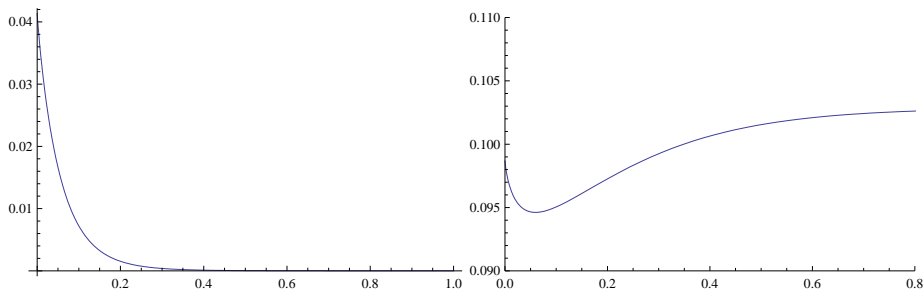


Figure 6.12: Case 5:  $\alpha = 0.8$ ; Left:  $S(\rho_t || \rho_\infty)$ ; Right:  $E[\rho_t]$

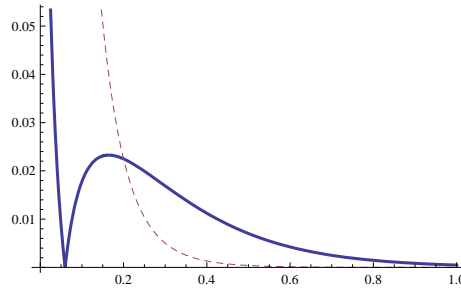


Figure 6.13: Case 5:  $\alpha = 0.8$ ;  $\sigma[\varrho_t]$  dashed line,  $|\sigma_E[\varrho_t]|$  continuous line

**Remark 12** In the last plot of the entanglement rate vs. the entropy rate, the cusp is due to the change of sign in the entropy of entanglement  $S(\varrho_t|\varrho_\infty)$  and to the fact that in the conjecture (6.18) the absolute value of the entanglement rate  $\sigma_E[\varrho_t]$  is considered. On the other hand, all the other plots of the entanglement rate present a continuous behavior which reflects the fact that the entropy of entanglement does not change sign, i.e. it either increases or decreases monotonically. Finally, the plots of the relative entropy show its monotonic behavior under the action of completely positive trace-preserving maps; and to this corresponds a monotonic decreasing behavior for the entropy rate.

## 6.5 Conclusions

The time-derivative of the quantum relative entropy serves as a measure of how fast an open quantum system tends to equilibrium dissipating free energy under a quantum dynamical semigroup of completely positive maps generated by a Lindblad-type master equation. On the other hand, via a variational formulation, the relative entropy may be used as a pseudo-distance of an entangled bipartite state from the convex subset of separable states (relative entropy of entanglement); therefore, its time derivative can be interpreted as the speed with which a time-evolving state moves toward, or away from, becoming separable.

Based on the expectation that the entanglement content of dissipatively-driven bipartite systems disappears asymptotically due to decoherence effects, in [12] a conjecture was put forward, namely that the entropy rate, measured by (minus) the time-derivative of the relative entropy of a dissipatively evolving state and its asymptotic state, should always be larger than the absolute value of the time-derivative of the relative entropy of entanglement.

However, beside being a source of decoherence, an environment can in some cases build quantum correlations that can even persist asymptotically: in this work, the fate of the above conjecture is studied in the case of a Lindblad-type master equation that presents a rich manifold of asymptotic states that may be more or less entangled with

respect to the initial states they emerge from. The entropy and entanglement rates have been explicitly calculated and numerically plotted for a class of initial states. It turns out that, when the asymptotic state is entangled, the conjecture is violated either at all times or after a finite time; instead, the conjecture is confirmed in all cases when the asymptotic state is separable. The conjecture put forward in [12] should be thus reformulated as follows:

$$\left| \sigma_E[\varrho_t] \right| \leq \sigma[\rho_t] \quad \forall \rho_t \text{ with } \varrho_\infty \text{ separable .} \quad (6.28)$$

While the asymptotic predominance of the entropy rate over the entanglement rate in the latter case has already been explained in [12] based on the fact that there are no entangled states in a suitable neighborhood of the separable asymptotic state, the truly remarkable fact about (6.28) is its validity at all  $t \geq 0$  in all the cases that have been checked.

# Summary and outlook

In this PhD work two main topics were considered: open quantum systems and their characterization, on one hand, and the behavior of entanglement in these systems, on the other, and some interesting results were found.

In Chapter 3 a way of characterizing properties of the environment through physical quantities of the system immersed within it is proposed. Here an open quantum system consisting of an electron propagating through a one-dimensional wire, in which a spin-1/2 impurity is embedded, is considered. There is a local magnetic interaction between the electron and the impurity, and the whole system is immersed in a bath whose noisy effects affect only the spin-1/2 impurity. In this scenario an explicit expression for the noise parameters (i.e. the Kossakowski matrix elements) is found in terms of the electron's transmission and reflection probabilities, which can be effectively measured. Further, this could represent a test for the Markovian approximation used: indeed, if the results of the probabilities lead to a Kossakowski matrix which is not positive semi-definite, i.e. to a dissipative map which is not completely positive, this could indicate that the particular approximation used is not correct.

Moreover, an example of the necessity of complete positivity for physical consistency is given: indeed, in the case of a diagonal Kossakowski matrix, it is shown that negative transmission probabilities arise for some entangled states, if the map governing the dissipative dynamics is positive but not completely positive.

This work could be further pursued both considering discretized systems consisting of wires or rings with  $N$  sites and an electron hopping along, and analyzing wires with more than one impurity embedded in it.

In Chapter 5, the sufficient condition presented in [10] for a bath to generate entanglement in an initially separable state of two qubits is proved to be also necessary, and an explicit example of this is given. Further, the sufficient condition for environment-induced entanglement is generalized to bipartite systems of arbitrary dimensions, generalizing the structure of the Kossakowski matrix. In this case, since the latter is of higher dimension, it is possible to obtain a larger number of conditions for environment-induced entanglement and thus a wider variety of entangling options in the higher-dimensional system. Indeed, an explicit example of this is also given, where entanglement can be gen-

erated in a four-qubit state, although it cannot be created between any pair of qubits of the system. So, on the one hand it could be of interest to find other such examples; while on the other, since multipartite entanglement has also become very important to study, as briefly mentioned at the end of Example 2, the generalization of the sufficient condition for environment-induced entanglement generation to higher-dimensional systems could be used to find analogous conditions fitted to the multipartite setting. Moreover, it could be of interest to try and use the different definitions of the geometric measure of entanglement considered in [49] to evaluate the environment-induced entanglement quantitatively in the multipartite setting.

Finally, in Chapter 6, the behavior of entanglement in time has been studied in detail for a particular class of states undergoing a dissipative dynamics. For the chosen class of states it is possible to analytically solve the master equation and find the explicit form of the asymptotic state. Therefore, the variation in time of entanglement (entanglement rate) measured with the so-called relative entropy of entanglement is analyzed together with the variation in time of entropy (entropy rate), and the amount of entanglement in the initial and in the asymptotic states is compared. Two results can be highlighted here. On one hand, following a conjecture put forward in [12], a new conjecture can be formulated here, namely:

- when the asymptotic state of the dissipative dynamics is separable, then the conjecture from [12] holds, i.e. the entanglement rate is always bounded by the entropy rate;
- when the asymptotic state is entangled, then the conjecture from [12] is violated, either for all times or after a finite amount of time, i.e. the entanglement rate is not bounded by the entropy rate.

Further, the dissipative dynamics considered here leads to various different behaviors in time of entanglement, depending on the chosen initial state and on the noise parameters: indeed, entanglement can be generated in initially separable two-qubit states; it can be partly dissipated or even vanish totally, if it was initially present; but, most interestingly, it can also increase during the dissipative dynamics and be non-zero in the asymptotic state.

It would be of interest to try and find a general framework to explain the behavior of entanglement and the entanglement rate versus the entropy rate with generic dissipative dynamics and a wider class of states.



# Acknowledgements

I am extremely grateful to my PhD supervisor, Dr. Fabio Benatti, for helping me grow scientifically, for transmitting enthusiasm to me, and for being my mentor during these three years of interesting work.



## Appendix A

# Calculation of transmission and reflection coefficients

The first two equations for the transmission and reflection probabilities in terms of the Kossakowski matrix elements and transmission coefficients, computed to the first order in  $t$ , are as follows:

$$\begin{aligned} \frac{P_0^T(t)}{t} &= K_{11}|t_0^E|^2 + K_{12}[-2\text{Im}(t_0^E)\text{Re}(t_1^E) + 2\text{Im}(t_1^E)\text{Re}(t_0^E)] \\ &+ K_{13}[2\text{Re}(t_0^E)\text{Re}(t_1^E) + 2\text{Im}(t_1^E)\text{Im}(t_0^E)] + K_{22}|t_1^E|^2 + 2K_{33}|t_1^E|^2, \end{aligned}$$

$$\begin{aligned} \frac{P_0^R(t)}{t} &= K_{11}[2 - 2\cos(2kx) + |t_0^E|^2 - 2\text{Re}(t_0) + 2\text{Re}(t_0)\cos(2kx) + 2\text{Im}(t_0)\sin(2kx)] \\ &+ K_{12}[-2\text{Im}(t_0^E)\text{Re}(t_1^E) + 2\text{Im}(t_1^E)\text{Re}(t_0^E) + 2\text{Im}(t_0^E) - 2\text{Im}(t_1^E)] \\ &+ 2\text{Re}(t_0)\sin(2kx) - \text{Im}(t_0)\cos(2kx) - 2\text{Re}(t_1)\sin(2kx) + \text{Im}(t_1)\cos(2kx)] \\ &+ K_{13}[4 - 4\cos(2kx) + 2\text{Re}(t_0^E)\text{Re}(t_1^E) + 2\text{Im}(t_1^E)\text{Im}(t_0^E) + 2\text{Re}(t_1)\cos(2kx) \\ &+ 2\text{Im}(t_1)\sin(2kx) - 2\text{Re}(t_1) - 2\text{Re}(t_0) + 2\text{Re}(t_0)\cos(2kx) + 2\text{Im}(t_0)\sin(2kx)] \\ &+ K_{22}[2 - 2\cos(2kx) + |t_1^E|^2 - 2\text{Re}(t_1) + 2\text{Re}(t_1)\cos(2kx) + 2\text{Im}(t_1)\sin(2kx)] \\ &+ 2K_{33}[2 - 2\cos(2kx) + |t_1^E|^2 - 2\text{Re}(t_1) + 2\text{Re}(t_1)\cos(2kx) + 2\text{Im}(t_1)\sin(2kx)]. \end{aligned}$$

The other four equations for  $P_a^{T,R}$ ,  $a = 1, 2$ , have the same form just with a different ordering of the elements  $K_{ij}$  in accordance with the rotation of the spin bases, as previously explained, using (3.16), (3.17), (3.18). In particular, taking  $x = \frac{n\pi}{4k}$  with  $n = 4m + 1$  and  $m = 0, 1, 2, \dots$ , it follows that  $\sin(2kx) = 1$ ,  $\cos(2kx) = 0$ : this leads to six distinct equations where the expressions for the reflection probabilities are somewhat simplified whereas those for the transmission probabilities remain unchanged. If this linear system is then written in vector form, equation (3.19) is obtained, where  $M$  is a matrix whose entries are the constants multiplying the elements  $K_{ij}$  in the system of equations. This

matrix explicitly reads:

$$M = \begin{pmatrix} a_0 & b & c & a_1 & 0 & 2a_1 \\ a_0 & -c & b & 2a_1 & 0 & a_1 \\ 2a_1 & 0 & -c & a_1 & b & a_0 \\ d_0 & e & f & d_1 & 0 & 2d_1 \\ d_0 & -f & e & 2d_1 & 0 & d_1 \\ 2d_1 & 0 & -f & d_1 & e & d_0 \end{pmatrix},$$

with

$$\begin{aligned} a_i &= \operatorname{Re}(t_i^E) = |t_i^E|^2, & i &= 0, 1, \\ b &= 2[-\operatorname{Im}(t_0^E)\operatorname{Re}(t_1^E) + \operatorname{Im}(t_1^E)\operatorname{Re}(t_0^E)], \\ c &= 2[\operatorname{Re}(t_0^E)\operatorname{Re}(t_1^E) + \operatorname{Im}(t_1^E)\operatorname{Im}(t_0^E)], \\ d_i &= 2 - |t_i^E|^2 + 2\operatorname{Im}(t_i^E), & i &= 0, 1, \\ e &= 2[\operatorname{Im}(t_0^E)\operatorname{Re}(t_1^E) + \operatorname{Im}(t_1^E)\operatorname{Re}(t_0^E) + \operatorname{Re}(t_0^E) - \operatorname{Re}(t_1^E) + \operatorname{Im}(t_0^E) - \operatorname{Im}(t_1^E)], \\ f &= 2[2 + \operatorname{Re}(t_0^E)\operatorname{Re}(t_1^E) + \operatorname{Im}(t_1^E)\operatorname{Im}(t_0^E) - \operatorname{Re}(t_0^E) - \operatorname{Re}(t_1^E) + \operatorname{Im}(t_0^E) + \operatorname{Im}(t_1^E)]. \end{aligned}$$

## Appendix B

# Integration of the master equation

In order to explicitly solve the master equation (6.1), firstly matrix  $\mathcal{A}$  is written in diagonal form:

$$\mathcal{A} = U \begin{pmatrix} 1 + \alpha & 0 & 0 \\ 0 & 1 - \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} U^\dagger, \quad U = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -i/\sqrt{2} & i/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and the dissipative term in (6.3) is recast in the form

$$\begin{aligned} \mathbf{D}[\varrho_t] &= 2(1 + \alpha) \left( \Sigma_- \varrho_t \Sigma_+ - \frac{1}{2} \{ \Sigma_+ \Sigma_-, \varrho_t \} \right) + 2(1 - \alpha) \left( \Sigma_+ \varrho_t \Sigma_- - \frac{1}{2} \{ \Sigma_- \Sigma_+, \varrho_t \} \right) \\ &+ \Sigma_3 \varrho_t \Sigma_3 - \frac{1}{2} \{ \Sigma_3 \Sigma_3, \varrho_t \}, \end{aligned} \quad (\text{B.1})$$

with  $\Sigma_\pm := \frac{1}{2}(\Sigma_1 \pm i\Sigma_2)$ . Since  $H = \frac{\Omega}{2} \Sigma_3$ , it follows that  $e^{iHt} \Sigma_\pm e^{-iHt} = e^{\pm i\Omega t} \Sigma_\pm$ . Thus, setting  $\tilde{\varrho}_t := e^{iHt} \varrho_t e^{-iHt}$ , in the interaction picture the master equation (B.1) becomes

$$\begin{aligned} \partial_t \tilde{\varrho}_t &= e^{iHt} \mathbf{D}[e^{-iHt} \tilde{\varrho}_t e^{iHt}] e^{-iHt} \\ &= 2(1 + \alpha) \left( \Sigma_- \tilde{\varrho}_t \Sigma_+ - \frac{1}{2} \{ \Sigma_+ \Sigma_-, \tilde{\varrho}_t \} \right) + 2(1 - \alpha) \left( \Sigma_+ \tilde{\varrho}_t \Sigma_- - \frac{1}{2} \{ \Sigma_- \Sigma_+, \tilde{\varrho}_t \} \right) \\ &+ \Sigma_3 \tilde{\varrho}_t \Sigma_3 - \frac{1}{2} \{ \Sigma_3 \Sigma_3, \tilde{\varrho}_t \}. \end{aligned} \quad (\text{B.2})$$

In order to solve it, it proves convenient to represent  $\tilde{\rho}_t = \sum_{i,j=1}^4 \rho_{ij}(t) |i\rangle\langle j|$  with respect to the orthonormal basis (6.6). Indeed, using that

$$\begin{cases} \Sigma_+ |1\rangle = 0 \\ \Sigma_+ |2\rangle = \sqrt{2}|3\rangle \\ \Sigma_+ |3\rangle = \sqrt{2}|1\rangle \\ \Sigma_+ |4\rangle = 0 \end{cases}, \quad \begin{cases} \Sigma_- |1\rangle = \sqrt{2}|3\rangle \\ \Sigma_- |2\rangle = 0 \\ \Sigma_- |3\rangle = \sqrt{2}|2\rangle \\ \Sigma_- |4\rangle = 0 \end{cases}, \quad \begin{cases} \Sigma_3 |1\rangle = 2|1\rangle \\ \Sigma_3 |2\rangle = -2|2\rangle \\ \Sigma_3 |3\rangle = 0 \\ \Sigma_3 |4\rangle = 0 \end{cases}, \quad (\text{B.3})$$

from (B.2) the following equations are derived:

$$\begin{aligned}
\dot{\rho}_{11} &= -4(1+\alpha)\rho_{11} + 4(1-\alpha)\rho_{33} & , & \dot{\rho}_{12} = -12\rho_{12} \\
\dot{\rho}_{13} &= -2(4+\alpha)\rho_{13} + 4(1-\alpha)\rho_{32} & , & \dot{\rho}_{14} = -2(2+\alpha)\rho_{14} \\
\dot{\rho}_{22} &= -4(1-\alpha)\rho_{22} + 4(1+\alpha)\rho_{33} & , & \dot{\rho}_{23} = -2(4-\alpha)\rho_{23} + 4(1+\alpha)\rho_{31} \\
\dot{\rho}_{33} &= 4(1+\alpha)\rho_{11} + 4(1-\alpha)\rho_{22} - 8\rho_{33} & , & \dot{\rho}_{24} = -2(2-\alpha)\rho_{24} \\
\dot{\rho}_{34} &= -4\rho_{34} & , & \dot{\rho}_{44} = 0 ,
\end{aligned}$$

plus the complex conjugated equations for  $\dot{\rho}_{ij}$ ,  $i \neq j$ ; whence

$$\begin{aligned}
\rho_{12}(t) &= \rho_{12} e^{-12t} & , & \rho_{14}(t) = \rho_{14} e^{-2(2+\alpha)t} \\
\rho_{24}(t) &= \rho_{24} e^{-2(2-\alpha)t} & , & \rho_{34}(t) = \rho_{34} e^{-4t} \\
\rho_{44}(t) &= \rho_{44} .
\end{aligned} \tag{B.4}$$

Of the remaining equations, two of them couple the off-diagonal terms  $\rho_{13}$  and  $\rho_{32}$ , yielding

$$\rho_{13}(t) = \rho_{13} F_+(t) + \frac{2(1-\alpha)\rho_{32} - \alpha\rho_{13}}{\sqrt{4-3\alpha^2}} F_-(t) \tag{B.5}$$

$$\rho_{32}(t) = \rho_{32} F_+(t) + \frac{2(1+\alpha)\rho_{13} + \alpha\rho_{32}}{\sqrt{4-3\alpha^2}} F_-(t) , \tag{B.6}$$

while the other three solutions couple the diagonal entries:

$$\begin{aligned}
\rho_{11}(t) &= \frac{(1-\alpha)^2}{3+\alpha^2} R + \frac{\sqrt{1-\alpha^2} (1+\alpha)^2 \rho_{11} - 2(1-\alpha)\rho_{22} + (1+\alpha)^2 \rho_{33}}{(1+\alpha)(3+\alpha^2)} E_-(t) \\
&+ \frac{2(1+\alpha)\rho_{11} - (1-\alpha)^2(\rho_{22} + \rho_{33})}{3+\alpha^2} E_+(t)
\end{aligned} \tag{B.7}$$

$$\begin{aligned}
\rho_{22}(t) &= \frac{(1+\alpha)^2}{3+\alpha^2} R - \frac{\sqrt{1-\alpha^2} 2(1+\alpha)\rho_{11} - (1-\alpha)^2(\rho_{22} + \rho_{33})}{(1-\alpha)(3+\alpha^2)} E_-(t) \\
&- \frac{(1+\alpha)^2 \rho_{11} - 2(1+\alpha)\rho_{22} + (1+\alpha)^2 \rho_{33}}{3+\alpha^2} E_+(t)
\end{aligned} \tag{B.8}$$

$$\begin{aligned}
\rho_{33}(t) &= \frac{(1-\alpha^2)}{3+\alpha^2} R + \frac{\sqrt{1-\alpha^2} (1+\alpha)^3 \rho_{11} + (1-\alpha)^3 \rho_{22} - 2(1-\alpha^2)\rho_{33}}{(3+\alpha^2)(1-\alpha^2)} E_-(t) \\
&+ \frac{2(1+\alpha^2)\rho_{33} - (1-\alpha^2)(\rho_{11} + \rho_{22})}{3+\alpha^2} E_+(t) ,
\end{aligned} \tag{B.9}$$

where  $R = \rho_{11} + \rho_{22} + \rho_{33} = \rho_{11}(t) + \rho_{22}(t) + \rho_{33}(t)$  is a constant of the motion and

$$E_{\pm}(t) = e^{-8t} \begin{cases} \cosh 4t\sqrt{1-\alpha^2} \\ \sinh 4t\sqrt{1-\alpha^2} \end{cases} , \quad F_{\pm}(t) = e^{-8t} \begin{cases} \cosh 2t\sqrt{4-3\alpha^2} \\ \sinh 2t\sqrt{4-3\alpha^2} \end{cases} . \tag{B.10}$$

are quantities which decay asymptotically with  $t \rightarrow +\infty$ . The remaining entries  $\rho_{ij}(t)$  follow from complex conjugation. By returning to the Schrödinger representation, using (B.3) the explicit solution of (B.1) reads

$$\varrho_t = \sum_{i,j=1}^4 \varrho_{ij}(t) e^{2i\omega t(\delta_{j1} + \delta_{i2} - \delta_{i1} - \delta_{j2})} |i\rangle\langle j| . \tag{B.11}$$

## Appendix C

# Solution of the maximization problem

In order to prove Proposition 7 in Chapter 6, consider the spectral decompositions  $\varrho_t = \sum_{i=1}^4 r_i(t) |i\rangle\langle i|$  (see (6.8)) and  $\varrho_{sep} = \sum_{j=1}^4 s_j |s_j\rangle\langle s_j|$ . Then

$$\begin{aligned} \text{Tr}(\varrho_t \log \varrho_{sep}) &= \sum_{i=1}^4 r_i(t) \langle i | \log \varrho_{sep} | i \rangle = \sum_{i=1}^4 r_i(t) \sum_{j=1}^4 |\langle i | s_j \rangle|^2 \log s_j \\ &\leq \sum_{i=1}^4 r_i(t) \log \left( \sum_{j=1}^4 s_j |\langle i | s_j \rangle|^2 \right) \\ &= \sum_{i=1}^4 r_i(t) \log \langle i | \varrho_{sep} | i \rangle = \text{Tr}(\varrho_t \log \Pi[\varrho_{sep}]), \end{aligned} \quad (\text{C.1})$$

where the inequality follows from the convexity of  $\log x$ ,

$$\log \sum_i \lambda_i x_i \geq \sum_i \lambda_i \log x_i, \quad \lambda_i \geq 0, \quad \sum_i \lambda_i = 1, \quad x_i \geq 0,$$

and  $\sum_{j=1}^4 |\langle i | s_j \rangle|^2 = 1$ . Also, the completely positive map

$$\varrho \mapsto \Pi[\varrho] := \sum_{i=1}^4 |i\rangle\langle i | \varrho | i\rangle\langle i|, \quad (\text{C.2})$$

on the two-qubit density matrices  $\mathcal{S}(\mathbb{C}^4)$  that diagonalizes its argument with respect to the orthonormal basis (6.6) has been introduced. This map has the following property which allows one to analytically solve the variational problem (C.1).

**Lemma**  $\Pi : \mathcal{S}(\mathbb{C}^4) \mapsto \mathcal{S}(\mathbb{C}^4)$  maps separable states into separable states.

**Proof:** Given the density matrix of an arbitrary two-qubit state in the standard basis

$$\varrho = \begin{pmatrix} \varrho_{00,00} & \varrho_{00,01} & \varrho_{00,10} & \varrho_{00,11} \\ \varrho_{01,00} & \varrho_{01,01} & \varrho_{01,10} & \varrho_{01,11} \\ \varrho_{10,00} & \varrho_{10,01} & \varrho_{10,10} & \varrho_{10,11} \\ \varrho_{11,00} & \varrho_{11,01} & \varrho_{11,10} & \varrho_{11,11} \end{pmatrix},$$

the action of the map  $\Pi$  transforms it into a density matrix of the form

$$\Pi[\varrho] = \begin{pmatrix} \varrho_{00,00} & 0 & 0 & 0 \\ 0 & \frac{\varrho_{01,01} + \varrho_{10,10}}{2} & \Re(\varrho_{01,10}) & 0 \\ 0 & \Re(\varrho_{01,10}) & \frac{\varrho_{01,01} + \varrho_{10,10}}{2} & 0 \\ 0 & 0 & 0 & \varrho_{11,11} \end{pmatrix}.$$

By partial transposition [16],  $\Pi[\varrho]$  is entangled if and only if  $|\Re(\varrho_{01,10})| \geq \sqrt{\varrho_{00,00}\varrho_{11,11}}$ . But then, the partially transposed  $\varrho$  (with respect to the second qubit),

$$\varrho^\Gamma = \begin{pmatrix} \varrho_{00,00} & \varrho_{01,00} & \varrho_{00,10} & \varrho_{01,10} \\ \varrho_{00,01} & \varrho_{01,01} & \varrho_{00,11} & \varrho_{01,11} \\ \varrho_{10,00} & \varrho_{11,00} & \varrho_{10,10} & \varrho_{11,10} \\ \varrho_{10,01} & \varrho_{11,01} & \varrho_{10,11} & \varrho_{11,11} \end{pmatrix}$$

cannot be positive semi-definite, for  $|\varrho_{01,10}| \geq |\Re(\varrho_{01,10})| > \sqrt{\varrho_{00,00}\varrho_{11,11}}$  in the sub-matrix  $\begin{pmatrix} \varrho_{11} & \varrho_{01,10} \\ \varrho_{10,01} & \varrho_{22} \end{pmatrix}$ . Therefore, if  $\varrho$  is separable, then also  $\Pi[\varrho]$  must be so.  $\square$

Observe that (C.1) implies  $\sup_{\varrho_{sep}} \text{Tr}(\varrho_t \log \varrho_{sep}) \leq \sup_{\varrho_{sep}} \text{Tr}(\varrho_t \log \Pi[\varrho_{sep}])$ ; on the other hand, since  $\Pi$  maps separable states into separable states,

$$\sup_{\varrho_{sep}} \text{Tr}(\varrho_t \log \varrho_{sep}) \leq \sup_{\varrho_{sep}} \text{Tr}(\varrho_t \log \Pi[\varrho_{sep}]) \leq \sup_{\varrho_{sep}} \text{Tr}(\varrho_t \log \varrho_{sep}).$$

Thus, the maximum in (C.1) is attained on the subset  $\mathcal{S}_{sep}^{diag}$  of separable qubit states that are diagonal with respect to the orthonormal basis, namely of the form (6.20) with the second bound on the real parameters  $x, y, u, v$  in (6.21) coming from the condition of positivity under partial transposition of matrices of the form (6.7), which is necessary and sufficient for separability.

It thus follows from (6.19) and (C.1) that for  $\varrho_t$  as in (6.8) the relative entropy of entanglement can be reduced to the computation of (6.22). In order to explicitly solve such a variational problem, it is sufficient to seek the stationary points of a function of the form

$$f(x, y, u, v) := a \log x + d \log y + b \log u + c \log v + \lambda(x + y + u + v - 1)$$



with given  $a, b, c, d \geq 0$  such that  $a + b + c + d = 1$ , relative to variations of the parameters  $x, y, u, v$  over values achieving separable states of the form (6.20). Stationarity implies

$$a = -\lambda x, \quad d = -\lambda y, \quad b = -\lambda u, \quad c = -\lambda v;$$

whence  $\lambda = -1$  and  $a = x, d = y, b = u, c = v$ . However, this can be the required solution only if the state  $\rho$  in  $E[\rho]$  is separable so that  $E[\rho] = 0$ . Otherwise, the solution must lie on the border of the subset of separable states of the form (6.20), where the inequality in (6.21) is saturated. From  $x + u + v + y = 1$  and  $(u - v)^2 = 4xy$ , one gets

$$u_{\pm} = \frac{1 - (\sqrt{x} \mp \sqrt{y})^2}{2}, \quad v_{\pm} = \frac{1 - (\sqrt{x} \pm \sqrt{y})^2}{2},$$

so that the function to be maximized becomes

$$f(x, y) = a \log x + d \log y + b \log \left( \frac{1 - (\sqrt{x} \mp \sqrt{y})^2}{2} \right) + c \log \left( \frac{1 - (\sqrt{x} \pm \sqrt{y})^2}{2} \right). \quad (\text{C.3})$$

Stationarity with respect to  $x, y$  leads to a system of two equations for the two unknowns  $x$  and  $y$  in terms of the coefficients  $a, b, c, d$ . From setting  $\partial_{x,y} f(x, y) = 0$  and from the condition  $a + b + c + d = 1$  it follows that  $y = x - a + d$  and that

$$\begin{aligned} x = & \frac{1}{8(-1+b)(a+b+d)} \left\{ -a^3 - d(-1+2b+d)^2 + a^2(-6+4b+d) \right. \\ & + a(-1+4(-1+b)+d^2) + \left[ (-1+a+2b+d)^2 (a^4 + 2a^3(-1+2b-2d) \right. \\ & + d^2(-1+2b+d)^2 + a^2(1+4b^2+2d+6d^2-4b(1+d)) \\ & \left. \left. + 2ad(1+d-2(2b(-1+b)+bd+d^2)) \right) \right]^{1/2} \left. \right\}. \end{aligned}$$

By inserting into it the values (6.9)–(6.11), this expression yields the separable state of the form (6.20) which is closest to an evolving entangled state of the form (6.8). Though cumbersome, the resulting entanglement rate (6.17) is amenable to numerical inspection.



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