University College London
Department of Physics and Astronomy

Transfer process and typicality of noisy quantum systems with discrete time dynamics

Author:
Michele Avalle

Supervisor:
Dr. Alessio Serafini

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Declaration

I, Michele Avalle, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Abstract

In the thesis, models of quantum systems characterized by discrete time dynamics are presented and applied to different problems. More specifically, aspects of excitation transport, quantum state transfer and thermalization are investigated mainly within the framework of quantum cellular automata (QCA), which are discrete time evolution quantum systems defined on a regular lattice of, in this case, qubits.

The peculiarities of QCA, together with the restriction to the first excitation sector of the Hilbert space, make it possible to define a transport dynamics on a one dimensional lattice that encompasses all classical Markov chains, as well as maps where quantum coherence between sites can build up over time. This allows for the possibility to make a direct comparison between a fully classical dynamics and a dynamics affected by quantum effects, which is of relevance both in the field of quantum biology, especially regarding the transport of electronic excitations in photosynthetic systems, and in quantum computing when dealing with the transport of an unknown quantum state.

In a quantum thermodynamics context, instead, QCA can serve the purpose to validate arguments of tipicality that have been brought forward in recent years in order to demonstrate the thermalization of closed quantum systems (i.e. the tendency of any small subsystems to evolve towards the maximally mixed state). Numerical results concerning this issue are presented.

Finally, a modelization of scattering-like processes, where the scattering consists of random unitary interactions between an environment and part of a quantum bipartite system is discussed. Relevant properties of the resulting state such as its mean purity and the correlations between the interacting and the "sheltered" part of the system can be analitically evaluated, and their fluctuations bounded.

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Questa tesi é dedicata ad ogni millimetro
degli svariati chilometri di filo da torcere
che mi hai dato in questi ultimi quasi tre anni
e che spero continuerai a darmi per molto tempo.

"I'm a rebel, mum!"

Skiantos

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Introduction

In the recently born and emerging field of quantum biology [1], much effort has been devoted so far to the study of excitation transfer in simple photosynthetic systems [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. In a light harvesting antenna, a photon hitting a receptor induces an electronic excitation which is transported with extreme efficiency to a molecular complex where it is eventually converted into chemical energy. It has been claimed that classical mechanisms alone may not be sufficient to explain that very high efficiency we find in nature [17] and this conjecture has been recently partially corroborated by experimental results showing the evidence of the presence of quantum coherences at some early stages of the dynamics [2, 19, 4, 5, 6]. However, what the role of quantum coherences is and even *if* quantum coherences do actually play a role in enhancing the transfering efficiency are still open questions. In this view, it is interesting to compare the efficiency of classical stochastic systems with that of systems driven by quantum effects to see whether these effects can lead to better performance[1]. On the other hand, trying to model a biological system, even a simple one, in terms of a quantum dynamics is a difficult task, the main reason being their coupling with a warm environment, whose fluctuations are expected to fastly decohere the system. In addition, the structural complexity and variety of biological systems does not allow for a complete knowledge and control of all necessary details. Nonetheless, several models aimed at predicting the presence and describing the role of coherences in transport processes have been proposed. Typically, a classical system is compared to the analogous, quantized model [12, 13, 22, 23, 24], although such a correspondence is by no means straightforward when open, dissipative systems are considered, as it should be in most cases of interest. Indeed, no real attempts have

[1]This is of course a longstanding, relevant question, which has already been tackled in the past [20, 21], establishing that, from a quantum information perspective, purely coherent quantum dynamics can provide qualitative performance improvements over classical systems.

been made so far in order to have a simple, "fair" comparison between a classical and a related quantum model, e.g.: What is the unequivocal equivalent classical dynamics to be compared to the quantum jump approach? In the work that will be presented in Chap.(3), instead of trying to get precise quantitative predictions for actual biological complexes, one looks for a minimal way to model excitation transfer in a generic open quantum system, with the aim of establishing a clear relationship between classical and quantum dynamics and to see whether there are qualitative differences in the outcomes obtained in these two regimes.

The resulting model enjoys a natural extension that allows to tackle another problem of great relevance within the context of quantum communication: quantum state transfer. The transfer of a quantum state between two or more different points in space is an important task in quantum information processing. When thinking for instance about quantum cryptography protocols, such as quantum key distribution, communication may need to be set over long distance so that the use of photons as information carriers represents the most natural choice, for they can travel easily through empty space or optical fibers. On the other hand though, the physical realization of a quantum computer would require the construction of an interacting network of components communicating over short distances, where interfacing between the physical systems carrying information and the ones performing the computation needs to be minimized. For such a scenario, it is thus highly desirable to find alternatives to photons. To this end, arrays of permanently coupled quantum systems in which quantum state transfer is accomplished through free dynamical evolution – also known as *spin chains* [25, 26] – have drawn substantial attention in the last ten years, up to the point of establishing themselves as a self standing area of study [27, 28, 29, 30, 31, 32],

A class of systems intimately related to spin chains [27, 28] is represented by quantum walks, the (either continuous or discrete time evolving) quantum counterpart to random walks on a lattice [33, 34, 35]. Although originally introduced to investigate quantum speedups over classical algorithms [20, 21], quantum walks have been applied to the problem of state transport as well, proving the capability to achieve perfect state transfer, even though usually under the engineering of rather restrictive dynamical protocols (e.g. [27, 28, 36]; see also [37] and references therein).

In the thesis, both coherent excitation transport and quantum state transfer are studied within the framework of quantum cellular automata (QCA). These systems are substancially different but nevertheless in a sense closely related to spin chains and quantum walks [38]. QCA are discrete time dynamics systems defined on a regular lattice, characterized by a strictly causal evolution arising from the locality and homogeneity of the interactions taking place among their components. These features, along with the further requirement of unitarity of evolution, make QCA a very natural tool to deal with quantum simulation and communication tasks [39, 40], as well as with more fundamental physical questions [41, 42].

The model we will discuss will detach itself from almost (see [43]) all the approaches present in the literature as the class of QCA we will consider is not restricted to unitary evolutions but actually defined within the more general formalism of CP-maps, in which quantum noise is naturally a part of the picture and the dynamics is suitable to describe the evolution of both open and closed quantum systems. That will lead us to introduce a strictly local model of energy transfer via a noisy quantum cellular automaton construction on a qubit lattice, which does provide the aimed "fair" comparison between classical and quantum energy transfer and can at the same time also be thought of being representative, to a certain extent, of the general quantum to classical transition mechanism. The same framework, properly extended, will then allow for a description of quantum state transfer processes in which the effects related to a certain degree of unavoidable coupling between system and environment can be taken into account. In the context of quantum state transfer, that represents a clear advantage over spin chains, as in that approach non-unitary evolutions have never been considered. As regards quantum walks, instead, despite one is provided with a rich literature concerning noisy dynamics, the application of such dynamics to the problem of transferring an unknown quantum state has been very little explored so far[2]. However, we remark that the QCA formalism we will develop, unlike discrete quantum walks, does not rely on a bipartition of the Hilbert space where the dynamics is defined, thus allowing for a more simple – and, arguably, natural – description of local noise in terms of just one-qubit CP-maps.

As QCA mimic actual physical interactions, they could prove useful for addressing fundamental problems like the explanation of thermalization at a quantum state

[2]With the notable exception of [44].

level, a mechanism underlying the foundation of statistical mechanics and quantum thermodynamics. In the last ten years, the topic has given rise to a whole new area of research where different approaches have provided many solid results concerning the mechanism of equilibration and thermalization of pure closed quantum states both at a kinematical and a dynamical level [45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55]. One such approach relies on the concept of *typicality*, the notion of which, although not explicitly, is rooted in probability theory. It was Boltzmann, in the 1870s [56], to first talk about typicality of behavior of a physical system in his famous explanation of the second law of thermodynamics, which identifies the impossibility for dissipative processes to be reversible with the vanishingly small probability of states with entropy far from the maximum. In this view, the concept of typicality can be regarded as the physical counterpart of Cournot's concept of *moral certainty*[3]. Transposed into a quantum mechanical context, reasoning in terms of typical properties of quantum states lead Gemmer *et al.* [49] and then Popescu *et al.* [45] to advance partial reformulations of the foundations of statistical mechanics based on their finding that almost all pure states are almost maximally entangled[4]. As shown in the thesis, similar typicality arguments can be applied to other contexts, like partial interactions of discretised quantum systems with a large environment (scattering-like processes).

The plan of the thesis is as follows.
In Chap.(1) and Chap.(2) we will introduce all the preliminary notions of quantum mechanics and quantum information theory that are necessary to deal with the arguments treated throughout the thesis. In Chap.(3), after providing a self-contained introduction to quantum cellular automata, we will present and discuss a QCA-based model of energy excitation transfer through a linear chain of qubits. The same model will be extended in Chap.(4) in order to deal with the transfer of a qubit state. In Chap.(5) we will give a brief introduction to the typicality approach to quantum thermodynamics issues, followed by numerical results concerning dy-

[3] In Cournot's words [57]: "*It is physically impossible for the frequency of an event in a long sequence of trials to differ substantially from the event's probability.*"

[4] In the sense that any small subsystem of a pure quantum state defined on a big Hilbert space, obtained by partial tracing, will almost certainly look maximally mixed, which is in agreement with the prescription given by the standard interpretation describing the unknown global state as a statistical ensemble. Small subsystems would then be well described by statistical ensembles not due to an observer's lack of knowledge, but due to their entanglement with the rest of the "universe" .

namical thermalization in QCA. Finally, Chap.(6) will be devoted to presenting a modelization of random scattering interactions for discrete quantum systems.

Part I

Preliminary concepts

Chapter 1

Elements of quantum information

This chapter is meant to introduce some of the fundamental concepts and mathematical tools of quantum mechanics and quantum information theory that will be used throughout the thesis. Most of the information contained in this chapter can be found in classical textbooks of quantum information, such as [58] and [59].

1.1 The postulates of quantum mechanics

Quantum mechanics is a mathematical model that provides a description of the physical world at a fundamental level. The structure of the model lies on a few postulates, sketched below, that aim at characterizing the concepts of *states*, *observables*, *measurement* and *evolution*.

- **States.** A state is a complete description of a physical system S and it is represented by a normalized vector $|\psi\rangle$ in the Hilbert space $\mathcal{H}_S$ associated with the system. The Hilbert space is separable, that is the Hilbert space of a composite system $S = \{s_1, s_2, \ldots, s_n\}$ is the tensor product of the state spaces associated to the subsystems: $\mathcal{H}_S = \bigotimes_{i=1}^{n} \mathcal{H}_i$.

- **Observables.** Observables are properties of the physical system that in principle can be measured and are represented by Hermitian operators on the Hilbert space $\mathcal{H}_S$.

- **Measurement.** The only possible outcome of a measurement of the observ-

able $O = \sum_i o_i |o_i\rangle\langle o_i|$ on a system is one of the eigenvalues $\{o_i\} \in \mathbb{R}$ of the operator O. Given a quantum state $|\psi\rangle$, prior to a measurement the probability of observing the outcome o_j is

$$p(j) = \langle\psi|P_j|\psi\rangle\,, \quad \text{with} \quad P_j = |o_j\rangle\langle o_j| \tag{1.1}$$

and right after measuring, if the outcome o_j is attained, the quantum state becomes

$$|\psi_j\rangle = \frac{P_j|\psi\rangle}{\sqrt{\langle\psi|P_j|\psi\rangle}}\,. \tag{1.2}$$

- **Evolution.** The time evolution of a quantum state is given by a unitary operator U_t acting on the state $|\psi\rangle$:

$$|\psi(t)\rangle = U_t|\psi\rangle. \tag{1.3}$$

The unitary evolution U_t is generated by a Hermitian operator H called the *Hamiltonian* of the system and can be written as[1] $U = e^{-iHt}$. The dynamics of the system is governed by the *Schrödinger equation*

$$\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle. \tag{1.4}$$

The whole structure of quantum theory is derived from these postulates. However, the formulation of the axioms just outlined is suitable for a description of entirely isolated systems. In most practical situations, instead, one either observes quantum systems that are somehow coupled to an environment, or is interested in describing just a (possibly small) part of a larger whole quantum system evolving unitarily. As we will see, to deal with such situations, the quantum "toolbox" must be enlarged to accommodate more general mathematical objects such as *density operators* for physical systems and *completely positive maps* for what concerns evolutions.

[1] Natural units ($\hbar = 1$) will be understood through all the thesis.

1.2 The qubit

The qubit is the quantum counterpart of the classical bit and, as such, it represents the fundamental "unit" of quantum information. A qubit describes the state of the simplest possible quantum system, namely a two-level system defined on a two dimensional complex Hilbert space. In this space, one can set an orthonormal basis formed by the two vectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \tag{1.5}$$

representing the values 0 and 1 of a classical bit. The basis composed of these two vectors is generally referred to as the *computational basis*. Any qubit state can then be written in a superposition form, up to a physically irrelevant overall phase, as

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \, , \tag{1.6}$$

where the amplitudes α and β are complex numbers constrained by the normalization condition

$$|\alpha|^2 + |\beta|^2 = 1 \, . \tag{1.7}$$

In practice, any two-level quantum system can be used as a qubit if:

1. It is possible to prepare it in some well-defined state (*fiducial state*);
2. any state of the qubit can be transformed into any other state by means of a unitary operation;
3. the qubit state can be measured in the computational basis.

1.3 Density matrix

In most practical situations the state of a quantum system is often not perfectly determined. This may for instance be due to either a lack of information or an imperfect control over the preparation procedure of the quantum system (or due to entanglement, see Sec. 1.7). When this happens, a statistical description of the state of the system is needed. That is provided by the density operator (or density

matrix) ρ, defined as

$$\rho = \sum_{k=1}^{n} p_k |\psi_k\rangle\langle\psi_k| \,, \tag{1.8}$$

where the vectors $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle\}$ represent the *ensemble* of states we estimate our system can be in, and the weights $\{p_1, p_2, \ldots, p_n\}$ are such that $\sum_{k=1}^{n} p_k = 1$. The density operator is thus interpreted as a statistical *mixture* of (not necessarily orthogonal with one another) *pure states* $\{|\psi_k\rangle\}$.

Recalling the measurement postulate given in Sec.(1.1), the probability that a measurement of the observable O yields outcome o_j is

$$p(j) = \sum_{k=1}^{n} p_k \langle\psi_k|P_j|\psi_k\rangle \,, \tag{1.9}$$

where $\{P_i\}$ are the projectors onto the subspaces associated with the eigenvalues $\{o_i\}$. Therefore

$$\langle O\rangle = \sum_{j=1}^{m} o_j p(j) = \sum_{k=1}^{n} p_k \langle\psi_k|O|\psi_k\rangle = \sum_{i=1}^{m} \langle i|\rho O|i\rangle = \mathrm{Tr}(\rho O) \tag{1.10}$$

where the second-last equality follows from the completeness relation $\sum_i |i\rangle\langle i| = \mathbb{1}$. It is also easy to check that

$$p(j) = \mathrm{Tr}(\rho P_j) \,. \tag{1.11}$$

The density operator then allows to both compute the mean value of any observable and to evaluate the probabilities to obtain the outcomes $\{o_j\}$ from a measurement, thus providing a complete characterization of the system. In fact, the density matrix can be considered as the most general object describing a quantum system and the postulates of quantum mechanics can be reformulated in the density operator picture.

The density operator ρ satisfies the following properties

1. It is Hermitian: $\rho = \rho^\dagger$;

2. It has unit trace;

3. It is non negative, that is $\forall|\psi\rangle \in \mathcal{H}$, then $\langle\psi|\rho|\psi\rangle \geq 0$.

Moreover, when the state is pure one has $\mathrm{Tr}(\rho^2) \leq 1$, whereas if the system is in a mixed state, then $\mathrm{Tr}(\rho^2) < 1$. The quantity $\pi(\rho) = \mathrm{Tr}(\rho^2) \in [(\dim\mathcal{H})^{-1}, 1]$,

accounting for the degree of "mixedness" of a quantum system, is called *purity*.

Besides providing a convenient means for describing quantum systems whose state is not completely known, the density operator formalism is also extremely useful when describing composite systems. Consider a quantum state $|\psi_{AB}\rangle$ defined on a bipartite Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. One may be interested in characterizing the observations that can be made on, say, system A alone. A generic observable $O = \sum_j o_j |o_j\rangle\langle o_j|$ acting only on the Hilbert space of A can be expressed as $O_A \otimes \mathbb{1}_B$, where $\mathbb{1}_B$ denotes the identity operator acting on $\mathcal{H}_B$. The expectation value of this observable on the state $|\psi_{AB}\rangle$ can be evaluated as

$$\langle O \rangle = \langle \psi_{AB} | (O_A \otimes \mathbb{1}_B) | \psi_{AB} \rangle = \mathrm{Tr}(\rho_A O)\,, \tag{1.12}$$

with

$$\rho_A := \mathrm{Tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|) \tag{1.13}$$

and $\mathrm{Tr}_X(\bullet)$ denoting partial tracing over the degrees of freedom of the Hilbert space $\mathcal{H}_X$. Also, the probability of obtaining the outcome o_i from a measurement reads

$$p(i) = \langle \psi_{AB} | (|o_i\rangle\langle o_i| \otimes \mathbb{1}_B) | \psi_{AB} \rangle = \mathrm{Tr}(\rho_A |o_i\rangle\langle o_i|)\,. \tag{1.14}$$

The *reduced density matrix* ρ_A defined in Eq.(1.13), obtained by partial tracing, fulfills the properties listed above and thus gives a complete description of subsystem A.

1.4 Bloch sphere

A single qubit in the density operator formalism is represented by a 2×2 hermitian matrix. The most general form of such a matrix has four real parameters and can be expressed as an expansion in the basis $\{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}$, as

$$\rho = c_0 \mathbb{1} + \sum_i c_i \sigma_i\,, \tag{1.15}$$

where $\mathbb{1}$ is the 2×2 identity and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \tag{1.16}$$

are the *Pauli matrices*. Since $\mathrm{Tr}\,(\sigma_i) = 0\,, \forall \sigma_i$, in order to have $\mathrm{Tr}(\rho) = 1$ we must set $c_0 = 1/2$, and upon defining the vectors $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^T$ and $\boldsymbol{n} = (n_x, n_y, n_z)^T$ we obtain a general parametrization of the density operator of a qubit that reads:

$$\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{n} \cdot \boldsymbol{\sigma}) \tag{1.17}$$

The determinant of ρ can be easily calculated: $\det(\rho) = \frac{1}{4}(1 - \boldsymbol{n} \cdot \boldsymbol{n})$; the non negativity of ρ then sets $\det(\rho) \geq 0$. Therefore, there is a one-to-one correspondence between the density operator of a single qubit and a 3-dimensional ball defined by the vector $\boldsymbol{n}$ satisfying the condition $0 \leq |\boldsymbol{n}| \leq 1$. This ball is commonly called *Bloch sphere* and it provides a useful geometrical picture of the qubit and the transformation one can operate on it. All points on the surface of the ball (where $|\boldsymbol{n}| = 1$) are pure states $|\psi_{|\boldsymbol{n}|=1}\rangle$ and correspond to density matrices with vanishing determinant. Hence, since $\mathrm{Tr}(\rho) = 1$, density matrices of pure states have the eigenvalues 0 and 1 and therefore are one-dimensional projectors. An alternative way of parametrizing pure states which is particularly useful when picturing them on the Bloch sphere is

$$|\psi_{|\boldsymbol{n}|=1}\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle \tag{1.18}$$

where $0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$ and the basis $\{|0\rangle, |1\rangle\}$ is formed by the eigenvectors of σ_z, with $\sigma_z|0\rangle = |0\rangle$ and $\sigma_z|1\rangle = -|1\rangle$. A point on the Bloch sphere is thus identified by the angles θ and ϕ, as depicted in Fig.(1.1). All points within the Bloch ball that do not lie on the surface are mixed states, the most mixed one corresponding to the center of the ball: $\rho = \frac{1}{2}\mathbb{1}$. Let us notice that the notion of Bloch sphere can be generalized to any dimension $N > 2$, though then the usefulness of the visualization is lost.

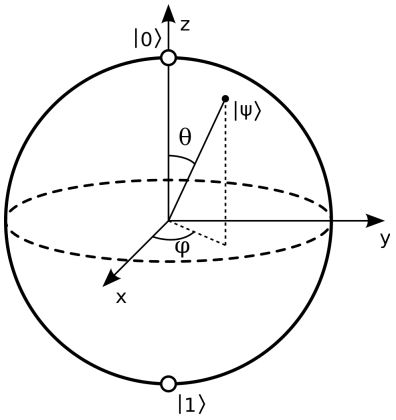


Figure 1.1: Bloch sphere representation of a qubit.

1.5 Schmidt decomposition

Consider a pure state of a bipartite quantum system $|\psi_{AB}\rangle$ defined in $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$. Given two basis $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ for, respectively, $\mathcal{H}_A$ and $\mathcal{H}_B$, it is always possible to write

$$|\psi_{AB}\rangle = \sum_{i=0}^{d_A-1} \sum_{j=0}^{d_B-1} c_{i,j} |i\rangle_A |j\rangle_B \,. \tag{1.19}$$

The *Schmidt decomposition theorem* states that there exist orthonormal states $\{|\alpha_i\rangle_A\}$ for $\mathcal{H}_A$ and $\{|\beta_i\rangle_B\}$ for $\mathcal{H}_B$ such that

$$|\psi_{AB}\rangle = \sum_{i=0}^{\tilde{d}-1} s_i |\alpha_i\rangle_A |\beta_i\rangle_B \,, \tag{1.20}$$

with $\tilde{d} = \min(d_A, d_B)$ and s_i positive real numbers satisfying the condition $\sum_{k=0}^{\tilde{d}-1} s_k^2 = 1$. Moreover, the *Schmidt coefficients* s_i are the square roots of the eigenvalues of the two reduced density matrices:

$$\begin{aligned} \rho_A &= \mathrm{Tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|) \\ &= \sum_{i=0}^{\tilde{d}-1} s_i^2 |\alpha_i\rangle\langle\alpha_i| \\ \rho_B &= \mathrm{Tr}_A(|\psi_{AB}\rangle\langle\psi_{AB}|) \\ &= \sum_{i=0}^{\tilde{d}-1} s_i^2 |\beta_i\rangle\langle\beta_i| \,. \end{aligned} \tag{1.21}$$

Notice that if ρ_A (or, equivalently, ρ_B) has non-degenerate eigenvalues other than zero, then the Schmidt decomposition of $|\psi_{AB}\rangle$ is uniquely determined, in that after diagonalizing ρ_A and ρ_B to find the states $\{|\alpha_i\rangle\}$ and $\{|\beta_i\rangle\}$ we can pair up the eigenstates with the same eigenvalues to obtain Eq.(1.20). As we shall see in Sec.(1.7), the Schmidt decomposition can be used as an entanglement criterion.

1.6 Von Neumann entropy

The Von Neumann entropy is the quantum analogue of the Shannon entropy of classical information. Given a random variable $X = \{x_1, x_2, \ldots, x_n\}$ with probability distribution $P(X = x_i) = p_i$, the Shannon entropy associated with this probability distribution is defined by

$$H(X) = -\sum_i p_i \log_2 p_i \tag{1.22}$$

and represents a measure of the unpredictability of the *source* generating the *message* X or, alternatively, the amount of information one gets after unraveling the content of the message. In quantum information, a quantitative estimate of the "ignorance" about the state ρ of a system is provided by the Von Neumann entropy, defined as

$$S(\rho) = -\mathrm{Tr}\,(\rho \log_2 \rho) \tag{1.23}$$

The analogy with the Shannon entropy is clarified by noting that when dealing with orthogonal pure states, i.e. $\rho = \sum_i p_i |i\rangle\langle i|$, which in practice is equivalent to a classical situation, the Von Neumann entropy reduces to the Shannon entropy.

Some properties that are satisfied by the Von Neumann entropy are the following:

- $S(\rho)$ is null for a pure state:

$$S(\rho) = 0\,,\ \forall \rho\ s.t.\ \mathrm{Tr}(\rho^2) = 1\,; \tag{1.24}$$

- $S(\rho)$ satisfies

$$0 \leq S(\rho) \leq \log_2 d_{\mathcal{H}}\,, \tag{1.25}$$

where $d_{\mathcal{H}}$ is the dimension of the Hilbert space of the system and the maximum

value is attained when the state is maximally mixed.

- $S(\rho)$ is invariant under unitary change of basis or, equivalently, under unitary evolution:

$$S(U\rho U^\dagger) = S(\rho)\,; \tag{1.26}$$

- $S(\rho)$ is additive for independent systems:

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B)\,. \tag{1.27}$$

The first two properties show that the Von Neumann entropy is tightly related to the degree of mixedness of a quantum state, which, as we have seen in Sec.(1.4), is quantified by the purity $\pi(\rho) = \mathrm{Tr}(\rho^2)$. As we will shortly see, both Von Neumann entropy and purity are extensively used in quantum information as quantum entanglement quantifiers.

1.6.1 Quantum mutual information

Defined through the Von Neumann entropy, the quantum mutual information is a measure of correlations between subsystems of a quantum state. It is, again, the generalization to the quantum realm of a classical concept, the mutual information between random variables X and Y, which can be expressed as

$$I_c(X;Y) = H(p(x)) + H(p(y)) - H(p(x,y))\,, \tag{1.28}$$

where $p(x,y)$ is the probability distribution of the two variables X and Y, $p(x) = \sum_y p(x,y)$ and $p(y) = \sum_x p(x,y)$ their respective marginal distribution, and $H(p(x,y))$ is the joint entropy. A direct calculation shows that the mutual information is actually equal to the *relative entropy*, which is a measure of the difference between two probability distributions.

Analogously, when classical probability distributions are replaced by density matrices, the quantum mutual information can be defined as

$$I(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})\,, \tag{1.29}$$

where $S(\rho_A)$ and $S(\rho_B)$ are the reduced Von Neumann entropies of subsystems A

and B of ρ_{AB} supported on $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, obtained by partial tracing. As will be clarified in the next section, the difference in the lack of information between the global state and the two reduced states, quantified by the Von Neumann entropies, can be regarded as to be translated in the correlations between the two subsystems. Clearly, the quantum mutual information estimates the total amount of correlations contained in the system, without distinguishing or quantifying the contribution of correlations of quantum or classical nature. Notice that $I \geq 0$, and that I is equal to zero for completely uncorrelated, i.e. separable states $\rho_{AB} = \rho_A \otimes \rho_B$ (cf. Eq.(1.27)).

1.7 Entanglement

Quantum entanglement is arguably considered to be the most non classical manifestation of the quantum formalism. First described by Einstein, Podolski and Rosen [60] and by Schrödinger [61] in 1935, this phenomenon is exploited in many founding protocols of quantum communication (such as quantum cryptography, dense coding and teleportation) and it is nowadays regarded as a key resource for quantum information theory. Entanglement occurs in composite systems and it is a manifestation of the tensor product structure of the Hilbert space and the superposition principle. In striking contrast to classical probability distributions, which can always be written as mixtures of product distributions, whenever a quantum state ρ of n systems is not *separable*, i.e. it cannot be written as a convex combination of product states:

$$\rho \neq \sum_{i=1}^{n} p_i \rho_1^i \otimes \rho_2^i \otimes \cdots \otimes \rho_n^i \,, \quad \text{with} \sum_{i=1}^{n} p_i = 1 \,, \tag{1.30}$$

it is called entangled. For a pure state $\rho = |\psi\rangle\langle\psi|$, that translates to

$$|\psi\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle \,. \tag{1.31}$$

For a bipartite pure state ρ_{AB} defined in $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ there is entanglement if and only if the reduced density matrices of its subsystems are not projectors: $\mathrm{Tr}_B(\rho_B^2) = \mathrm{Tr}_A(\rho_A^2) \neq 1$. Looking at Eq.s(1.21), it is easy to realize that this is equivalent to saying that in order for the state ρ_{AB} to be entangled the number of non-zero coefficients of the Schmidt decomposition must be greater than one[2].

[2]The Schmidt decomposition thus represents an entanglement criterion for bipartite pure states. The qualification of entanglement for bipartite mixed states turns out to be a much more complicated

The above consideration suggests a relation between entanglement and mixedness of reduced states. The connection between the two features can be further elucidated by means of a simple example. Consider the following two-qubit state

$$|\psi^+\rangle = \frac{1}{\sqrt{2}}(|0_A\rangle|1_B\rangle + |1_A\rangle|0_B\rangle) \tag{1.32}$$

This is one of the four *Bell states*, states that provide the maximal achievable violation of Bell inequalities [63, 64]. Bell states have remarkable non-local properties, as for such states the combined results of measurements of local observables performed on the subsystems are perfectly correlated: they are "maximally entangled" . But, if one takes into account the state of, say, qubit A by partial tracing over the degrees of freedom of B, the resulting reduced state is proportional to the identity, namely, the maximally mixed one. This is a general feature of quantum mechanics: for any pure states of an n-dimensional bipartite system, maximally entangled states lead to maximally mixed reduced states. Of course, this is at odds with our classical intuition and notion of correlation: On one hand we have maximal knowledge of the whole system because the system is pure, but on the other hand we know nothing about the subsystems[3]. Indeed, the information regarding the pure quantum state is lost when addressing its components individually but in turn it is utterly encoded in the quantum correlations – the entanglement – among them.

Since, when the global state is pure, the degree of entanglement and the degree of mixedness of the partial trace are strongly connected, a quantity that well describes the entanglement content of a quantum system is the Von Neumann entropy of the reduced state:

$$E(|\psi\rangle) = S\left(\mathrm{Tr}_B(|\psi\rangle\langle\psi|)\right) \tag{1.33}$$

This pure state entanglement measure, often called *entropy of entanglement*, is null

and mostly unresolved issue, since mixed states are affected by an "ignorance" about the global state and both classical and quantum correlations may be present. However, for low dimensional ($\dim_{\mathcal{H}} \leq 6$) mixed systems, the *Positivity of Partial Transpose* (PPT) criterion, introduced by Peres [62], is a simple, sufficient test to detect entanglement. Another difficult task is represented by the characterization of entanglement in multipartite systems – systems with generally more than two parties – the main reason being the possible dependence of the entanglement on the partition chosen for the subsystems. In this section we will always be concerned with pure bipartite states.

[3] In Schrödinger's words [61] [as translated in [65], page 167] "*Thus one disposes provisionally (until the entanglement is disposed by actual observation) of only a common description of the two in that space of higher dimension. This is the reason that knowledge of the individual systems can decline to the scantiest, even to zero, when that of the combined system remains continually maximal. Best possible knowledge of a whole does not include best possible knowledge of its parts - and this is what keeps coming back to haunt us.*"

for separable states and invariant under local unitary transformations. Notice that the mutual information of a pure state is reduced to the entropy of entanglement, as it must be since no classical correlations are present in such an instance.

1.8 Measures of distinguishability for quantum states

To determine how close two quantum systems are, the notion of *distance* in the Hilbert space must be introduced. In order for a distance function $\mathcal{D}(\rho, \sigma)$ between two quantum states ρ and σ to be well-defined, the following properties must be satisfied:

i) **Positivity**

$$\mathcal{D}(\rho, \sigma) \geq 0 \qquad \forall \rho, \sigma \tag{1.34}$$

$$\mathcal{D}(\rho, \sigma) = 0 \qquad iff \quad \rho = \sigma\,; \tag{1.35}$$

ii) **Symmetry**

$$\mathcal{D}(\rho, \sigma) = \mathcal{D}(\sigma, \rho)\,; \tag{1.36}$$

iii) **Triangular inequality**

$$\mathcal{D}(\rho, \sigma) \leq \mathcal{D}(\rho, \pi) + \mathcal{D}(\pi, \sigma)\,. \tag{1.37}$$

Given an arbitrary operator norm $\|O\|_x$, which automatically satisfies the above listed properties, it is always possible to define a distance as

$$\mathcal{D}_x(\rho, \sigma) = C\|(\rho - \sigma)\|_x \tag{1.38}$$

where C is a multiplying constant.

Different distances can be defined for different purposes. Here we introduce three widely used ones, the *trace distance*, the *Hilbert-Schmidt distance* and the *fidelity*.

1.8.1 Trace distance

The trace distance is related to the trace norm $\|O\|_1$ of a matrix:

$$\|O\|_1 := \mathrm{Tr}(\sqrt{O^\dagger O}) = \mathrm{Tr}(|O|)\,, \tag{1.39}$$

where $\sqrt{O^\dagger O}$ is a positive semidefinite matrix. The trace distance is defined as half of the trace norm of the difference of two matrices:

$$\mathcal{D}_1(\rho,\sigma) \equiv \frac{1}{2}\|(\rho-\sigma)\|_1 = \frac{1}{2}\mathrm{Tr}\left(\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}\right)\,. \tag{1.40}$$

The choice $C = \frac{1}{2}$ ensures that $0 \leq \|(\rho-\sigma)\|_1 \leq 1\,, \forall \rho, \sigma$. Since density operators are Hermitian,

$$\|(\rho-\sigma)\|_1 = \frac{1}{2}\mathrm{Tr}(|\rho-\sigma|) = \frac{1}{2}\sum_i |\lambda_i|\,, \tag{1.41}$$

where $\{\lambda_i\}$ are the real eigenvalues of the (not necessarily positive) matrix $(\rho-\sigma)$.

The trace distance satisfies the following additional properties:

- It is invariant under unitary transformations:

$$\|U\rho U^\dagger - U\sigma U^\dagger\|_1 = \|(\rho-\sigma)\|_1\,; \tag{1.42}$$

- It is contractive under trace-preserving CP maps (see Sec.(2.1)):

$$\|(\mathcal{M}(\rho)-\mathcal{M}(\sigma))\|_1 \leq \|(\rho-\sigma)\|_1\,; \tag{1.43}$$

- It is subadditive under tensor product:

$$\|(\rho_1\otimes\sigma_1 - \rho_2\otimes\sigma_2)\|_1 \leq \|(\rho_1-\rho_2)\|_1 + \|(\sigma_1-\sigma_2)\|_1\,. \tag{1.44}$$

It can be shown [58] that the trace distance provides a measure of the maximum probability of distinguishing between two states with an optimal measurement. This operational meaning makes the trace distance a particularly "natural" measure of distinguishability. However, there is a catch: Evaluating Eq.(1.41) requires the diagonalization of $(\rho-\sigma)$, which is often a challenging procedure, especially when dealing with infinite-dimensional operators.

1.8.2 Hilbert-Schmidt distance

A more mathematical friendly, but unfortunately less "physical" measure of distinguishability is the Hilbert-Schmidt distance, defined through the Hilbert-Schmidt norm

$$\|O\|_2 \equiv \sqrt{\mathrm{Tr}(O^\dagger O)}\,. \tag{1.45}$$

The Hilbert-Schmidt (HS) distance between two quantum states is

$$\begin{aligned} \mathcal{D}_2(\rho-\sigma) &\equiv \sqrt{\frac{1}{2}}\|(\rho-\sigma)\|_2 \\ &= \sqrt{\frac{1}{2}\mathrm{Tr}\left((\rho-\sigma)^2\right)} \\ &= \sqrt{\frac{1}{2}(\mathrm{Tr}\left(\rho^2\right)+\mathrm{Tr}(\sigma^2)-2\mathrm{Tr}(\rho\sigma))}\,. \end{aligned} \tag{1.46}$$

As for the trace norm, the HS distance is invariant under unitary transformations and $0 \leq \|(\rho-\sigma)\|_2 \leq 1$, $\forall \rho, \sigma$. We see that the evaluation of the HS distance only requires the computation of the purity of the two quantum states and a term representing the overlap between the two; no diagonalizations are implied. For high-dimensional systems though, $\|(\rho-\sigma)\|_2$ can be small even when the two states are orthogonal. However, the HS distance and the trace distance can be related to each other by noting that, for any $n \times n$ matrix M with eigenvalues $\{\lambda_i\}$, by convexity of the square function:

$$\begin{aligned} \|M\|_1^2 &= n^2\left(\frac{1}{n}\sum_i |\lambda_i|\right)^2 \\ &\leq n^2\frac{1}{n}\sum_i |\lambda_i|^2 \\ &= n\|M\|_2^2\,. \end{aligned} \tag{1.47}$$

This bound will prove useful in the last part of the thesis.

1.8.3 Fidelity

Unlike the distances introduced so far, the fidelity is not a metric in the space of density matrices[4]. Given two density matrices ρ and σ, the fidelity is defined[5] by

$$F(\rho,\sigma) = \mathrm{Tr}\left(\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right) . \tag{1.48}$$

Even though a clear operational interpretation of F is not known, it represents a generalization to the quantum realm of the classical fidelity $F_c(p_i,q_i) = \sum_i \sqrt{p_i}\sqrt{q_i}$, which is a measure of distance between probability distributions $\{p_i\}$ and $\{q_i\}$ over the same alphabet. In fact, if $[\rho,\sigma]=0$, by diagonalizing the two density matrices in the same basis $\rho = \sum_i r_i|i\rangle\langle i|$, $\sigma = \sum_i s_i|i\rangle\langle i|$ we have:

$$\begin{aligned} F(\rho,\sigma) &= \mathrm{Tr}\left(\sqrt{\sum_i r_i s_i |i\rangle\langle i|}\right) \\ &= \mathrm{Tr}\left(\sum_i \sqrt{r_i s_i}|i\rangle\langle i|\right) \\ &= \sum_i \sqrt{r_i s_i} \\ &= F_c(r_i,s_i)\,, \end{aligned} \tag{1.49}$$

i.e. the classical fidelity between the eigenvalue distributions r_i of ρ and s_i of σ. The analogy between the two quantities is further strengthened by the fact that, since $\sum_i(\sqrt{p_i})^2 = \sum_i(\sqrt{q_i})^2 = 1$, the classical fidelity is nothing but the inner product between two vectors lying on a unit-sphere, while when pure states $\rho = |\psi\rangle\langle\psi|$ and $\sigma = |\phi\rangle\langle\phi|$ are considered, $F(|\psi\rangle\langle\psi|,|\phi\rangle\langle\phi|) = |\langle\phi|\psi\rangle|$ clearly represents the overlap between two states living on the surface of the Bloch sphere. Notice also that in this case the fidelity is equivalent to the Hilbert-Schmidt distance (cf. Eq.(1.46)).

Another characterization of the fidelity is provided by the following theorem

Theorem 1 *(Uhlmann's theorem) Given ρ and σ two states defined on a Hilbert space $\mathcal{H}_A$, then*

$$F(\rho,\sigma) = \max_{|\Psi\rangle,|\Phi\rangle} |\langle\Psi|\Phi\rangle|\,, \tag{1.50}$$

where $|\Psi\rangle$ and $|\Phi\rangle$ are respectively purifications of ρ and σ, i.e. states defined on a

[4] Even though it can be used to define the *Bures metric* [66].

[5] It is actually customary to define it as in Eq.(1.48) or as $F'(\rho,\sigma) = \left(\mathrm{Tr}(\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}})\right)^2$

larger Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ *such that*

$$\begin{aligned} \rho &= Tr_B(|\Psi\rangle\langle\Psi|) \\ \sigma &= Tr_B(|\Phi\rangle\langle\Phi|) \end{aligned} \tag{1.51}$$

The definition given in Eq.(1.50) makes it clear that the fidelity is symmetric in its input and that $0 \leq F(\rho, \sigma) \leq 1$. It is also easy to show that F is unitarily invariant. Unlike a distance defined by means of an underlying metric though, $F(\rho, \sigma) = 1$ if and only if $\rho = \sigma$, and $F(\rho, \sigma) = 0$ if and only if ρ and σ have support on orthogonal subspaces. Also, as opposed to the trace distance, F is monotonically increasing under completely positive maps: $F(\mathcal{M}(\rho), \mathcal{M}(\sigma)) \geq F(\rho, \sigma)$. Finally, fidelity and trace distance are related by the following bound (*Fuchs-van de Graaf inequality* [67])

$$1 - F(\rho, \sigma) \leq \|\rho - \sigma\|_1 \leq \sqrt{1 - F(\rho, \sigma)^2}\,. \tag{1.52}$$

1.9 Invariant measure over the unitary group

In order to be able to draw unitaries U at random or, equivalently, draw pure states $|\psi\rangle$ at random, one needs to introduce a probability measure on the unitary group.

The unitary group

$$U(d) := \{U \in \mathbb{C}^{d \times d} \,|\, U^\dagger U = \mathbb{1}\} \tag{1.53}$$

is a compact Lie group, hence it is equipped with the *Haar measure* [68]:

Theorem 2 *(Haar measure): Every compact Lie group* G *possesses a regular measure* μ *such that for every Borel measurable function* $f : G \to \mathbb{R}$, μ *is right and left invariant with respect to multiplication with group elements, i.e.:*

$$\begin{aligned} \int_G f(xy) d\mu(y) &= \int_G f(y) d\mu(y) \quad \forall y \in G \\ \int_G f(yx) d\mu(y) &= \int_G f(y) d\mu(y) \quad \forall y \in G\,. \end{aligned} \tag{1.54}$$

The measure μ *is unique up to a constant factor. If that factor is chosen such that* $\mu(G) = 1$, *then* μ *is called the Haar measure.*

The property of being invariant with respect to multiplication with group elements makes it possible to identify the integral of a function on the unitary group with the expectation value of that function with respect to a random choice of U:

$$\int_{U(d)} f(U)\mathrm{d}U = \mathbb{E}_U f(U) =: \langle f \rangle_H \,. \tag{1.55}$$

That means the Haar measure allows one to compute expectation values of functions or observables with respect to a random choice of transformation, or a random choice of initial pure quantum states.

That represents a mathematical privileged, widely exploited in approaching several problems in quantum physics (see Chap.(5) and Chap.6). However, despite being an extremely useful mathematical tool, actual physical interactions are always selected by the nature of the system under study which inevitably put constraints on the relevance of different regions of the Hilbert space where the system itself is defined: Drawing states at random from the uniform measure on the whole Hilbert space is thus a fruitful but rather abstract procedure, whose physical questionable nature must always be taken into account.

Chapter 2

Open quantum systems

This chapter is devoted to introducing the basic notions of open quantum system dynamics. The concepts presented here will be important for the understanding of the second part of this thesis. We will discuss the two different approaches to the description of the evolution of open quantum systems: Quantum operations, which implement a discrete-time dynamics, and whose formalism will be employed in Chap.(3) and (4); and the complementary, continuous-time approach based on the master equation. Despite the fact that the latter is less general than the former – for it is suitable for describing Markovian evolutions only – and that we will not make use of it in our models, it is nonetheless important to introduce the master equation approach, as the overwhelming majority of models in quantum biology rely on it. Contextually to the discussion on the general formalism of open quantum systems dynamics, two remarkable examples of quantum noise, namely dissipation and dephasing, described in terms of quantum operations by respectively the amplitude damping channel and the phase damping channel, will be presented. We will then conclude the chapter with an introduction to the concept of decoherence, a dynamical mechanism which provides a plausible explanation to the emergence of classicality from a quantum world. It will be shown how the phase damping channel arguably plays a central role in the transition from quantum to classical. As for the previous chapter, most of what follows can be found in e.g. [58, 59] and [69].

2.1 Superoperators

In the previous chapter we focused the attention on closed quantum systems, namely systems that are perfectly isolated from their environment. We did, however, talk about bipartite systems and introduced the concepts of partial trace and reduced density matrix, through which a complete description of the state of a part of the whole physical system is attained. Let us consider now the case in which the bipartition of the state ρ_{SE} supported on $\mathcal{H}_S \otimes \mathcal{H}_E$, evolving unitarily, represents a quantum system S immersed – interacting in some way – in an environment E, and we wish to describe the dynamics of system ρ_S alone. Suppose, for simplicity, that initially the environment is in a pure state and it is also not entangled to the system:

$$\rho_{SE} = \rho_S \otimes |0\rangle\langle 0|_E \,. \tag{2.1}$$

The global evolution is governed by a unitary operator, thus after a time t the global state is

$$\rho_{SE}(t) = U\rho_{SE}U^\dagger = U\left(\rho_S \otimes |0\rangle\langle 0|_E\right)U^\dagger \,. \tag{2.2}$$

Now, performing a partial trace over the environment, the density matrix of the system S at time t is given by:

$$\begin{aligned} \rho_S(t) &= \mathrm{Tr}_E\left(U(\rho_S \otimes |0\rangle\langle 0|_E)U^\dagger\right) \\ &= \sum_j \langle j_E|U|0_E\rangle \rho_S \langle 0_E|U^\dagger|j_E\rangle \,, \end{aligned} \tag{2.3}$$

where $\{|j_E\rangle\}$ is an orthonormal basis for $\mathcal{H}_E$ and $\langle j_E|U|0_E\rangle$ is an operator acting on the Hilbert space $\mathcal{H}_S$ associated with system S. Upon denoting $K_j \equiv \langle j_E|U|0_E\rangle$, with $K_j^{lm} = \langle l_S|\langle j_E|U|0_E\rangle|m_S\rangle$, we may express $\rho_S(t)$ as

$$\mathcal{M}(\rho_S) \equiv \rho_S(t) = \sum_j K_j \rho_S K_j^\dagger \,. \tag{2.4}$$

Notice that, since U is unitary, the operators $\{K_j\}$ satisfy the property: $\sum_j K_j^\dagger K_j = \mathbb{1}$. The map $\mathcal{M}$, which is not a unitary operator, is called *superoperator* or *quantum operation* and its explicit form in terms of $\{K_j\}$ is known as the *operator-sum representation* or *Kraus representation* of $\mathcal{M}$. A superoperator maps density matrices to density matrices since it can be easily verified that $\rho_S(t)$ is still a Hermitian, trace-

one, non-negative operator. The operator-sum representation is important in that, as evident in Eq.(2.4), it describes the dynamics of the system of interest without having to explicitly consider properties of the environment.

As a Kraus representation for the evolution of a subsystem can always be associated to a unitary evolution of the composite system, the reverse is also true: given a Kraus representation of a superoperator describing the evolution of S, it is always possible to derive a corresponding unitary representation. Define an orthonormal basis $\{|j_E\rangle\}$ on a Hilbert space $\mathcal{H}_E$ whose dimension is equal to the number of operators appearing in the Kraus representation and consider the operator U acting as follows:

$$U|\psi\rangle_S|0\rangle_E = \sum_j K_j|\psi\rangle_S|j\rangle_E\,. \tag{2.5}$$

For any two arbitrary states $|\psi\rangle_S$, $|\phi\rangle_S$ the operator U preserves the inner product: $\langle\psi_S|\langle 0_E|U^\dagger U|\phi_S\rangle|0_E\rangle = \langle\psi_S|\phi_E\rangle$ and can thus be extended to a unitary operator acting on the Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_E$ of the composite system. The evolution of the pure state is then:

$$\rho_S(t) = \mathrm{Tr}\left(U|\psi_S\rangle|0_E\rangle\langle\psi_S|\langle 0_E|U^\dagger\right) = \sum_j K_j|\psi_S\rangle\langle\psi_S|_S K_J^\dagger \tag{2.6}$$

and since any density matrix can be expressed as an ensemble of pure states, the Kraus representation of Eq.(2.4) is recovered.

It is now possible to state the following theorem[1]:

Theorem 3 *(Kraus representation theorem): A map $\mathcal{M} : \mathcal{M}(\rho) \to \rho'$ which:*

1. *Is linear;*
2. *preserves trace;*
3. *preserves hermiticity;*
4. *is completely positive,*

is a quantum operation, i.e. it can be given an operator-sum representation (Eq.(2.4)) and a unitary representation (Eq.(2.5)) on a larger Hilbert space.

Complete positivity of $\mathcal{M}$ formally means that for any possible extentions of $\mathcal{H}_S$ to a larger Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_E$, the map $\mathcal{M} \otimes \mathbb{1}_E$ is positive for all $\mathcal{H}_E$. Physically

[1] A proof of which can be found in [70].

this condition accounts for the fact that, in general, it cannot be excluded that one is unaware that the system under study is initially entangled with some other system E which evolves trivially. If this is the case, the requirement of complete positivity assures that any density matrix of the combined system is mapped to a valid density matrix. For this reason, quantum operation are often called *completely positive (CP) maps*.

Quantum operations are composable, meaning that given two superoperators $\mathcal{M}_1$ and $\mathcal{M}_2$, one can define a new superoperator as: $\mathcal{M}(\rho) = \mathcal{M}_2(\mathcal{M}_1(\rho))$. Quantum operations are invertible if and only if there is only one term in the operator sum representation, i.e. if the dynamics of the system is unitary. Physically, this means that in open quantum dynamics an arrow of time arises for the system, the evolution of which cannot be described backwards in time by means of superoperators. This irreversibility of the dynamics is interpreted as the impossibility of retrieving the information continually flowing from the system to its surrounding environment due to their interaction (cf. Sec.(2.3)). Notice that the operator sum representation of a superoperator is not unique: As prooved in e.g. [70] or [58], different representations $\mathcal{M}(\rho) = \sum_j K_j \rho K_j$ and $\mathcal{M}'(\rho) = \sum_j L_j \rho L_j$ coincide if and only if there exist a unitary matrix V such that $L_k = \sum_l V_{kl} K_l$.

We will now analise two remarkable examples of quantum operations (or *noisy quantum channels*, following the classical terminology of quantum communication theory) on a single qubit that will be part of the model presented in the second part of this thesis.

2.1.1 Amplitude damping

The amplitude-damping channel may be regarded as the quantum operation description of energy dissipation processes. Though its general formulation can be adapted and extended to the characterization of various physical scenarios, the straightforward interpretation of the amplitude damping channel is that of a schematic model of the decay of an excited state of a two-level atom due to spontaneous emission of a photon.

The unitary representation of the channel can be formulated following this line of reasoning. For the two-level system S there is a probability p that after a certain amount of time the excited state $|1_S\rangle$ has decayed to the ground state $|0_S\rangle$. If that

happened, a photon was emitted and the environment made a transition from a "vacuum" state $|0_E\rangle$ to the "one photon" state $|1_E\rangle$. The unitary evolution may therefore be expressed as

$$\begin{aligned} U|0_S\rangle|0_E\rangle &= |0_S\rangle|0_E\rangle \\ U|1_S\rangle|0_E\rangle &= \sqrt{1-p}|1_S\rangle|0_E\rangle + \sqrt{p}|0_S\rangle|1_E\rangle \end{aligned} \tag{2.7}$$

which, taking the partial trace over the environment, leads to the Kraus operators:

$$K_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \; K_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}, \quad \text{with} \quad \sum_{j=0}^{1} K_j^\dagger K_j = 1\,. \tag{2.8}$$

One application of the channel gives

$$\rho \to \begin{pmatrix} \rho_{00} + p\rho_{11} & \sqrt{1-p}\rho_{01} \\ \sqrt{1-p}\rho_{10} & (1-p)\rho_{11} \end{pmatrix}, \tag{2.9}$$

from which we notice that by applying the channel a number $n \gg 1$ of times the coherences as well as the probability of being in the excited state are exponentially suppressed, eventually leading, for $n \to \infty$, the system to its (pure) ground state.

2.1.2 Phase damping

The phase damping channel, or *dephasing channel*, describes a uniquely quantum mechanical effect, namely the loss of quantum information without loss of energy. The physical picture is that of an environment whose constituents (for instance photons), by interacting with probability p with the system, "scatter" off of it resulting in one of two distinguishable states, say $|1_E\rangle$ if the system was in $|0_S\rangle$ and $|2_E\rangle$ if it was in $|1_S\rangle$. The unitary representation is thus

$$\begin{aligned} U|0_S\rangle|0_E\rangle &= \sqrt{1-p}|0_S\rangle|0_E\rangle + \sqrt{p}|0_S\rangle|1_E\rangle \\ U|1_S\rangle|0_E\rangle &= \sqrt{1-p}|1_S\rangle|0_E\rangle + \sqrt{p}|1_S\rangle|2_E\rangle\,, \end{aligned} \tag{2.10}$$

which, evaluating the partial trace over the environment basis, gives the following Kraus operators

$$K_0 = \begin{pmatrix} \sqrt{1-p} & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} , \; K_1 = \begin{pmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{pmatrix} , \; K_2 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix} . \tag{2.11}$$

By applying the channel once, the density operator becomes

$$\rho \to \begin{pmatrix} \rho_{00} & (1-p)\rho_{01} \\ (1-p)\rho_{10} & \rho_{11} \end{pmatrix} . \tag{2.12}$$

Hence the channel leaves untouched the diagonal elements while suppressing the coherences. After a number of scattering interactions $n \gg 1$ such that $(1-p)^n \simeq 0$, the state is left in the incoherent superposition $\rho_{00}|0\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|$. The decay of the off-diagonal terms represents, in a broad sense, the process of *decoherence*, which will be presented in some detail in Sec.(2.3).

2.2 Master equation

The master equation, as opposed to quantum operations, describes the evolution of open quantum systems in continuous time, using differential equation. In this respect it represents a complementary formalism to deal with quantum noise and it is actually very often the privileged approach to modelling biological systems within the field of quantum biology. That is why, although we will not make use of master equations in the remainder of the thesis, it is nonetheless important to at least give a general presentation of this formalism, highlighting the connections and differences with the quantum operations framework.

It is actually possible to obtain a derivation of the master equation from the superoperator formalism. Consider an infinitesimal time interval dt. The density matrices of the system at times t and $t + dt$ are related by

$$\rho_S(t+dt) \equiv \mathcal{M}(t; t+dt)(\rho(t)) = \sum_j K_j \rho_S(t) K_j^\dagger = \rho_S(t) + \mathcal{O}(dt) . \tag{2.13}$$

It follows from the condition $\mathcal{M}(t;t)(\rho_S(t)) = \mathbb{1}\rho_S\mathbb{1}$ that one Kraus operator will have the form $K_0 = \mathbb{1} + \mathcal{O}(dt)$ and the others will be of order $\sqrt{dt}$. We may then

write

$$\begin{aligned} K_0 &= \mathbb{1} + (-iH + M)dt \\ K_j &= L_j\sqrt{dt}\,, \quad j = 1, 2, 3, \ldots \end{aligned} \tag{2.14}$$

where both H and M are Hermitian and the operators L_j are known as *Lindblad operators*. The form of M can be determined through the normalization condition $\sum_j K_j^\dagger K_j = \mathbb{1}$, which results in

$$M = -\frac{1}{2}\sum_{j>0} L_j^\dagger L_j \tag{2.15}$$

Inserting Eq.s(2.14) and (2.15) in Eq.(2.13), by writing $\rho(t+dt) = \rho(t) + \dot{\rho}(t)dt$ and equating terms of order dt we obtain the master equation in the Lindblad form:

$$\dot{\rho}_S = -i[H, \rho_S] + \sum_{j>0}\left(L_j\rho_S L_j^\dagger - \frac{1}{2}L_j^\dagger L_j\rho_S - \frac{1}{2}\rho_S L_j^\dagger L_j\right). \tag{2.16}$$

The first term in the equation accounts for the free evolution of the system, the operator H actually being the (renormalized) Hamiltonian of the system in absence of coupling to the environment; the other terms describe the interaction with the environment. The probabilistic transitions, sometimes called *quantum jumps*, that the system may undergo are enclosed in each term $L_j\rho_S L_j^\dagger$, while the remaining terms ensure normalization when no transitions occur.

The master equation relies on the *Markov approximation*, which states that at each time t, for an infinitesimal time interval dt the state of the system at time $t+dt$ only depends on the state of the system at time t. This assumption is a non-trivial requirement, since in general information acquired by the environment through the interaction with the system can flow back to the system at later times $t' > t$, making in principle the knowledge of the total density matrix $\rho_{SE}(t)$ necessary to determine $\rho_S(t')$. In the Markov approximation the information can only flow from the system to the environment, which in practice means that the memory of any effect the system has on the environment is limited to a time scale much shorter than that of interest for the description of the dynamics of the system. Whenever this assumption is physically well motivated, the master equation can safely be used. Let us remark though that, for this very reason, the master equation approach is less general than

the quantum operation formalism. Indeed, the latter does not describe continuous time evolution but only state changes, hence providing a good framework for the description of non-Markovian dynamics as well.

2.3 Decoherence and quantum to classical transition

In its broader meaning, the term *decoherence*[2] indicates the effectively irreversible disappearance of quantum coherence as a dynamical consequence of the interaction between a quantum system and the environment. The intuitive picture of the process is that of an environment continuously "monitoring" the system, acquiring information about its state and consequently diluting this information content into a larger Hilbert space in the form of quantum correlations, i.e. entanglement. Indeed, open quantum system dynamics in its general formulation can be thought of as a process in which the environment performs indirect measurements on the system. In such indirect measurements a non-destructive interaction between a probe-like environment E and the system S is followed by a projective measurement on E. Consider an initial joint state $\rho_{SE}(0) = \rho_S(0) \otimes |0\rangle\langle 0|_E$[3] evolving unitarily under the action of $U(t)$. If $\{|j\rangle\}$ and $\{j\}$ are the eigenvectors and associated eigenvalues of the environment, the density matrix of S at time t conditioned on the outcome j of a projective measurement on E is:

$$\begin{aligned} \rho_S^{(j)}(t) &= \frac{\mathrm{Tr}_E\{[\mathbb{1} \otimes |j\rangle\langle j|_E]U(t)(\rho_S(0) \otimes |0\rangle\langle 0|_E)U^\dagger(t)[\mathbb{1} \otimes |j\rangle\langle j|_E]\}}{\mathrm{Prob}(j|\rho_S(t))} \\ &= \frac{\langle j_E|U(t)|0_E\rangle \rho_S(0) \langle 0_E|U^\dagger(t)|j_E\rangle}{\mathrm{Prob}(j|\rho_S(t))}\,. \end{aligned} \tag{2.17}$$

In almost all practical situations the degrees of freedom of the environment are out of the experimental control, namely, if the environment is big, the actual outcome of the measurement is out of reach and the density operator of the system must be described by the sum over all possible conditional states $\rho_S^{(j)}(t)$ weighted by their

[2]The seminal papers on decoherence are [71, 72, 73]; For comprehensive reviews on the topic, see [74] and [75].

[3]Let us remark that the assumption of an initial absence of correlations between system and environment is shared by both the quantum operations formalism and the master equation approach to open quantum systems dynamics. We also note that there is no loss of generality in considering an initial pure state for the environment in that by expanding the Hilbert space $\mathcal{H}_E$ an initial mixed state $\rho_E(0)$ can always be *purified* [58, 59].

probabilities $\mathrm{Prob}(j|\rho_S(t))$. Upon defining the measurement operators

$$E_j = \langle j_E|U(t)|0_E\rangle\,, \quad \text{with} \sum_i E_i^\dagger E_i = \mathbb{1}\,, \tag{2.18}$$

we thus have

$$\begin{aligned} \rho_S(t) &= \sum_j \mathrm{Prob}(j|\rho_S(t))\rho_S^{(j)}(t) \\ &= \sum_j E_j \rho_S(0) E_j^\dagger\,. \end{aligned} \tag{2.19}$$

The formal equivalence between Eq.(2.19) and the operator sum formalism (cf. Sec.(2.1)) implies that the effect of a general environmental interaction on the state of the system, when the environment is not read out, can be understood as an environmental monitoring on the system, resulting in an increase of entanglement between the system and the degrees of freedom of the environment. As discussed in Sec.(1.7), the more a bipartite quantum system ρ_{SE} gets entangled, the more the information about ρ_S is delocalized into quantum correlation: Phase relations become locally (i.e. with respect to S) inaccessible and the state of S becomes more mixed. In turn, purely quantum phenomena, like superpositions and interference, are suppressed and eventually become unobservable at the level of the system. This suggests that the decoherence mechanism provides an explanation to the problem of the quantum-to-classical transition, namely the emergence of classicality from an underlying world governed by the laws of quantum mechanics. Indeed, decoherence theory gives prescriptions to single out some preferred states, called *pointer states*, which persist in spite of environmental monitoring. These states, which lack coherence and therefore do not exhibit quantum behaviors, arise through a process called *einselection* [72, 73, 74] which effectively rules out nonclassical superposition states.

In light of the considerations above, an illustrative example of a stylized mechanism accounting for the transition from the quantum to the classical world is represented by the phase damping channel. One may interpret this channel as describing the scattering interaction between a heavy "classical" particle and a bath of photons. The particle position is initially in a superposition of two eigenstates $|\psi\rangle = \frac{1}{\sqrt{2}}(|x\rangle + |-x\rangle)$. We can introduce a scattering rate τ such that (cf. Sec.(2.1.2)) $p = \tau\delta t \ll 1$ for a fixed time δt. After a time $t = n\delta t$, the off-diagonal damping

factor is $(1-p)^n = (1-\tau\delta t)^{t/\delta t}$ which, in the limit $\delta t \to 0$ takes an exponential form $e^{-\tau}$. Hence, after a time $t \gg \tau^{-1}$ coherence in the position basis is almost totally suppressed, and quantum effects like interference are no longer observable. We also remark that, whenever dealing with coherent superpositions of macroscopically distinguishable states of a "heavy" object, the decoherence time scale is much quicker than that of dissipation [76]. Physically, following this interpretation of the phase damping channel, the position-eigenstate basis is selected because the particle-photon interactions are localized in space, and photons impinging on the particle get scattered into different (not necessarily mutually orthogonal) states according to the different distinguishable position of the particle (the "monitoring" process previously described). In general, the spatial locality of the interaction of the system with its environment is the cause of the rise of a preferred basis for decoherence and the example just presented is considered to be representative of the transition between a quantum and a classical behavior in many physical situations.

Part II

Quantum cellular automata for transport processes

Chapter 3

Excitation transfer through noisy QCA

In this chapter, based on [77], we introduce a model of energy transfer via a noisy quantum cellular automaton construction on a one-dimensional qubit lattice. The model represents the first strictly local discrete-time dynamics approach to the problem, since prior to this all others were based on a master equation.

We begin in the first section by presenting a brief but self-contained introduction to quantum cellular automata, providing the fundamental notions underlying these systems and highlighting the interplay between their axiomatic definition and their privileged constructive representation. In the second section we will consider the problem of constructing a class of one-qubit CP maps that, in a certain limit, reproduce all classical Markov transition matrices on dichotomic probability distributions. Then, in the third section, we will embed this construction into a quantum cellular automaton structure and in the final section we will present a numerical study of the resulting dynamics applied to the problem of excitation transfer, comparing the performance of classical and quantum dynamics with equal local transition probabilities.

3.1 An informal introduction to QCA

Quantum Cellular Automata can be described as a set of quantum systems (cells) on a d-dimensional regular lattice evolving in discrete time steps according to a certain fixed transition rule. This rule has to be local (information cannot travel faster

than some fixed number of cells per time step) and the global dynamics must be translationally invariant, such that the physics is homogeneous across the lattice. Because of this "physics-like"structure and the inherent parallelism, QCA were first envisaged as potentially versatile and interesting models for quantum computation and quantum simulation [39, 78]. In recent years, unitary QCA have attracted attention as models for both specific quantum information processing tasks [40] and as underlying models of emergent causal theories such as quantum field theory [79, 80, 81, 82, 83] and quantum gravity [41, 42]. Their classical counterparts (CA), first introduced by Von Neumann [84], have been successfully used in many different fields, mostly for simulations of complex physical phenomena [85, 86, 87] (fluid dynamics, non-linear diffusion, phase transitions, traffic jam models, biological colony growth...) and have also been shown to be Turing complete [84, 88].

In order to better understand how QCA work, it is perhaps useful to begin by describing briefly how classical automata do. Consider a CA on an n-dimensional regular lattice. At each node of the lattice there is a system (the cell of the CA) which can only be in one of a finite set of possible states (dead-alive, black-white, 0-1...). Each one of these cells interacts only with a finite fixed number of neighboring cells, defining a neighborhood scheme, which is the same for every site of the lattice. Within this neighborhood an interaction rule is defined, which again has to be the same for all neighborhoods across the lattice. At every discrete time step this local interaction rule is applied in parallel to all cells simultaneously, updating their internal status. Notice that here by interaction we mean that the rule determines what is going to be the status of each cell by just reading the content of all cells within the neighborhoods. A rigorous general definition reads:

Definition 1 ***(Cellular automata)*** *A cellular automaton is a* $4-$*tuple* $(L, \Sigma, \mathcal{N}, f)$ *consisting of* (1) *a d-dimensional lattice of cells* L *indexed* $i \in \mathbb{Z}^d$, (2) *a finite set of states* Σ, (3) *a finite neighborhood scheme* $\mathcal{N} \subset \mathbb{Z}^d$ *and* (4) *a local interaction rule* $f : \Sigma^{\mathcal{N}} \to \Sigma$.

The freedom of choosing the neighborhood scheme and the local interaction rule translates into a rich variety of different behaviors for the evolution of CA (for a more than comprehensive reference on this, see Wolfram [88]).

The reasons why it is interesting to extend the theory of CA to the quantum domain are multiple. The importance of building a theory of quantum cellular

automata was first suggested by Feynman in his famous 1981 seminal lecture on quantum computation [39][1]. He argued that QCA are similar to nature as their structure is intrinsically local and causal and because of that they could represent a powerful computational tool as well as natural frameworks for simulating quantum systems. It is indeed evident that QCA would have the benefit of modeling phenomena together with their spatial structure, and, from a computational standpoint, they would have clear advantages over the circuit model. This is due to the fact that having uniform rules applied in parallel across the lattice means reducing the depth of the circuit. Moreover, as individual qubits in the lattice would not need to be separately addressed one by one, very little external control would be needed and thus the main source of decoherence would be dramatically reduced. Although, as we will see in the remainder of this section, the theory of QCA has nowadays reached a certain degree of maturity and completeness, experimentally nothing has been done so far. The two most natural and promising candidates for realizing QCA in labs in the next future are microtraps arrays [90] and optical lattices [91, 92].

The path towards a satisfactory development of a theory of quantum cellular automata has been quite troubled, as the problem of how to translate cellular automata into a quantum mechanical framework turned out not to be trivial. That is why throughout the years QCA have been given many different, sometimes competing, definitions. While the earliest ones [89, 93, 94, 95] were plagued by unphysical behaviors[2], more recent proposals failed in a sense to build a comprehensive model of QCA, in that either an axiomatic [97, 98, 38] or a constructive approach [43, 99, 100, 95] to the problem would be chosen, depending on the authors' taste. Fortunately enough though, it has been very recently shown that the two different approaches can be reconciled [101], and in order to justify the constructive approach we will follow in the next sections to define noisy QCA, it is beneficial to see how unitary QCA structures may emerge in an axiomatic framework.

Consider a QCA on an n-dimensional lattice and set a neighboring scheme for the local interactions[3]. At each node of the lattice is placed a quantum system (a qubit,

[1] He did not explicitly develop a notion of QCA in that lecture, though. His formal approach to QCA can be found in [89].

[2] For instance Feynmann's [89] definition allowed for negative probability transitions, whilst Grössing and Zeilinger's [93] first and Watrous' [94] later did not rule out non-local behaviours [96, 38].

[3] The following definitions are taken from [101, 97]. In those works, the axiomatization given

for instance), whose internal states belong to a discrete finite set Σ. All the possible *finite* configurations $c \in \mathcal{C}^{\Sigma}$ the global state of the analogus classical automaton can be in are now associated to an orthonormal basis $\{|c\rangle\}$ for the global Hilbert space $\mathcal{H}_{\mathcal{C}^{\Sigma}}$ of the QCA. The state of the QCA at any time t is a unit vector in $\mathcal{H}_{\mathcal{C}^{\Sigma}}$ and it can of course be expressed as a superposition of the basis vectors $\{|c\rangle\}$. The action of a QCA can be represented by a linear global map $\mathcal{G} : \mathcal{B}(\mathcal{H}_{\mathcal{C}^{\Sigma}}) \to \mathcal{B}(\mathcal{H}_{\mathcal{C}^{\Sigma}})$. In order for a QCA to be axiomatically well defined, the map $\mathcal{G}$ must satisfy the following definitions

Definition 2 ***(Unitarity)*** *A linear operator $G : \mathcal{H}_{\mathcal{C}^{\Sigma}} \to \mathcal{H}_{\mathcal{C}^{\Sigma}}$ is unitary iff $\{G|c\rangle \mid c \in \mathcal{C}^{\Sigma}\}$ is an orthonormal basis of $\mathcal{H}_{\mathcal{C}^{\Sigma}}$.*

Definition 3 ***(Shift invariance)*** *let σ be the one-site shift operator on the lattice; A linear operator G is shift invariant iff $\sigma G = G\sigma$.*

Definition 4 ***(Causality)*** *Let the global state of the QCA be identified with a trace-one positive operator ρ; A linear map $\mathcal{G} : \mathcal{B}(\mathcal{H}_{\mathcal{C}^{\Sigma}}) \to \mathcal{B}(\mathcal{H}_{\mathcal{C}^{\Sigma}})$ is said to be causal iff for any ρ, ρ' two states over $\mathcal{H}_{\mathcal{C}^{\Sigma}}$, and for any site x:*

$$\mathrm{Tr}_{\mathcal{L}\setminus\mathcal{N}_x}(\rho) = \mathrm{Tr}_{\mathcal{L}\setminus\mathcal{N}_x}(\rho') \quad \Rightarrow \quad \mathrm{Tr}_{\mathcal{L}\setminus x}\left[\mathcal{G}(\rho)\right] = \mathrm{Tr}_{\mathcal{L}\setminus x}\left[\mathcal{G}(\rho')\right], \tag{3.1}$$

where $\mathrm{Tr}_{\mathcal{L}\setminus\mathcal{N}_x(x)}$ means tracing over the entire lattice but the neighborhood $\mathcal{N}_x$(the site x). In words, this definition means that to know the state of a site x after one application of the automaton we only need to know the state of its neighborhood before the evolution. Hence:

Definition 5 ***(Quantum Cellular Automata)*** *An n-dimensional Quantum Cellular Automaton is an operator G which is unitary, shift invariant and causal.*

Now, the last definition gives a precise axiomatization to QCA but it does not say anything about the actual structure of the operator G, so a constructive representation is also needed. The gap between axiomatic and constructive representations was bridged by Arrighi and Grattage [101] using the concepts of *partitioning*[4] and

by Schumacher and Werner in [38] working with C^* algebra formalism on an infinite lattice is translated into the more manageable Schrödinger picture in Hilbert space. Again, the lattice is infinite, but the set of possible configurations a QCA can take is defined to be countable and finite. Notice that such a lattice entails the notion of a *quiescent state*, a state that does not change under the action of the local transition function. However, being it unnecessary in the present context, we will not introduce such notion.

[4] which was already used in [38], as well as in [95, 94].

intrinsic simulation. The concept of partitioning can be clarified by highlighting a fundamental distinction between CA and QCA. In the former case, the possibility of synchronously update all cells can be achieved by, for instance, storing the current CA configuration in a temporary register, where the update of all the even indexed cells is performed in parallel with the update of all the odd indexed ones in the original CA. The next time step configuration is then obtained by simply merging the two registers. For QCA this procedure cannot be applied as quantum states cannot in general be copied due to the *no-cloning* theorem, thus making parallel update for these systems impossible. One way around this problem is given by the introduction of a periodic partitioning scheme of the lattice into blocks such that every cell belongs to exactly one block and any two blocks are connected by a lattice translation. Looking at Fig.(3.1) for the case of a 4×4 neighborhood scheme on a 2-dimensional lattice, the time-step evolution is divided into two, meaning that at first an interaction on a non-overlapping partition of neighborhoods on the lattice is applied followed by the same interaction performed on the same partition shifted by one cell in all directions.

The concept of intrinsic simulation is related to the ability of a computational

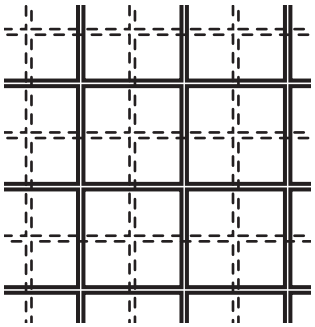


Figure 3.1: A schematization of the so-called Margolus partitioning scheme in $s = 2$ dimensions. Operations are alternatingly applied to the solid and to the dashed partitioning into 2×2 squares. Here cells are represented as squared, but their actual shape can be different, as it only serves to label localized quantum systems.

model to efficiently simulate other instances of the same model. In a nutshell, we say that a QCA F can be simulated by another QCA H if[5]:

1. There exists a procedure to map F into H and vice-versa.

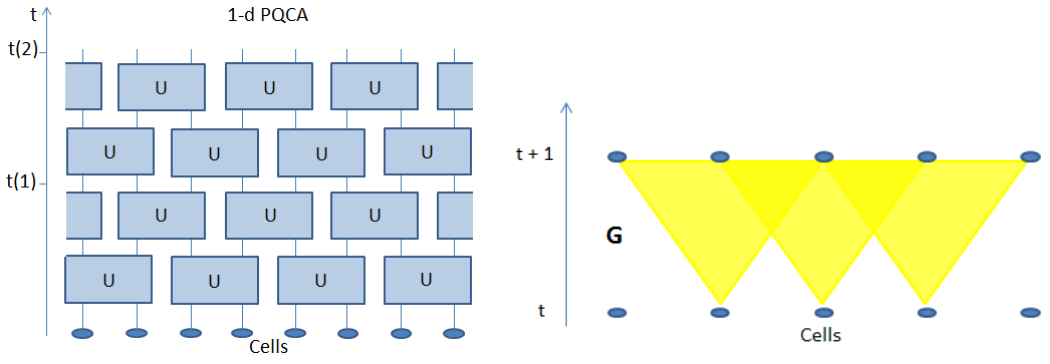
[5]This is a rough simplification of [101], where the whole procedure is made rigorous through the definition of *isometric coding*, *direct simulation* and *grouping*. However, introducing those notions lies outside the scope of this brief presentation, so we deliberately skip them and point the interested reader to the aforementioned reference.

2. The state of F after t time-steps of evolution is retrievable from the state of H after H has undergone s time-steps of evolution (s can be either different or equal to t).

The two automata can in general have different neighborhood schemes and different Hilbert space dimension of the cells. It was shown in [101] that any n-dimensional QCA (defined as in Def.(5)) can be simulated by an n-dimensional partitioned QCA (PQCA) and that, at the cost of a rather complicated mapping, there exists an intrinsically universal instance of PQCA, i.e. an n-dimensional PQCA capable in principle of simulating any other n-dimensional QCA [102]. Notice that PQCA are the simplest possible valid QCA setups and therefore they represent the most valuable model to deal with in most applications. Ours, which will be introduced in the next sections, will not make an exception. As a matter of fact, in the following we will be always concerned with $1-$dimensional PQCA, whose global evolution (depicted in Fig.(3.2)) can be expressed as:

$$\rho(t+1) = \mathcal{G}(\rho) = G\rho(t)G^{\dagger}, \quad \text{with} \quad G = \left[\sigma_{-1}\left(\bigotimes_{\mathcal{N}_x} U\right)\sigma_{+1}\left(\bigotimes_{\mathcal{N}_x} U\right)\right], \tag{3.2}$$

where U is the local unitary acting upon each neighborhood, $\sigma_{\pm 1}$ is the one-site right/left shift of the lattice and $\mathcal{N}_x$ labels the xth neighborhood.



(a) (b)

Figure 3.2: (a) Sketch of the 1-dimensional $\frac{1}{2}-$nearest neighbor QCA evolution in time. Wires are cells, time flows upwards. One iteration of the automaton corresponds to the application of two layers of local two-qubit unitaries. (b) The light cone of a QCA.

As a final remark for this introduction, let us notice that from a *physical* standpoint there is in particular one reason why one should be interested in developing

models of physical phenomena in a QCA framework instead of a more usual regular lattice *plus* Hamiltonian evolution setup. That is due to the fact that for any Hamiltonian continuous time evolution the Lieb-Robinson bounds[6] [103] allow for an exponentially vanishing but nonetheless non-zero probability of correlating instantaneously any two different regions of the lattice. That undoubtedly sounds unphysical as it would be desirable to have a model in which no correlations can be established (not even in principle) outside a causality light-cone. One can then either choose to adopt a loose attitude and simply not care about this "accident" – which is actually what happens most of the times – or be somewhat concerned and try to switch the attention towards models in which this issue does not arise. QCA fall within such models, in that the very strict notion of causality of Def.(4) leads to a sharp definition of information light cones (Fig.(3.2.b)), thus *structurally* ruling out unwanted exponential probability tails.

3.2 CP map representation of classical stochastic maps

The transport model we are about to build is based on the architecture described by Eq.(3.2) and Fig.(3.2).a, but, as we will consider noise, we will not have, in general, a unitary scattering acting on a two-qubit Hilbert space. Let us anticipate though that this will not be just a straightforward substitution ($U \rightarrow$ CP-map), in that the class of local CP-maps that will be introduced only acts on the one excitation subspace of a two-qubit neighborhood. As we shall see in this section, the constructive approach we will use will be dictated by specific arguments related to the possibility of embedding classical stochastic processes (Markov chains) within the more general, quantum, dynamics.

With this spirit, consider a classical random walk between two sites. This is the prototypical Markov process, represented by a general stochastic transition matrix

[6] There are several possible formulations of these bounds. Perhaps the most direct way of stating them is to say that for any two observables O and O'

$$[O(t), O'] \leq c\|O\|\|O'\|\min\{|O|, |O'|\}\exp(-\mu(d(O, O') - v|t|)) \,. \tag{3.3}$$

In the above equation, c and μ are positive constants, while v has the role of a group velocity; $\mathrm{d}(O, O')$ is the distance between the supports (the region of the lattice where the operators act) of the two operators, and $|O|$, $|O'|$ is the size of their supports.

of the form

$$T_{p,q} = \begin{pmatrix} 1-p & q \\ p & 1-q \end{pmatrix}, \quad \text{with} \quad 0 \leq p, q \leq 1 \tag{3.4}$$

acting on dichotomic probability distribution vectors of the kind $v_m = (m, 1-m)^{\mathsf{T}}$, with $0 \leq m \leq 1$. In the random walk picture, the parameters p and q represent the probabilities to jump from one site to the other at each discrete time step of the evolution. When there is no bias between the two directions of the walk, i.e. $p = q$, the transition matrix $T_{p,p}$ is called doubly stochastic. This classical dynamics may be related to a quantum dynamics if one takes into account a specific class $\mathcal{C}$ of completely positive maps that, once a privileged basis is set, send diagonal density operators into diagonal density operators.[7] It is possible to find a simple construction which allows one to reproduce any possible two-dimensional stochastic matrix by considering a subset of $\mathcal{C}$ acting on a one-qubit system.

First, note that one-qubit diagonal density matrices can be trivially bijectively mapped into dichotomic probability distribution vectors, as per $B : \rho_m = \mathrm{diag}(m, 1-m) \mapsto v_m = (m, 1-m)^{\mathsf{T}}$, where we have denoted such a bijection by B. We will conventionally refer to the parameter m as the probability of populating the excited state of the qubit, or "excitation probability" . Two different kinds of quantum noise, ultimately selecting the classical basis, will enter the picture of the dynamics. The dephasing channel Φ_ξ, which, as discussed in Sec.(2.3), arguably represents the most natural decoherence mechanism in several practical cases, has the effect of damping all coherences in a density matrix by a factor $\sqrt{1-\xi}$, while leaving the diagonal elements untouched. Its Kraus operators (cf. Sec.(2.1.2)) are:

$$D_0 = \sqrt{1-\xi}\mathbb{1},\ D_1 = \sqrt{\xi}(\mathbb{1} + \sigma_z)/2,\ D_2 = \sqrt{\xi}(\sigma_z - \mathbb{1})/2\,, \tag{3.5}$$

where the dephasing strength parameter ξ is such that $0 \leq \xi \leq 1$, and σ_j for $j = x, y, z$ stand for the Pauli matrices. We shall refer to the CP-map Φ_1, whose effect is setting to zero all the off-diagonal elements, as "total" , or "complete" dephasing. The amplitude damping channel (cf. Sec.(2.1.1)) Ξ_η, is defined by the Kraus operators

$$L_{0,\eta} = (\mathbb{1} + \sigma_z)/2 + \sqrt{1-\eta}(\mathbb{1} - \sigma_z)/2,\ L_{1,\eta} = \sqrt{\eta}(\sigma_x + i\sigma_y)/2\,, \tag{3.6}$$

[7] Quite significantly, another class of such maps has been recently adopted to establish a resource theory of quantum coherence [104].

with $0 \leq \eta \leq 1$. As the dephasing, it damps all coherences by a factor $\sqrt{1-\eta}$, while also affecting the populations on the diagonal. It will be convenient to introduce the "swapped" amplitude damping channel, the extention of the definition of Ξ_η to negative η ($-1 \leq \eta \leq 0$), characterized by the Kraus operators $\sigma_x L_{0,|\eta|}\sigma_x$ and $\sigma_x L_{1,|\eta|}\sigma_x$.

We can now show two statements relating classical stochastic maps and single qubit dynamics:

Proposition 1 *Any two-dimensional doubly stochastic map may be represented on diagonal density matrices by the action of a unitary map followed by complete dephasing.*

Proof: Let $U_{\theta,\boldsymbol{\varphi}}$ be a generic 2×2 unitary matrix parametrized as

$$U_{\theta,\boldsymbol{\varphi}} = \begin{pmatrix} \cos\theta & \sin\theta \mathrm{e}^{i\varphi_2} \\ -\sin\theta \mathrm{e}^{i\varphi_1} & \cos\theta \mathrm{e}^{i(\varphi_1+\varphi_2)} \end{pmatrix} \tag{3.7}$$

with $0 \leq \theta \leq \pi$, $\boldsymbol{\varphi} = (\varphi_1, \varphi_2)$ and $0 \leq \varphi_1, \varphi_2 \leq 2\pi$. The action of the map $B \circ \Phi_1 \circ U_{\theta,\boldsymbol{\varphi}}$ on a diagonal density matrix $\rho_m = \mathrm{diag}(m, 1-m)$ (where $U_{\theta,\boldsymbol{\varphi}}$ is understood to act by similarity) is analogous to the action of the stochastic map $T_{p,p}$ of Eq.(3.4) on the probability vector $v_m = (m, 1-m)^{\mathsf{T}}$:

$$B\left(\Phi_1\left(U_{\theta,\boldsymbol{\varphi}}\rho_m U^\dagger_{\theta,\boldsymbol{\varphi}}\right)\right) = T_{\sin^2\theta,\sin^2\theta}\boldsymbol{v}_m \ , \tag{3.8}$$

upon identifying $p = \sin(\theta)^2$. It is thus always possible to reproduce any doubly stochastic maps through a proper choice of θ.

□

Proposition 2 *Any two-dimensional stochastic map may be represented on diagonal density matrices by the action of a completely dephased unitary map, followed by an amplitude damping channel.*

Proof: By direct application of the map $\Xi_\eta \circ \Phi_1 \circ U_{\theta,\boldsymbol{\varphi}}$ we find a state $\rho_{m'}$ with excitation probability ($c \equiv \cos(2\theta)$):

$$m' = \cos(2\theta)(1-|\eta|)m + \frac{1+|\eta|\cos(2\theta) - \cos(2\theta) + \eta}{2} \ , \tag{3.9}$$

while the action of $T_{p,q}$ on the vector v_m gives a vector $v_{m'}$, with $m' = (1-p-q)m+q$. By equating the two new excitation probabilities one obtains the desired relationships between the parameters defining the two different maps:

$$\eta = q - p \; ; \qquad \cos(2\theta) = \frac{1-p-q}{1-|q-p|} \; . \tag{3.10}$$

Proposition (2) (and hence (1)) can then be translated into:

$$B\left[\Xi_{|q-p|}\left(\Phi_1\left(U_{f(p,q),\boldsymbol{\varphi}}\rho_m U^\dagger_{f(p,q),\boldsymbol{\varphi}}\right)\right)\right] = T_{p,q}v_m \; , \tag{3.11}$$

where

$$f(p,q) := \frac{1}{2}\arccos\left(\frac{1-p-q}{1-|q-p|}\right). \tag{3.12}$$

□

Even though there is no claim here for this embedding to be the only possible or the most general one, it is clear that all values of p and q, and thus all two-dimensional stochastic maps, can be reproduced by the open dynamics we considered by an appropriate choice of η and θ.

3.3 The noisy cellular automaton model

Using the embedding of two-dimensional stochastic maps into dissipative qubit dynamics described in the previous section, it is now possible to define an extended single excitation dynamics on a 1-d lattice of qubits employing a partitioned quantum cellular automata structure. Let us consider the case of a single excitation transfer from one end to the other of a chain composed of N qubits. As it is customary when dealing with excitation transport processes, we shall restrict to the single excitation subspace of the global, 2^N-dimensional Hilbert space. This assumption, which dramatically simplifies the treatise, is biologically well justified when modeling photosynthetic systems, which host only one excitation at a time during a transport dynamics. In this sector, the Hilbert space (whose dimension is now equal to N) is spanned by the basis $\{|n\rangle\}$ $(1 \leq n \leq N)$, with $|n\rangle$ representing the state in which the n-th qubit is in an excited state, while all the others are in the ground state. Let us now define the CP-map $\Omega^{(n)}_{\eta,\xi,\theta,\boldsymbol{\varphi}}$ as the map acting as the composition of a unitary $U^{(n)}_{\theta,\boldsymbol{\varphi}}$, a dephasing $\Phi^{(n)}_{\xi}$ and an amplitude damping $\Xi^{(n)}_{\eta}$ on the two-dimensional

subspace spanned by $|n\rangle$ and $|n+1\rangle$, and as the identity on the remainder of the single excitation subspace: $\Omega^{(n)}_{\eta,\xi,\theta,\boldsymbol{\varphi}}(\rho) = \Xi^{(n)}_{\eta}\left(\Phi^{(n)}_{\xi}\left(U^{(n)}_{\theta,\boldsymbol{\varphi}}\rho U^{(n)\dagger}_{\theta,\boldsymbol{\varphi}}\right)\right)$, where ρ is a density matrix with support in the single excitation subspace. We can then define a noisy quantum cellular automaton on the lattice as the following map [97, 38, 101]

$$\Omega_{\eta,\xi,\theta,\boldsymbol{\varphi}} = \bigotimes_{l\,\mathrm{odd}} \Omega^{(l)}_{\eta,\xi,\theta,\boldsymbol{\varphi}} \bigotimes_{l\,\mathrm{even}} \Omega^{(l)}_{\eta,\xi,\theta,\boldsymbol{\varphi}} \,. \tag{3.13}$$

Here, the "odd" and "even" prescriptions in the labels realise a partitioning of the lattice, taking into account the non-commutativity of CP-maps acting on overlapping subsystems: One step of the automaton consists first in applying the map on disjoint pairs of neighbouring qubits, and then in applying the same operation shifted by one lattice position (cf. Fig.(3.2) and Fig.(3.3)). The lattice may be a ring – in which case the map $\Omega^{N}_{\eta,\xi,\theta,\boldsymbol{\varphi}}$ acts on the state $|N\rangle$ and $|1\rangle$ – or open – in which case the map $\Omega^{N}_{\eta,\xi,\theta,\boldsymbol{\varphi}}$ is not applied [8]. As we saw in Sec.(3.1), any unitary quantum cellular automaton may be realised, up to shift operations, by adopting such a partitioning, based on the iteration of the same map between alternate pairs of neighbouring qubits and, although no corresponding general theorem exists for noisy CP-maps [105], the above maps are by construction causal and – on infinite lattices – invariant under the squared shift operator, so that it seems appropriate to maintain the denomination of (noisy) quantum cellular automata for them[9].

A classical transfer process may be modeled on such a lattice by a chain of identical stochastic transition matrices which, in the light of Proposition 2, can be represented by the CP-map $\Omega_{\eta,1,\theta,\boldsymbol{\varphi}}$ acting on diagonal (classical) states, where the dephasing channel is set to a total dephasing, with strength $\xi = 1$. Hence, the class of cellular automata just designed is such that one can study classical transfer by setting $\xi = 1$, and then enter the quantum regime by decreasing the dephasing strength ξ from 1 to 0. While still in a sense arbitrary, it can be argued that this model is – though in a very simple way – representative of the classical to quantum transition in actual physical systems, in that it enacts such a transition entirely by

[8] In the case of odd N, a lattice on a ring would require specific prescriptions for the partition used. However, this is really a matter of technicalities, which have very little bearing on what follows.

[9] Although derived from a definition on the full tensor product Hilbert space, the automaton of Eq.(3.13) is, in a sense, a generalization to CP-maps of the unitary automata in direct space (1-excitation subspace) first considered in [93]. It has been argued that these should be considered as an example of "quantum walks" [38].

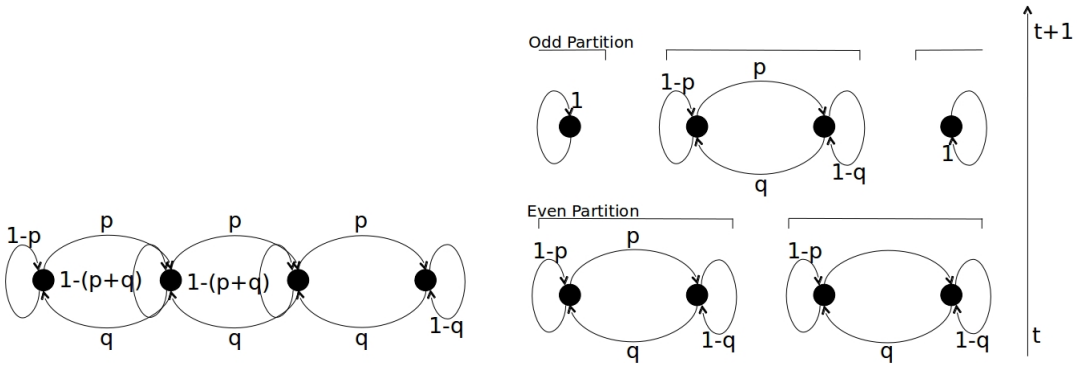


Figure 3.3: (*left*) The classical homogeneous random walk on an open chain of $N = 4$ sites; (*right*) One time step scheme of the equivalent partitioned random walk, which represents the classical dynamics QCA (3.13) is reduced to when total dephasing ($\xi = 1$) is applied.

changing a dephasing strength, which is the main decoherence mechanism in any open quantum system. In practical cases, dephasing results from the coupling with the environment, which sets the privileged basis.

Given p and q of a classical stochastic transfer process, one can construct the corresponding class of quantum cellular automata $\Omega_{\eta,\xi,\theta,\boldsymbol{\varphi}}$ by setting $\eta = q-p$ (whose sign will determine the privileged direction of travel of the excitation along the lattice) and $\theta = \arccos\left(\frac{1-p-q}{1-|q-p|}\right)/2$, and letting ξ vary from the classical automaton for $\xi = 1$ to the "most quantum" (where no dephasing acts and coherent off-diagonal terms are only suppressed by the amplitude damping) for $\xi = 0$. The phases φ_1 and φ_2 are completely free, as one should expect since they cannot be determined by the limiting classical process where they do not appear at all. Such phases do potentially play a role in applications, as we will see in the next section.

3.4 Energy excitation transfer

Now that the structure of the dynamics is established, the model can be applied to the study of energy excitation transfer through the lattice [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16] by comparing, at given local transition probabilities p and q, the performance of a classical process with that of quantum dynamics where coherent phases are allowed to develop and interfere along the chain. Let us stress once again that the equality of the local transition probabilities ensures that all the difference between the classical and quantum cases is exclusively down to quantum coherence.

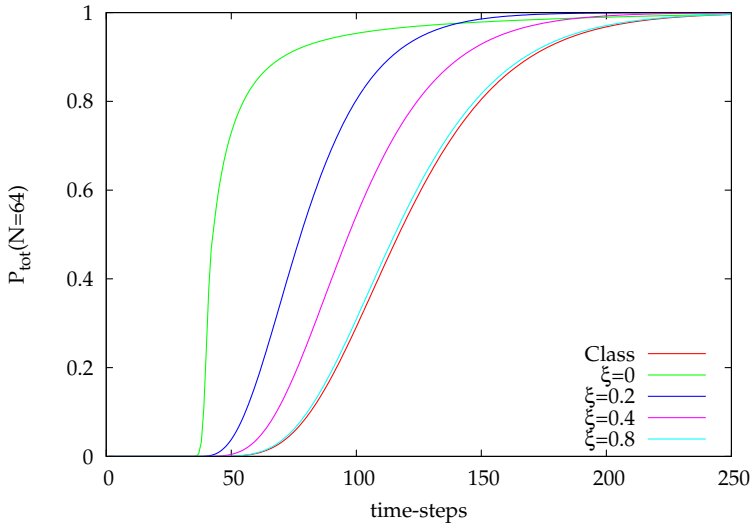


Figure 3.4: Integrated probability of absorption through an open chain with $N = 64$, $p = 0.7$, $q = 0.5$, $\varphi_1 + \varphi_2 = \pi$ (the probability only depends on the sum $\varphi_1 + \varphi_2$) and various values of ξ, from classical ($\xi = 1$, denoted by "Class") to most quantum ($\xi = 0$).

Energy transfer will be studied by assuming the pure initial state $|1\rangle$, with a single excitation localized on the first site of the chain. The excitation absorption by a receptor located at site $|N\rangle$ and $|N/2+1\rangle$ for, respectively, an open chain and a ring of N sites (taking, for simplicity, N to be even), is modeled by a quantum measurement with elements $M_0 = \mathbb{1} - |N\rangle\langle N|$ and $M_1 = |N\rangle\langle N|$ (replacing N with $N/2+1$ for a ring). This measurement process can be expressed in the following (unconditional) form:

$$\begin{aligned} \rho &\rightarrow \frac{|0_N\rangle\langle 0_N| \otimes \langle 0_N|\rho|0_N\rangle}{\mathrm{Tr}_{\mathcal{L}\setminus N}(\langle 0_N|\rho|0_N\rangle)} + \frac{|1_N\rangle\langle 1_N| \otimes \langle 1_N|\rho|1_N\rangle}{\mathrm{Tr}_{\mathcal{L}\setminus N}(\langle 1_N|\rho|1_N\rangle)} \\ &= \frac{|0_N\rangle\langle 0_N| \otimes \langle 0_N|\rho|0_N\rangle}{1 - P_N} + \frac{|1_N\rangle\langle 1_N| \otimes \langle 1_N|\rho|1_N\rangle}{P_N}, \end{aligned} \tag{3.14}$$

where $\mathrm{Tr}_{\mathcal{L}\setminus N}$ means tracing over the entire lattice excluding the last site and $P_N = \rho_{NN}$ is the probability of finding the excitation on the last site. Whenever the result of the measurement is 0, the form of the density matrix changes accordingly: $\rho_{Nj} = 0 \quad \forall j, \quad \rho_{jN} = 0 \quad \forall j$ (i.e. the Nth row and Nth column of ρ are killed by the measurement) and all the other elements of ρ are renormalized by a factor $1 - P_N$. The next time step of the evolution is then applied to this new density operator, and the dynamics goes on until outcome 1 occurs, whereby the excitation is captured at the receptor and the transfer process stops.

The quantity we keep track of during the evolution of the automaton is the total probability of absorption after t time steps of the dynamics. More precisely, this is the total integrated probability that after t iterations of the automaton after which a measurement on site N has been performed at some fixed rate Δt, the system has measured the excitation. In formulae, when $\Delta t = 1$:

$$\begin{aligned} P_N^{tot}(t=1) &= \rho_{NN}(t=1) \\ P_N^{tot}(t=2) &= [1 - \underbrace{(1-\rho_{NN}(t=1))}_{1-P_N^{tot}(t=1)}(1-\rho_{NN}(t=2))] \\ P_N^{tot}(t=3) &= [1 - \underbrace{(1-\rho_{NN}(t=1))(1-\rho_{NN}(t=2))}_{1-P_N^{tot}(t=2)}(1-\rho_{NN}(t=3))] \\ &\dots \end{aligned} \tag{3.15}$$

and so on.

As a preliminary investigation, the optimal rate of measurement at the receptor site, in terms of maximizing the absorption probability, was considered. In the classical case ($\xi = 1$), where the only effect of measuring 0 is renormalizing the probability distribution, the optimal rate is measuring after every step of the automaton. In the quantum case, a failed absorption has the additional effect of destroying the off-diagonal terms involving the receptor site: nonetheless, it turns out that in the vast majority of cases that have been considered measuring after every step is still the optimal strategy, with very marginal gains when measuring every two steps in few specific cases. In the following, we will hence always consider absorption measurements performed at each step of the automaton.

Let us start by considering an open chain of $N = 64$ sites[10]. The case $p = 0.7$ and $q = 0.5$ is illustrated in Fig.(3.4)[11]. The advantage granted by quantum coherence is manifest, in that, for $\varphi_1 + \varphi_2 = \pi$, the presence of the off-diagonal terms of the density matrix increases dramatically the absorption probability at each step in the early dynamics (reflected in the increased slope in Fig.(3.4)). Interestingly, after such an initial boost, systems with stronger quantum coherence are slower in saturating the integrated probability to 1 than more classical counterparts. Increasing the

[10] Notice that in the absence of periodic boundary conditions one drops *global* translational invariance.

[11] Figures from 3.4 to 3.8 are reprinted from [77]. Copyright (2014) by the American Physical Society.

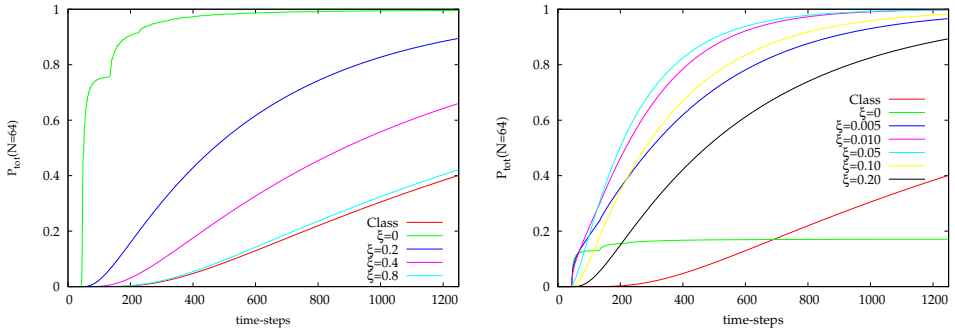


Figure 3.5: Integrated probability of absorption through an open chain with $N = 64$, $p = 0.5$, $q = 0.5$, various values of ξ, from classical ($\xi = 1$, denoted by "Class") to most quantum ($\xi = 0$), and phases $\varphi_1 + \varphi_2 = \pi$ (a) and $\varphi_1 = \varphi_2 = 0$ (b).

bias $\eta = |q - p|$ enhances the effect of the amplitude-damping channel, and thus diminishes the difference between the corresponding quantum and classical cases. In point of fact, note that, when $\eta = 1$, the map becomes classical regardless of the choice of ξ and other parameters: this is, so to speak, the ballistic limit, where the excitation is deterministically transferred through the chain in $N/2$ steps. While trivially optimal, this is not such an interesting regime when modeling stochastic transfer phenomena. Further, notice that, because of the way the partitioning was defined, any case with $p = 1$, including the one with $q = 1$ that can be obtained by chains of unitary swap operations, also results in ballistic transfer. The benefit granted by stronger amplitude damping in this model is distinct from the seminal cases of noise assistance flagged up in [7, 8, 9, 10, 11], where local dephasing is responsible for suppressing destructive interference [12]. As we will see, the latter can also be reproduced within the present framework.

Intriguing effects become apparent setting $p = q = 0.5$, as reported in Fig.(3.5).a for an open chain with optimized phases (such that $\varphi_1 + \varphi_2 = \pi$). In this instance, the gap between quantum and classical dynamics is at its widest, and purely quantum distinctive features emerge. In particular, the integrated absorption probability shows stationary points, whereby the instantaneous absorption probability is zero, followed by sudden increases. This effect, for which heuristic analytical evidence is provided in the next subsection, is a manifestation of destructive interference due to the off-diagonal terms of the density matrix, and disappears as soon as any amount

[12] It must be said that, although expedient to comply with the literature on single-qubit channels, the terminology "amplitude damping" is in this case slightly misleading, since here the environment is not locally draining excitations, but rather acting at the interface between two qubits by pushing the excitation along a privileged direction.

of dephasing is introduced. It is however a purely quantum effect, which could in principle be observed.

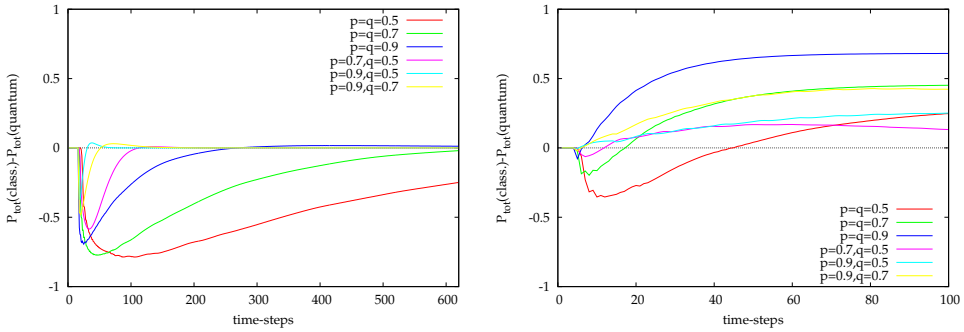
Dephasing-assisted transfer is apparent in Fig.(3.5).b, where the parameters are set as in Fig.(3.5).a except for the coherent phases $\boldsymbol{\varphi}$ (also, a different set of values for ξ is taken into account). In this case destructive interference is clear in the quantum case ($\xi = 0$), where the integrated probability soon encounters a plateau, and is suppressed as soon as some dephasing noise is introduced. An optimal value around $\xi = 0.05$ can be determined with this choice of parameters. This is at variance with the stationarity encountered for optimized phases, where each stationary point is followed by a steep ramp of constructive interference. This provides a clear indication that this framework is capable of highlighting the dependence of noise-assistance on the phases of coherent interactions (the unitary U, in our discrete treatment): for certain choices of phases (such as the one in Fig.(3.5).a), dephasing noise helps only marginally and at long times (after the initial quantum boost)[13].

The case of a ring with $N = 64$ is depicted in Fig.(3.6).a, and confirms that the advantage granted by quantum coherence is most apparent in the case $p = q = 0.5$, and tends to vanish as the difference between p and q increases. The quantum advantage in the transfer probability critically depends on the number of qubits N: with more qubits, the effect of constructive interference becomes more relevant and enduring. This advantage is reminiscent of the speed-up occurring in random [34] or Hamiltonian [20] quantum walks – where by "random" quantum walk we refer to dynamics featuring a coin Hilbert space – which share similarities with the present approach. For instance, the analogous of Fig.(3.6).a for $N = 18$ is reported in Fig.(3.6).b, and shows that the classical maps surpasses their quantum counterparts (with optimally chosen phases) after at most 70 time-steps.

3.4.1 Coherent effects on absorption

Let us conclude this chapter by giving a plausible explanation regarding the mechanism underlying the dephasing-assisted transfer observed in Fig.s(3.5). Recalling the partitioning induced on the lattice by the automaton, the global operators composing the map Eq.(3.13) are block diagonal matrices, where for the *even* partitioning all the blocks are 2×2, while for the *odd* partitioning the first and last

[13]Notice that the action of local dephasing on each qubit is equivalent to the action of our dephasing channel in the single excitation subspace.



(a) (b)

Figure 3.6: Difference between most classical ($\xi = 1$) and most quantum ($\xi = 0$) integrated probabilities of absorption through a ring with $\varphi_1 = \varphi_2 = 0$, various values of p and q, and $N = 64$ (a) and $N = 18$ (b).

blocks are just the 1-dimensional identity. Because of the neighbouring scheme of the automaton, only 3 sites directly interact with each other at each iteration.

Focusing only on the last 3 sites of the $N \times N$ global density matrix ρ, the action of the unitary part of the map (Eq.(3.13)) is given by [14]:

$$U^{odd}_{(3\times3)} U^{even}_{(3\times3)} \rho_{(3\times3)} U^{even\dagger}_{(3\times3)} U^{odd\dagger}_{(3\times3)}, \tag{3.16}$$

with

$$\rho_{(3\times3)} = \begin{pmatrix} \rho_{N-2,N-2} & \rho_{N-2,N-1} & 0 \\ \rho^*_{N-2,N-1} & \rho_{N-1,N-1} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{3.17}$$

and

$$U^{even}_{(3\times3)} = \begin{pmatrix} u_{22} & 0 & 0 \\ 0 & u_{11} & u_{12} \\ 0 & u_{21} & u_{22} \end{pmatrix}, U^{odd}_{(3\times3)} = \begin{pmatrix} u_{11} & u_{12} & 0 \\ u_{21} & u_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.18}$$

which gives a probability of absorption at time $t+1$:

$$\rho^{(t+1)}_{NN} = |u_{21}|^2 \left[|u_{21}|^2 \rho^{(t)}_{N-2,N-2} + |u_{22}|^2 \rho^{(t)}_{N-1,N-1} + \left(u_{21} u^*_{22} \rho^{(t)}_{N-2,N-1} + c.c. \right) \right]. \tag{3.19}$$

In the case $p = q = 0.5$, using Eq.(4.4), the equation above reads

$$\rho^{(t+1)}_{NN} = \frac{\rho^{(t)}_{N-2,N-2} + \rho^{(t)}_{N-1,N-1}}{4} - |\rho^{(t)}_{21}| \cos(\varphi_2 - \omega(t)), \tag{3.20}$$

where we have introduced a notation such that the complex off-diagonal terms of

[14] Let us remind the reader that all the entries in the Nth row and column of the global state of the system ρ are set to 0 due to the measurement that took place at the previous time step.

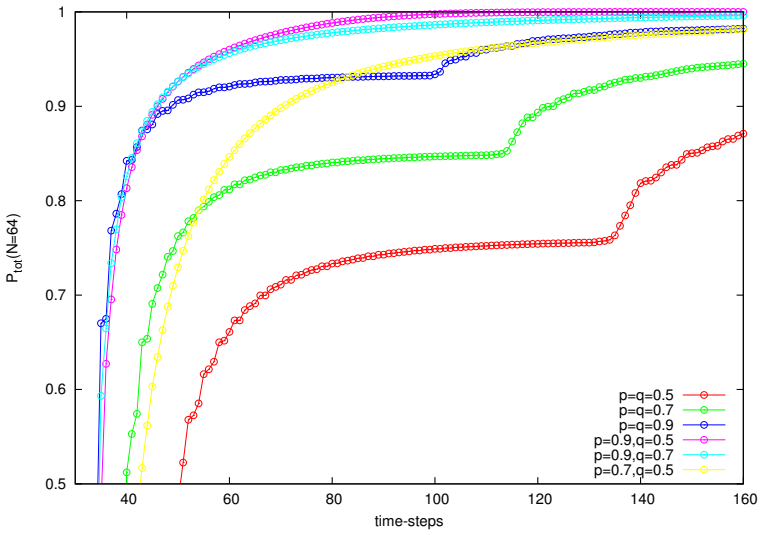


Figure 3.7: Integrated probability of absorption through an open chain with $N = 64$, $\varphi_1 + \varphi_2 = \pi$ and various values of p, q. The dephasing channel is switched off ($\xi = 0$).

ρ are written as $\rho^{(t)}_{N-2,N-1} \equiv e^{i\omega(t)}|\rho_{21}(t)|$. The stationarity of the total probability of absorption we can see in Fig.(3.7) occurs when $\rho^{(t+1)}_{NN} \simeq 0$ at some time-step. It can be easily shown that such a condition is only possible when $\rho^{(t)}_{N-2,N-2} \simeq \rho^{(t)}_{N-1,N-1}$, $\omega(t) = \varphi_2$ and, most importantly, when the off-diagonal term is such that $|\rho^{(t)}_{N-2,N-1}| = \sqrt{\rho^{(t)}_{N-1,N-1}\rho^{(t)}_{N-2,N-2}}$, which is the maximum value compatible with the positivity condition on ρ[15]. This is the reason why any amount of dephasing will prevent the cancellation above, and hence stationarity from happening (Fig.(3.8)).

Recalling that the amplitude damping channel (Eq.(3.6)) also suppresses coherent off-diagonal terms by a factor $\sqrt{1-|q-p|}$, the same argument heuristically explains why stationarity is ruled out for any dynamics with $p \neq q$ (Fig.(3.7)).

We point out that the mechanism just described, even though convincing enough, is likely not to be the end of the story. Another *localization* effect driven by quantum coherence and directly dependent on the values of the free phases φ_1 and φ_2, may affect significantly the transport performance. Evidence for this effect will be provided numerically in Sec.(4.2), within the context of quantum state transfer.

[15]The positivity condition is equivalent to saying that any reduced state of ρ must in turn be positive. Since partial tracing in the first excitation sector is equivalent to renormalizing, we have $|\rho^{(t)}_{N-2,N-1}|^2 \leq \rho^{(t)}_{N-2,N-2}\rho^{(t)}_{N-1,N-1}$, $\forall\, t$.

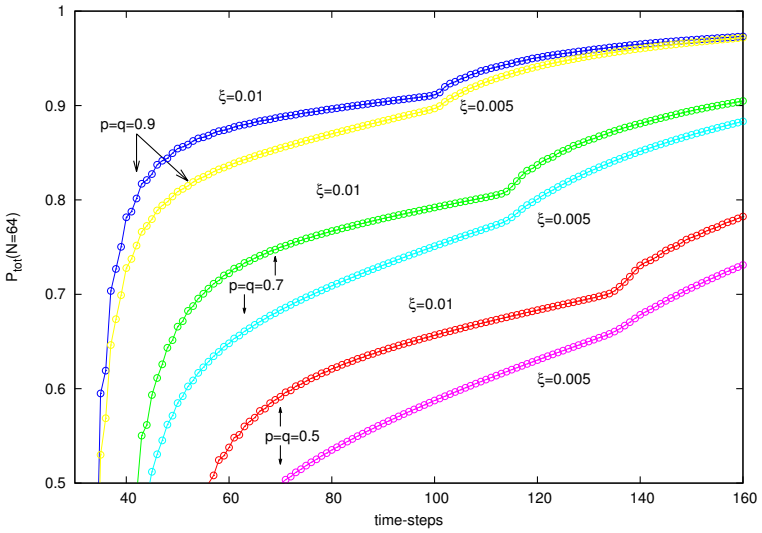


Figure 3.8: Integrated probability of absorption through an open chain with $N = 64$, $\varphi_1 + \varphi_2 = \pi$ and different values of p, q. The dephasing channel is now switched on: $\xi = (0.005; 0.01)$.

Chapter 4

Quantum state transfer through noisy QCA

In general, when dealing with spatially discrete quantum systems, the aim of a quantum state transfer protocol is to transfer with unit fidelity an unknown arbitrary quantum state from a sender to a receiver through a network of interacting quantum systems, which is initially in its ground (or "vacuum") state. If qubits are considered, then a generic state prepared on the sender qubit s ($|\psi\rangle_s = \alpha|0\rangle_s + \beta|1\rangle_s$) must be dynamically transported through the network in a finite time t^* to the receiver qubit r (and possibly read out):

$$|\psi\rangle_s \otimes |00\ldots0\rangle_{network} \otimes |0\rangle_r \quad \stackrel{t^*<\infty}{\longrightarrow} \quad |\phi\rangle \otimes |\psi\rangle_r \tag{4.1}$$

where the resulting state of network and sender $|\phi\rangle$ at the end of the process does not matter. Of course a sequence of unitary swap gates would be a straightforward solution, but it would require a considerable amount of control over the dynamics as well as complete absence of noise. Since we are interested in venturing into the noisy regime, Eq.(4.1) must be recast into:

$$|\psi\rangle_s \otimes |00\ldots0\rangle_{network} \otimes |0\rangle_r \quad \stackrel{t^*<\infty}{\longrightarrow} \quad \rho(t^*) \text{ s.t. } \rho_r(t^*) \equiv \mathrm{Tr}_{\neg r}\left(\rho(t^*)\right) = |\psi\rangle\langle\psi|, \tag{4.2}$$

where $Tr_{\neg r}(\rho)$ denotes partial tracing on the whole network but the receiver qubit r. As already mentioned in the introduction, by far the two prominent approaches to quantum state transfer are represented by spin chains – which are continuous-

time, unitary dynamics – and quantum walks; so far, only the latter has developed a formalism in which noise can be taken into account. However, to the author's best knowledge, the whole literature on quantum state transfer through noisy quantum walks is comprised of only one paper [44], where in turn quite stringent restrictions are imposed to the dynamics[1].

This chapter, based on [106][2], is devoted to studying the transport of a quantum state through qubit lattices governed by noisy QCA evolutions. The QCA structure allows to define a discrete time dynamics in which one does not need to resort to an arguably unpractical bipartition of the Hilbert space into internal and position degrees of freedom (as in quantum walks), and at the same time grants the development of the first strictly local model of noisy quantum state transfer.

In the first section, the QCA dynamics introduced in the previous chapter will be extended to a Hilbert space equipped with a global vacuum state, leading us to determine the dynamical constraints that define the class of noisy QCA in this subspace. In the second section we will study the transport performance through numerical simulations, showing that for some instances of the dynamics perfect quantum state transfer is attainable and discussing the impact of the different types of quantum noise taken into account in the model.

4.1 Noisy QCA dynamics in the $0 \oplus 1$ sector

While in the previous chapter we defined a framework which was sufficient to study single excitation transport, our aim now is to apply the same dynamics to the transport of a quantum state, i.e. we want to investigate how well our noisy QCA dynamics can transport initial on-site coherences, besides excitations. In order to do that, i.e. to transport the state of a qubit (as in Eqs.(4.1) or (4.2)), we need to extend the action of the automata CP maps from the single excitation sector (SES), to a Hilbert space which must also include a global vacuum state, the state in which there are no excitations in the chain. Let us recall that the full Hilbert space $\mathcal{H}^{\otimes N}$ (where $\mathcal{H}$ indicates the Hilbert space of a qubit) can always be decomposed into the

[1] Symmetry in the left/right propagation and, above all, absence of backflow of the wavefunction out of the receiver site, which acts as a sink.

[2] Online version at `http://stacks.iop.org/1751-8121/48/i=19/a=195304`.

direct sum of its number conserving sectors:

$$\mathcal{H}^{\otimes N} = \bigoplus_{e=0}^{N} \mathcal{H}_e \ . \tag{4.3}$$

With the assumption that no other sectors are populated, our maps will then be defined in the subspace with 0 and 1 excitations, $\mathcal{H}_0 \oplus \mathcal{H}_1$. Let us stress that there is a systematic way of going from this reduced subspace to the full $\mathcal{H}^{\otimes N}$, making the notion of partial trace (and thus reduced state) still meaningful and well defined (see Appendix A).

In terms of the operators involved in the evolution of the system, including a global vacuum simply translates into adding a row and a column to the global density matrix ρ and to the Kraus operators composing the global channel. Let us then focus on the Kraus operators formalism representing the map in Eq.(3.13).

First, using Eq.(3.7) and Eq.(3.10-3.12) we can express $U_{\theta,\boldsymbol{\varphi}}$ explicitly in terms of the transition probabilities p and q[3]

$$U^{(l)}_{p,q,\boldsymbol{\varphi}} = \frac{1}{\sqrt{1-\eta}} \begin{pmatrix} \sqrt{1-p} & \sqrt{q}e^{i\varphi_2} \\ \sqrt{q}e^{i\varphi_1} & -\sqrt{1-p}e^{i(\varphi_1+\varphi_2)} \end{pmatrix} . \tag{4.4}$$

We will be regarding p and q as the probability of the classical stochastic dynamics to jump one site on the left and on the right, respectively. We will always consider the case $p \geq q$, as we also arbitrarily choose to set the transfer direction in the chain from left to right. The superscript (l) will be used throughout the rest of the chapter to indicate local operators. As regards the general expression of the local channel representing the map $\Omega^{(n)}_{\eta,\xi,\theta,\boldsymbol{\varphi}}$ (Eq.(3.13)), we find:

$$K^{(l)}_0 = \sqrt{\frac{1-\xi/2}{1-\eta}} \begin{pmatrix} \sqrt{1-\eta}\sqrt{1-p} & \sqrt{1-\eta}\sqrt{q}e^{i\varphi_2} \\ \sqrt{q}e^{i\varphi_1} & -\sqrt{1-p}e^{i(\varphi_1+\varphi_2)} \end{pmatrix} , \tag{4.5}$$

$$K^{(l)}_1 = \sqrt{\frac{\xi/2}{1-\eta}} \begin{pmatrix} \sqrt{1-\eta}\sqrt{1-p} & \sqrt{1-\eta}\sqrt{q}e^{i\varphi_2} \\ -\sqrt{q}e^{i\varphi_1} & \sqrt{1-p}e^{i(\varphi_1+\varphi_2)} \end{pmatrix} , \tag{4.6}$$

[3]Eq.(4.4) represents the case $p \geq q$. When $q > p$, then $U^{(l)}_{p,q,\boldsymbol{\varphi}} \to U^{(l)}_{q,p,\boldsymbol{\varphi}}$. Notice also that the parametrization presented here corresponds to Eq.(3.7) provided $\varphi_1 \to \varphi_1 + \pi$.

$$K_2^{(l)}\sqrt{\frac{\eta}{1-\eta}} = \begin{pmatrix} 0 & 0 \\ \sqrt{1-p} & \sqrt{q}e^{i\varphi_2} \end{pmatrix}. \tag{4.7}$$

The above operators are obtained by changing to a unitary equivalent representation for the dephasing channel (Eq.(3.5)) composed of only two Kraus operators and then by multiplying $U^{(l)}_{p,q,\boldsymbol{\varphi}}$ by the combination of the application of the new dephasing channel followed by the amplitude damping channel of Eq.(3.6).

Given the QCA structure, the global channel in the SES is identified by three $N\times N$ block diagonal matrices $\{K_\mu^{(s)}\}$ (the superscript (s) identifies operators acting on the SES) in which the blocks are the corresponding local operators $\{K_\mu^{(l)}\}$. In the full (SES plus vacuum) Hilbert space $\tilde{\mathcal{H}}$ we can write[4]

$$\tilde{K_\mu} = \begin{pmatrix} z_\mu & \boldsymbol{V}_\mu^\dagger \\ \boldsymbol{W}_\mu & K_\mu^{(s)} \end{pmatrix}, \quad \mu = (0,1,2), \tag{4.9}$$

where $\{\boldsymbol{V}_\mu\}$ and $\{\boldsymbol{W}_\mu\}$ are N-dimensional vectors, $\{z_\mu\}$ are the $|0\rangle\langle 0|$ scalar entries in the enlarged Hilbert space, and we have introduced a *tilde*-notation such that $\tilde{X}$ represents an $(N+1)$-dimensional operator. One time step of the QCA evolution of the system (Eqs.(3.13)) can then be explicitly written as:

$$\tilde{\Omega}(\tilde{\rho}) = \sum_{\nu=0}^{2} \tilde{K}_\nu^{(odd)} \left[\sum_{\mu=0}^{2} \tilde{K}_\mu^{(even)} \tilde{\rho} \tilde{K}_\mu^{(even)\dagger}\right] \tilde{K}_\nu^{(odd)\dagger} \tag{4.10}$$

The condition for the new Kraus operators to sum up to the identity $\sum_\mu \tilde{K_\mu}^\dagger \tilde{K_\mu} = \mathbb{1}$ now reads:

$$\sum_\mu \begin{pmatrix} |z_\mu|^2 + ||\boldsymbol{W}_\mu||_2^2 & c.c. \\ (z_\mu \boldsymbol{V}_\mu + K_\mu^{(s)\dagger}\cdot \boldsymbol{W}_\mu) & (\boldsymbol{V}_\mu \cdot \boldsymbol{V}_\mu^\dagger + K_\mu^{(s)\dagger}\cdot K_\mu^{(s)}) \end{pmatrix} = \mathbb{1}, \tag{4.11}$$

[4] Assuming the operators in Eq.(4.9) refer to the even partition of the lattice, the odd partition's ones will simply be:

$$\tilde{K_\mu} = \begin{pmatrix} z_\mu & \boldsymbol{V}_\mu^\dagger \\ \boldsymbol{W}_\mu & \sigma K_\mu^{(s)} \sigma^\dagger \end{pmatrix}, \quad \mu = (0,1,2), \tag{4.8}$$

where σ is the one site shift operator. Some extra care must be taken when applying the shift to chains with no periodic boundary conditions (see later on).

which leads to a set of constraints:

$$\begin{cases} \sum_\mu (|z_\mu|^2 + ||\boldsymbol{W}_\mu||_2^2) = 1 \\ \sum_\mu {K_\mu^{(s)}}^\dagger \cdot \boldsymbol{W}_\mu = 0 \\ \boldsymbol{V}_\mu = 0, \quad \forall \mu \end{cases} \tag{4.12}$$

where $\boldsymbol{V}_\mu = 0$, $\forall \mu$, is due to the fact that the outer product of a vector with itself gives a nonnegative matrix, and we already had $\sum_\mu K_\mu^{(s)\dagger} K_\mu^{(s)} = \mathbb{1}$.

Looking at Eq.(4.9), we see that the two vectors $\boldsymbol{W}_\mu$ and $\boldsymbol{V}_\mu$ can be thought of, respectively, as excitation "pumping" and dissipation processes, in that the former represents the entries of $\{\tilde{K}_\mu\}$ that account for the creation of an excitation from the vacuum ($\{\boldsymbol{W}_\mu\} \leftrightarrow \{(|n\rangle\langle 0|)_\mu\}_{\mu=1}^N$), while the latter provides those entries such that excitations are annihilated into the vacuum ($\{\boldsymbol{V}_\mu\} \leftrightarrow \{(|0\rangle\langle n|)_\mu\}_{\mu=1}^N$). Notice that we do not allow for more than one excitation in the lattice during the transport and thus the role of the $\{\boldsymbol{W}_\mu\}$ vectors in the dynamics is to increase at each time step of the evolution the probability of having the excitation somewhere in the chain. Nonetheless, the two sets of vectors are in a broad sense representative of dissipation and excitation effects when hypothesizing a physical realization of a QCA quantum state transport device.

Given the Kraus operators of the single excitation sector, $K_\mu^{(s)}$, Eqs.(4.12) leave one with a certain freedom in the choice of the $\boldsymbol{W}_\mu$. In other words, for each noisy QCA dynamics in the SES, we are left with a whole class of dynamics in the extended Hilbert space. We notice that one can take advantage of the peculiar block structure of the QCA dynamics (Eq.(3.13)) in order to characterize the vectors $\boldsymbol{W}_\mu$. For closed chains with N even, each of the two QCA partitions are formed of $N/2$ blocks of local (2×2) Kraus operators lying on the diagonal of the global operator. Looking back at the set of constraints (Eq.(4.12)), the aforementioned block structure implies that $\sum_\mu {K_\mu^{(s)}}^\dagger \cdot \boldsymbol{W}_\mu = 0$ can be regarded as a local condition, as it can be rewritten in the form:

$$\sum_\mu {K_\mu^{(l)}}^\dagger \cdot \boldsymbol{w}_\mu(\mathcal{N}_i) = 0, \quad \forall i, \tag{4.13}$$

where the vectors $\boldsymbol{w}_\mu(\mathcal{N}_i)$ are $N/2$ 2-dimensional local vectors defined at each neighborhood $\{\mathcal{N}_i\}_{i=1}^{N/2}$. These vectors could in principle be different from each other. However, we can state the following:

Proposition 3 *The extention to the* $0 \oplus 1$ *sector of the Hilbert space of the class of noisy quantum cellular automata defined in Eq.(3.13) preserves invariance under the squared shift operator iff the vectors* $\boldsymbol{W}_\mu$ *defined in Eq.(4.9) are block translational invariant.*

Proof: The 2-site block translational invariance condition can be checked by directly computing the sum of the commutators between the squared lattice shift operator σ^2 and the operators defining the QCA map:

$$\begin{aligned}\sum_\mu \left[\tilde{\sigma^2}, \tilde{K_\mu}\right] &= \sum_\mu \left\{ \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \sigma^2 \end{pmatrix} \begin{pmatrix} z_\mu & \mathbf{0} \\ \boldsymbol{W}_\mu & K_\mu^{(s)} \end{pmatrix} - \begin{pmatrix} z_\mu & \mathbf{0} \\ \boldsymbol{W}_\mu & K_\mu^{(s)} \end{pmatrix} \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \sigma^2 \end{pmatrix} \right\} \\ &= \begin{pmatrix} 0 & \mathbf{0} \\ \sum_\mu \left(\sigma^2 \cdot \boldsymbol{W}_\mu - \boldsymbol{W}_\mu\right) & \sum_\mu \left[\sigma^2, K_\mu^{(s)}\right] \end{pmatrix} . \end{aligned} \tag{4.14}$$

In the SES with periodic boundary conditions, the block diagonal structure of $K_\mu^{(s)}$ ensures that $\sum_\mu \left[\sigma^2, K_\mu^{(s)}\right] = 0$. The translational invariance of the extended QCA dynamics is thus retained when the $\boldsymbol{W}_\mu$ vectors are translationally invariant, as in that case the order with which a squared shift of the lattice and the QCA map are applied does not matter:

$$\sum_{\mu\nu} \tilde{\sigma}^2 \left(\tilde{\sigma} \tilde{K_\mu} \tilde{\sigma}^\dagger \tilde{K_\nu} \tilde{\rho} \tilde{K_\nu}^\dagger \tilde{\sigma} \tilde{K_\mu}^\dagger \tilde{\sigma}^\dagger\right) \tilde{\sigma}^{2\dagger} = \sum_{\mu\nu} \tilde{\sigma} \tilde{K_\mu} \tilde{\sigma}^\dagger \tilde{K_\nu} \left(\tilde{\sigma}^2 \tilde{\rho} \tilde{\sigma}^{2\dagger}\right) \tilde{K_\nu}^\dagger \tilde{\sigma} \tilde{K_\mu}^\dagger \tilde{\sigma}^\dagger \tag{4.15}$$

□

Hence, in light of Prop.(3), we must set the vectors $\boldsymbol{w}_\mu(\mathcal{N}_i)$ to be the same (for a given superoperator μ) in every neighborhood, thus dropping the neighborhood index dependence $\mathcal{N}_i$: $\boldsymbol{W}_\mu = \bigoplus \boldsymbol{w}_\mu$, with $\boldsymbol{w}_\mu = (w_\mu^0, w_\mu^1)$, $\forall \mu$. This way this source of noise represents another homogeneous property of the dynamics.

There is still an even more important issue to be considered. In fact, the introduction of a global vacuum implies that our extended interactions may not fulfill the stringent causality definition of Eq.(3.1), which is a crucial property for a QCA evolution. Indeed, it turns out that additional constraints need to be added to the dynamics. The question of which of our extended CP-maps are still causal – hence representing a well-defined noisy QCA – is settled by the following statement:

Proposition 4 *The class of proper – i.e. causal and translational invariant – noisy*

quantum cellular automata on a 1-dimensional qubit lattice, when the dynamics is restricted to the $0 \oplus 1$ *sector of the Hilbert space, is defined by the set of constraints:*

$$\begin{cases} \boldsymbol{W}_\mu = \bigoplus^{N/2} \boldsymbol{w}_\mu \ , & \forall \mu \\ \boldsymbol{V}_\mu = 0 \ , & \forall \mu \\ \sum_\mu (|z_\mu|^2 + \frac{N}{2} ||\boldsymbol{w}_\mu||_2^2) = 1 & \\ \sum_\mu K_\mu^{(l)\dagger} \cdot \boldsymbol{w}_\mu = 0 & \\ \sum_\mu z_\mu w_\mu^i = \sum_\mu w_\mu^i = 0 \ , \quad i = 0,1 & \end{cases} \tag{4.16}$$

Proof: Given a global density matrix $\tilde{\rho} = \sum_{j,k=0}^{N} \rho_{jk} |j\rangle\langle k|$, we have (see Appendix A) that the reduced state of a qubit at any site x and the reduced state of the neighborhood $\mathcal{N}_x$ ($\mathcal{N}_x = \{x,\ y \equiv x+1\}$) are, respectively:

$$\rho_x = \begin{pmatrix} \sum_{l \neq x} \rho_{ll} & \rho_{0x} \\ \rho_{0x}^* & \rho_{xx} \end{pmatrix} \ , \quad \rho_{\mathcal{N}_x} = \begin{pmatrix} \sum_{l \neq (x,y)} \rho_{ll} & \rho_{0x} & \rho_{0y} \\ \rho_{0x}^* & \rho_{xx} & \rho_{xy} \\ \rho_{0y}^* & \rho_{xy^*} & \rho_{yy} \end{pmatrix} \ . \tag{4.17}$$

In order to check the causality condition Eq.(3.1), it is sufficient to directly calculate the reduced state of qubit x after an application of half step of the QCA, the step where the lattice partition is such that the two qubits in $\mathcal{N}_x$ interact through one of the local maps composing the global dynamics of Eq.(3.13). After a straightforward calculation, we find that the new state of qubit x can be expressed in the form:

$$\rho_x^{(new)} = \begin{pmatrix} 1 - f_{x|2} - \rho_{00} \sum_\mu w_\mu^{x|2} & g_x + \rho_{00} \sum_\mu z_\mu w_\mu^{x|2} \\ c.c. & f_{x|2} + \rho_{00} \sum_\mu w_\mu^{x|2} \end{pmatrix} \ , \tag{4.18}$$

where $\bullet|2$ means $\bullet$ modulo 2 and $f_{x|2} = f_{x|2}(\rho_{0x}, \rho_{0y}, \rho_{xx}, \rho_{yy}, \rho_{xy})$, $g_x = g_x(\rho_{0x}, \rho_{0y})$. The value of functions f and g is determined only by the parameters of the dynamics (through $\{K_\mu\}$, $\{\boldsymbol{W}_\mu\}$ and $\{z_\mu\}$) and the components of the reduced state of the neighborhood before the evolution (Eq.(4.17)). Two global states $\tilde{\rho}$ and $\tilde{\rho}'$ having $\rho_{\mathcal{N}_x} = \rho'_{\mathcal{N}_x}$ before the evolution will thus give new reduced states on x such that:

$$\rho_x^{(new)} - \rho_x^{\prime(new)} = \begin{pmatrix} (\rho'_{00} - \rho_{00}) \sum_\mu w_\mu^{x|2} & (\rho_{00} - \rho'_{00}) \sum_\mu z_\mu w_\mu^{x|2} \\ c.c & (\rho_{00} - \rho'_{00}) \sum_\mu w_\mu^{x|2} \end{pmatrix} \tag{4.19}$$

In order to have causality, the above difference must be zero for all ρ_{00} and ρ'_{00}.

We thus find that, when preserving the dynamics Eq.(3.13) in the single excitation sector, the class of causal QCA is selected by the following constraints

$$\begin{cases} \sum_\mu z_\mu w_\mu^0 = \sum_\mu z_\mu w_\mu^1 = 0 \\ \sum_\mu w_\mu^0 = \sum_\mu w_\mu^1 = 0 \end{cases} \tag{4.20}$$

which, combined with Prop.(3) and Eqs.(4.12), verify the claim of Prop.(4).

□

As a concluding remark for this section, we note that the fact that $\{\boldsymbol{V}_\mu\}$ (Eqs.(4.16)) are null means that the probability of having no excitations in the chain cannot increase during the evolution. Hence, the system is not subject to dissipation-like effects.

Of course one can in principle obtain other CP-maps in the enlarged Hilbert space, possibly with $\boldsymbol{V}_\mu \neq 0$, by rescaling the SES process (e.g. $K_\mu^{(s)} \to cK_\mu^{(s)}$, $\forall\mu$, with $|c| < 1$). However, we are interested in preserving the SES dynamics previously introduced, so we will only deal with the case characterized by Eqs.(4.12).

4.2 Quantum state transfer

We can now proceed to analise numerically the quantum state transfer performance of the QCA dynamics. We will consider two different settings: an open linear chain and a ring composed of an even number N of qubits. In both cases we will assume the transfer of the quantum state to take place from left to right ($p \geq q$), from the first site to the antipodal one, i.e. site N for a chain and $N/2 + 1$ for a ring. To quantify the transport, we will be employing the Uhlman fidelity (cf. Sec.(1.8.3)) between quantum states σ an ρ: $F(\sigma, \rho) = Tr(\sqrt{\sigma}\rho\sqrt{\sigma})$. Since the initial state to be trasferred will be pure, in our case the fidelity is reduced to the form $F(t) = \langle\psi(0)|Tr_{\mathcal{L}\setminus x}(\rho(t))|\psi(0)\rangle$, where the reduced state of the target x qubit is obtained by tracing the global state ρ over the entire lattice $\mathcal{L}$ but the qubit itself (see Appendix A). For any given setting, we will be considering as our figure of merit the average of the fidelities obtained by simulating the transfer of an ensemble of initial states drawn at random according to the Haar measure.

By observing the form of the local Kraus operators composing the channel, Eqs.(4.5,4.6,4.7), the first thing to note is that the closest the dynamics to unitarity, the more it is driven by the action of $K_0^{(l)}$; when the dynamics is purely unitary ($\xi = 0$, $\eta = 0$) $K_1^{(l)}$ and $K_2^{(l)}$ vanish. Since we are investigating a quantum dynamics, it is legitimate to be mostly interested in both the unitary and an "almost unitary"regimes, the study of the latter being relevant when envisaging a physical device which would naturally be exposed to some noise due to unavoidable coupling with the environment. Thus, when in these two regimes, it seems appropriate to privilege a tuple of the form $\{c_\mu\} = (a, b, c)$, $a \gg b \simeq c$, for the relative weights of the global channel's $\{z_\mu\}$ of Eq.(4.9). Moreover, it is reasonable to expect that with such $\{c_\mu\}$ the transfer fidelity will be higher. The same reasoning can be applied to the single excitation sector of the dynamics when dealing with the *odd* partition of an open chain. In that case, the $N/2 - 1$ local operators do not act on the first and last qubits, so that the first and last entries of the global operators of the *odd* partition are just scalars which have to be set such that they sum up to one to meet the identity condition for the Kraus operators. In this case we decide to set $\tilde{K}_0^{11} = \tilde{K}_0^{NN} = 1$; $\tilde{K}_i^{11} = \tilde{K}_i^{NN} = 0$, for $i \neq 0$; for the global dynamics we set $\{c_\mu\} = (1, 0, 0)$.

Let us start analyzing our numerical results by focusing on a linear open chain. In Fig.(4.1) we show the average fidelity of transfer on a chain of $N = 8$ qubits for a fully unitary dynamics (i.e. $\eta = 0$, $\xi = 0$ and $\boldsymbol{W}_\mu = 0$, $\forall\mu$) with $p = q = 0.5$. The three lines plotted correspond to three different choices for the two free phases appearing in the general parametrization of $U^{(l)}$ (Eq.(3.7)). As it can be clearly seen, these phases do play a role in the transferring process, in that for both phases set to zero $\langle F(t)\rangle$ fluctuates around ~ 0.5 (which is merely the average fidelity between two random Haar distributed states), whereas when either $(\varphi_1, \varphi_2) = (0, \pi)$ or $(\varphi_1, \varphi_2) = (\pi, 0)$ the amplitude of the average fidelity fluctuations in time are much wider and there are several times at which the fidelity is considerably higher than $2/3$ [107], which is the maximum value attainable using only classical transmission of information (*measure and prepare* strategies).

This phase dependence could be related to an analogue effect observed when dealing with the single excitation transport dynamics. By tuning the sum of the

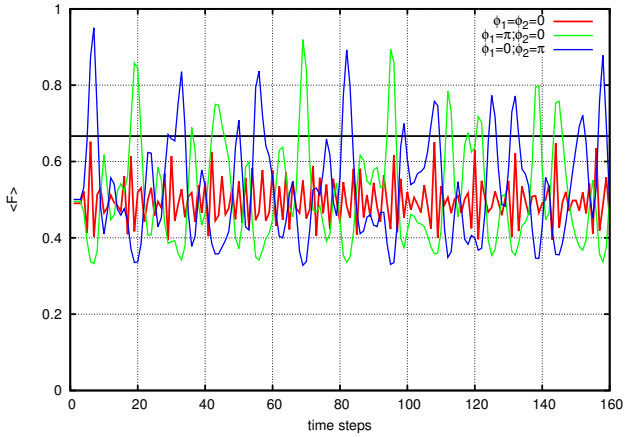
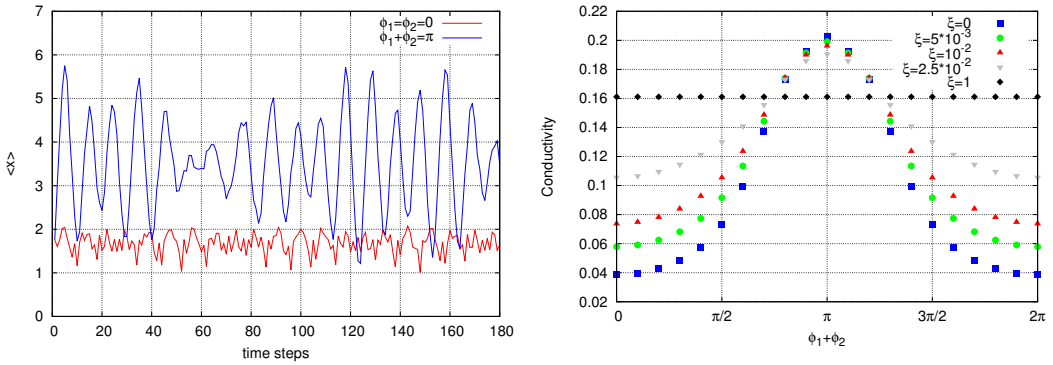


Figure 4.1: Average fidelity $\langle F(t)\rangle$ over a sample of 1000 evolutions starting from initial states drawn at random from the Haar measure, for $p = q = 0.5$ and three different choices of (φ_1, φ_2) on a linear chain of $N = 8$ qubits. No noise applied. The straight horizontal line at $F = 2/3$ shows the highest fidelity for classical transmission of a quantum state.



(a) (b)

Figure 4.2: (a) Mean excitation position in time along a chain of $N = 6$ qubits and $p = q = 0.5$ for a dynamics in the sigle excitation sector. When $\varphi_1 + \varphi_2 = 0$ a localization effect between the first two sites of the chain takes place. (b) Excitation transport performance measured by the channel's conductivity $C(t_{end}) = (1/t_{end}) \sum_{t=1}^{t_{end}} \rho_{NN}(t)$ to the last site at the end of the evolution ($t_{end} = 160$) vs $\varphi_1 + \varphi_2$ (same setting as in (a)). When no dephasing is present (blue squares), by tuning the sum of the two phases $\varphi_1 + \varphi_2$ the transport can be highly suppressed due to the observed localization effect. Interestingly enough, the introduction of some dephasing relaxes the localization, thus enhancing the transfer performance when $\varphi_1 + \varphi_2$ is not close to the optimal value of π. When total dephasing $\xi = 1$ is applied, the system undergoes a classical stochastic dynamics and the two phases cease to play any role (black diamonds).

two phases, in the SES an interesting localization phenomenon takes place for which the probability of finding the excitation can be highly concentrated between the first two sites of the chain at all times of the evolution (Fig.(4.2).a). This of course affects negatively the transport performance, as shown in Fig.(4.2).b. A detailed analysis of a similar localization effect, possibly related to what we observe here, in

a modelization of some biological systems, can be found in [108]. The analogy is strengthened by the fact that in [108], like in our model, there is a phase parameter that plays the same role in transport suppression. In the rest of the section we will be showing results obtained with the optimized choice of phases $(\varphi_1, \varphi_2) = (0, \pi)$, unless explicitly stated.

An even more dramatic effect on the transport performance is evident when comparing settings in which the main two dynamical parameters p and q take equal or different values. As Fig.(4.3) shows, when $p = q$ the wide oscillations allow for high fidelity peaks, whereas for $p \neq q$ these oscillations are quickly damped to a steady state close to 1/2. This is ascribable to the fact that turning on the amplitude damping component ($\eta \neq 0$) of the channel means that coherences in the SES get suppressed by a factor $\sqrt{1-\eta}$ at each time step and that should affect the transport of initial coherences with the vacuum state as well. In the limit of maximum amplitude damping ($p = 1, q = \epsilon$, $\epsilon \simeq 0$), the channel does not allow for coherences to build up in time in the SES. However, in such a limit the transfer is almost perfect and the excitation is locked at the end of the chain, as it can be easily understood by recalling that for vanishingly small values of q the excitation cannot travel back along the chain. The steady classical maximum value of $\langle F(t) \rangle$ in Fig.(4.3).b is due to the fact that initial vacuum coherences are perfectly transported at the beginning till the end of the chain and then progressively absorbed, as one can realize by directly computing the action of the channel in this particular case.

At the opposite extremum, when $p = q = 1$ (and $\xi = 0$), the channel is reduced to the sole action of $K_0^{(l)}$, which for $\varphi_1 = \varphi_2 = 0$ is a swap channel. The peak structure that can be observed in Fig.(4.3).b is obtained because the swap channel makes the entries $\tilde{\rho}_{11}$ bounce back and forth along the diagonal and similarly moves back and forth the two coherences along their row(column), as we can see by directly computing the first time step evolution on a three qubit QCA (with $\boldsymbol{W}_\mu = 0$, $\forall \mu$):

$$\tilde{\rho}(0) = \begin{pmatrix} \rho_{00} & \rho_{10} & 0 & 0 \\ \rho_{01} & \rho_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \tilde{\rho}(1) = \begin{pmatrix} \rho_{00} & 0 & 0 & |c_0|^2 \rho_{10} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ |c_0|^2 \rho_{01} & 0 & 0 & \rho_{11} \end{pmatrix}, \tag{4.21}$$

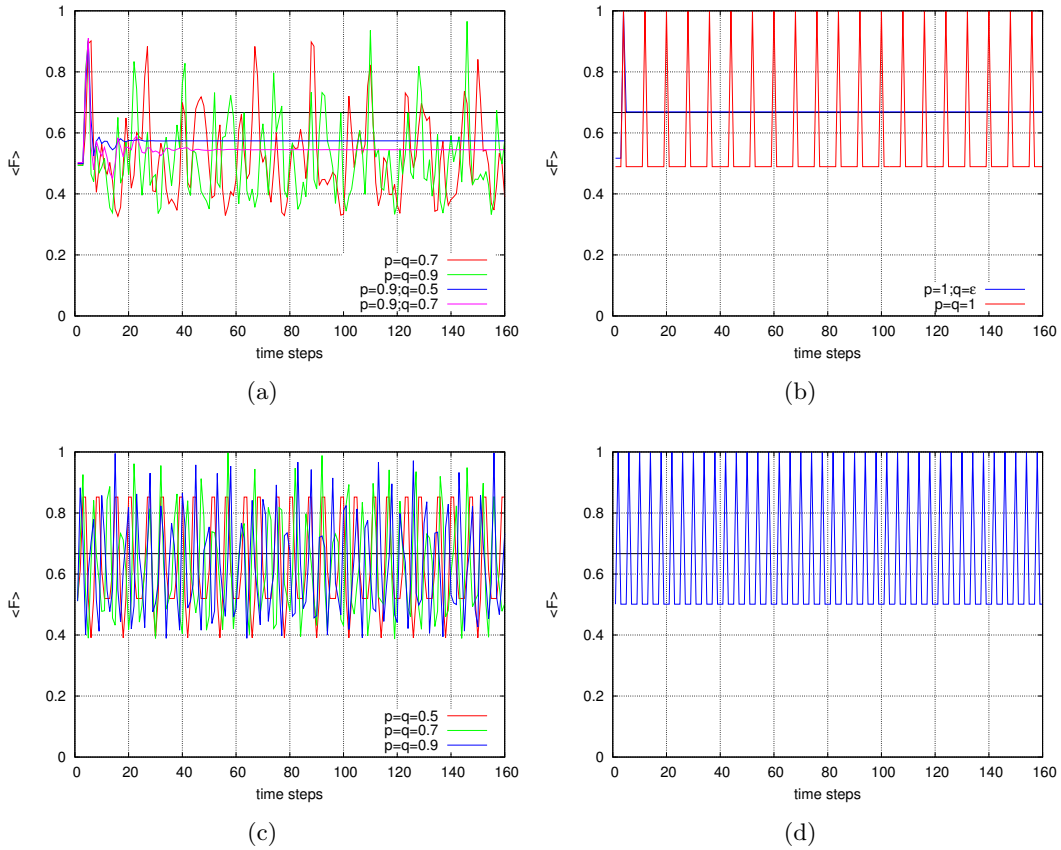


Figure 4.3: Average fidelity in time for a chain of $N = 8$ qubits, with $\xi = 0$,$\{\boldsymbol{w}_\mu\} = 0$, for (a) a linear chain for different values of p and q; (c) a ring for $p = q = (0.5, 0.7, 0.9)$; the two extreme cases of a dynamics driven by an almost maximum amplitude damping strength parameter ($p = 1$, $q = \epsilon$; in the plots $\epsilon = 5 \cdot 10^{-3}$) and a swap channel ($p = q = 1$) for a linear chain (b) and a ring (d) (where the two resulting trends in $\langle F(t) \rangle$ are perfectly superimposed).

The result above is obtained without specifying a priori any values for the tuple $\{c_\mu\}$. As already anticipated at the beginning of this section, when the dynamics is fully unitary ($K_1^{(l)} = K_2^{(l)} = 0$) only terms proportional to c_0 will survive in the first row(column) of the global density matrix $\tilde{\rho}(t)$, hence choosing $\{c_\mu\} = (1, 0, 0)$ is crucial in order to have perfect state transfer.

Let us now add periodic boundary condition to the chain. Numerics show that two considerations can be made about the differences in quantum state transfer performance between this ring-like configuration and the previous one. The first one is specific to the case of maximum amplitude damping $\eta \simeq 1$ where, as opposed to what happened in an open chain, now we find that vacuum coherences are not absorbed after a transient time but are perfectly periodically transported

back and forth along the chain together with the excitation, giving rise to exactly the same maximum peaks structure resulting from a "swap"dynamics (Fig.(4.3).d). Secondly, we note that in general, when equal settings are compared, introducing periodic boundary conditions considerably improves the state transfer's fidelity. As an example of this general trend, compare Fig.(4.3).c and (4.3).a.

4.2.1 The noise

Finally, let us conclude this chapter by discussing the role of noise in our system. In our dynamics the system-environment coupling is modeled through the action of three different general kinds of noise: amplitude damping, phase damping and "excitation pumping" -like noise. When transferring excitations only (SES), the former two could represent an advantage over a pure unitary dynamics. In fact, the amplitude damping is needed in order to introduce an asymmetry between the two directions of propagation, acting as a driving force to draw the excitation towards the end of the chain, whereas the introduction of some dephasing may smooth the localization effect previously discussed (Fig.(4.2).a,b) and/or contrast negative coherent effects on absorption (see Sec.(3.4.1)), allowing for a better transfer [77]. For quantum state transfer though, coherences play a fundamental role and, as expected, all the sources of noise we considered are always (apart from the very specific case of Fig.(4.3).d) detrimental. More specifically, amplitude damping and dephasing result in a damping of the coherent oscillations of $\langle F(t) \rangle$ (see Fig.(4.3).a and (4.4)), whereas the restrictions imposed by the causality condition on $\{\boldsymbol{w}_\mu\}$ and $\{z_\mu\}$ (last two lines of Eqs.(4.16)) make a quantum state transfer dynamics with $\{\boldsymbol{w}_\mu\} \neq 0$ strongly unfavorable. Assuming either $\{z_\mu\} \in \mathbb{R}$ or $\{\boldsymbol{w}_\mu\} \in \mathbb{R}$ (the case where both belong to $\mathbb{C}$ only complicates the picture without changing the results), we have that the only solutions to Eq.(4.16) where $\{\boldsymbol{w}_\mu\} \neq 0$ are such that $z_\mu = z$, $\forall \mu$, and we find that this condition, whatever the other parameters of the dynamics may be, always translates into very poor quantum state transfer performance.

For the sake of the argument, one can think of relaxing the causality requirement. In that case, as the third line in Eqs.(4.16) is just a matter of normalization, one can build the vectors by satisfying $\sum_\mu {K_\mu^{(l)}}^\dagger \cdot \boldsymbol{w}_\mu = 0$, which, upon substituting

Eqs.(4.5,4.6,4.7), reads:

$$\begin{cases} \sqrt{1-\frac{\xi}{2}}\sqrt{1-\eta}w_0^0 + \sqrt{\frac{\xi}{2}}\sqrt{1-\eta}w_1^0 + \sqrt{\eta}w_2^1 = 0 \\ \sqrt{1-\frac{\xi}{2}}w_0^1 - \sqrt{\frac{\xi}{2}}w_1^1 = 0 \end{cases} . \tag{4.22}$$

where we introduced a notation such that w_μ^a stands for the component a, $a = (0, 1)$ of each local vector pertaining to the Kraus operator μ. Of course, a whole set of solutions for Eqs.(4.22) is possible. In order not to give too big a bias among the different $\tilde{K}_\mu$ driving the dynamics, it is reasonable to privilege the most "balanced"solutions, the ones where $|w_\mu^a - w_\nu^b| \leq d, \forall \mu, \nu, a, b$, with the smallest possible d. To this aim, it is thus necessary to avoid solutions proportional to $(\xi/2)^{-1/2}$, $(1-\eta)^{-1/2}$ or $\eta^{-1/2}$, where for some regimes of the dynamics some components w_μ^a could be arbitrarily big. One such solution reads:

$$\begin{cases} w_0^0 = w_0^1 = -\frac{T}{\sqrt{3N}}\sqrt{\frac{\xi/2}{1-\xi/2}} \\ w_1^0 = \frac{T}{\sqrt{3N}}(1-\sqrt{\eta}); \quad w_1^1 = -\frac{T}{\sqrt{3N}} \\ w_2^0 = w_2^1 = \frac{T}{\sqrt{3N}}\sqrt{\xi/2}\sqrt{1-\eta} \end{cases} \tag{4.23}$$

Above, we assumed $\{\boldsymbol{w}_\mu\} \in \mathbb{R}$ and we arbitrarily chose a normalization proportional to $T/\sqrt{N}$, where the free parameter T tunes the strength of the noise. Notice that Eqs.(4.23) assure that $\{w_\mu^a\} \in \left[\pm T/\sqrt{3N}\right]$. As a result of relaxing causality, the components of $\{\boldsymbol{w}_\mu\}$ and $\{z_\mu\}$ are now "decoupled" and a tuple $\{z_\mu\} = (c, 0, 0)$ – which allows for the best quantum state transfer performance – can be selected. However, as it can be appreciated in Fig.(4.4), the effect of this kind of noise is very similar to that of the dephasing.

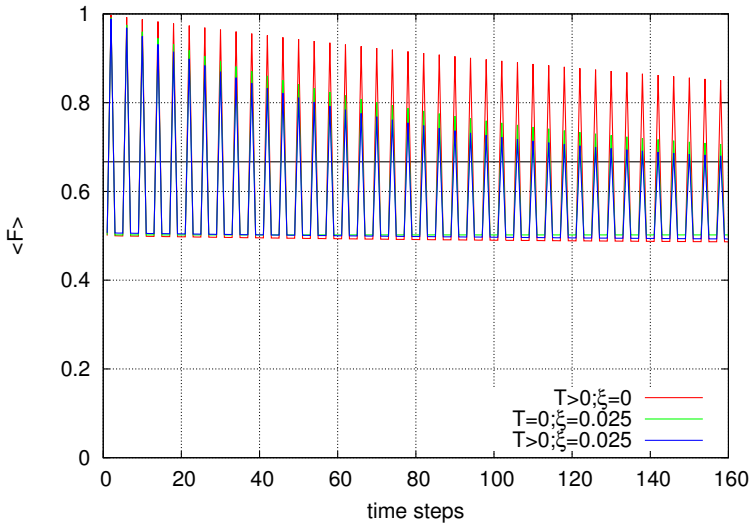


Figure 4.4: Noisy dynamics for a ring of $N = 8$ qubits and $p = q = 1$. In the depicted case $T > 0$ corresponds to the value $T = 0.1$ (see Eq.(4.23)). However, the magnitude chosen for the two parameters ξ and T does not acquire any particular meaning here, as the figure is intended to be only a representative example of the damping in $\langle F(t) \rangle$ resulting from introducing noise (cfr. Fig.(4.3).d).

Part III

Typicality

Chapter 5

Thermalization of finite quantum systems

In this brief chapter we introduce the concept of typicality in quantum thermodynamics. The attention will be focused on the issue of thermalization of quantum states. In Sec.(5.2) numerical results concerning thermalization of locally-interacting closed quantum systems are shown.

5.1 Thermalization and the typicality approach, in a nutshell

It is a known, well-established empirical fact that a physical system weakly coupled to a large bath will eventually evolve to a state which is independent from all initial state, bath and bath-state interaction conditions, but only characterized by a few macroscopic parameters of the bath, like its temperature. This thermalization phenomenon holds for both classical and quantum systems. Furthermore, the final "local" (when system and environment are considered as a whole) state will no longer exhibit any macroscopically visible evolution, despite the underlying dynamics being unitary, hence not leading to any fixed points. This ubiquitous, generic behavior thus seems to be paradoxical, to some extent, when addressed within the framework of quantum theory: In a sense, asking whether closed quantum systems thermalize is equivalent to asking whether quantum mechanics alone – which is governed by the time-reversal symmetric Schrödinger equation – is capable of describing irreversable dynamics.

The typicality approach to the problem [46, 47, 45, 49] aims at giving an explanation relying on the concept that an overwhelmingly large region of the portion of the Hilbert space accessible[1] to the evolving system is almost entirely filled with *typical* states, i.e. states that possess similar properties, like expectation values of a set of relevant observables, the probability to measure certain values for some functions, or reduced density matrices. Here we choose to privilege an approach focused on estimating the form of the latter, mostly because reduced density matrices amount to the set of all observables that can be locally defined for the system. To demonstrate thermalization, one then wishes to show that for the vast majority of pure states within a certain energy interval, the reduced density matrices pertaining to a small subsystem are the same as the ones that would be obtained by tracing out from the microcanonical ensemble corresponding to the same energy interval [45, 46]. Let us stress that these arguments primarily address relative frequencies, while delegating the dynamical mechanism leading to thermalization to the reasonable expectation that, if what discussed above is verified, any dynamics will bring and leave the system within the region filled by such typical states.

5.2 Kinematics versus dynamics

As already pointed out, although providing with valuable insights regarding fundamental issues in thermodynamics and statistical mechanics, the typicality approach to thermalization has the limit of treating the problem only from a kinematical point of view, without actually saying anything about the dynamical process leading to thermal states. Indeed, although being a very generic behavior, when trying to get to a rigorous derivation of fundamental dynamical laws explaining the thermalization of small systems in contact with a much larger bath, one usually needs very specific and technical hypothesis[2]. Of course, dynamics and kinematics are two related aspects and heuristic reasonings linking the two can be presented, for instance as follows (as detailed in [49]). Consider a dynamics that preserves the volume of the microstates and partition the accessible region Ω of the Hilbert space into two sets of states A and B according to some function $f(\tilde{\rho} \in \Omega)$: Let $\tilde{\rho}$ belong

[1] The accessible region of the Hilbert space is defined by some macroscopic constraint, or conserved quantity such as the energy of the system.

[2] The interested reader is pointed to Ref.[52], which provides a comprehensive overview of progress and open questions concerning most approaches to the problem, along with a vast list of references.

to A if

$$|f(\tilde{\rho}) - \langle f \rangle| \leq \epsilon \,, \quad \text{with}\, \epsilon \ll f_{max} - f_{min} \,, \tag{5.1}$$

and to B otherwise. Upon indicating the volume of the Hilbert space of A and B by $\Gamma(A)$, $\Gamma(B)$ respectively, by typicality we expect $\Gamma(A) \gg \Gamma(B)$. Also, if $\Gamma(X \to Y)$ denotes the size of the set of microstates X that has evolved to the set Y in a certain time t, assuming that the dynamics preserves the volume of microstates implies $\Gamma(A \to B) = \Gamma(B \to A)$, and thus

$$\frac{\Gamma(A \to B)}{\Gamma(A)} \ll \frac{\Gamma(B \to A)}{\Gamma(B)} \,. \tag{5.2}$$

The above equation can be viewed as an explanation of the second law, in that it expresses the statistical tendency of the microstates to evolve towards the "typical" set.

Of course, the argument just introduced is nothing more than a qualitative conceptual clarification. Following earlier results [48, 53, 54, 55], rigorous, analytic proof of dynamical thermalization have been obtained recently for weekly interacting systems [51] and, above all, translational invariant systems with finite-range interactions [50].

Given the peculiarities of quantum cellular automata, especially the distinguishing strict causality of information propagation, it is interesting to see whether dynamical thermalization occurs in these systems as well. A loose (see e.g. [52]) but nevertheless legitimate definition of thermalization when in absence of a clear way to define a temperature, reads as follows:

Definition 6 ***Local thermalization*** *Regardless of the initial conditions at time $t_0 = 0$, after a certain time $t > 0$, and for almost all times $t' > t$, any reduced state of a small subsystem of a quantum many-body system evolving unitarily will be in the maximally mixed state, or, equivalently, will have maximal reduced Von Neumann entropy.*

Interpreted in terms of typicality, as a consequence of the structure of the Hilbert space, the above statement is analogue to saying that drawing a state at random from the Haar measure over the unitary group, the larger the Hilbert space, the bigger the probability of the state to be maximally entangled, hence locally thermal.

Although at the time of writing no analytical proof is available, numerical evidence suggest that indeed QCA show local thermalization, in that, with reference to Fig.(5.1), for the overwhelming majority of unitary evolutions of a one-dimensional QCA any small subsystem of the QCA after some equilibration time is characterized by (almost) maximal Von Neumann reduced entropy S.

The plot below is obtained by simulating the evolution of a linear QCA of qubits with periodic boundary conditions, initially prepared in a state of the computational basis $|\Psi\rangle$. At each run, a local two-qubit unitary U is drawn at random from the Haar measure, forming a global evolution G such as in Eq.(3.2). At each time step $0 < t \leq t_{max}$, the Von Neumann reduced entropy $S(\rho_i(t))$ is computed for all qubits i in the chain, where $\rho_i(t) = Tr_{\mathcal{L}\setminus i}\left[G^t|\Psi\rangle\langle\Psi|\left(G^\dagger\right)^t\right]$ are the reduced states. After time t_{max}, the QCA is set back to state $|\Psi\rangle$ and a new local unitary is drawn. The scheme is repeated N times and the algebraic mean of all local entropies $\langle S(\rho_i(t))\rangle = N^{-1}\sum_{n=1}^{N} S_n(\rho_i(t))$ is computed for all i and all t. As can be inferred from the plot – net of an effect due to the finite size of the system which affects the maximum values of the reduced entropies – all locally interacting evolutions $U \in U_{4\times4}$ (except for a set of Haar measure $\varnothing$) show the signs of local thermalization.

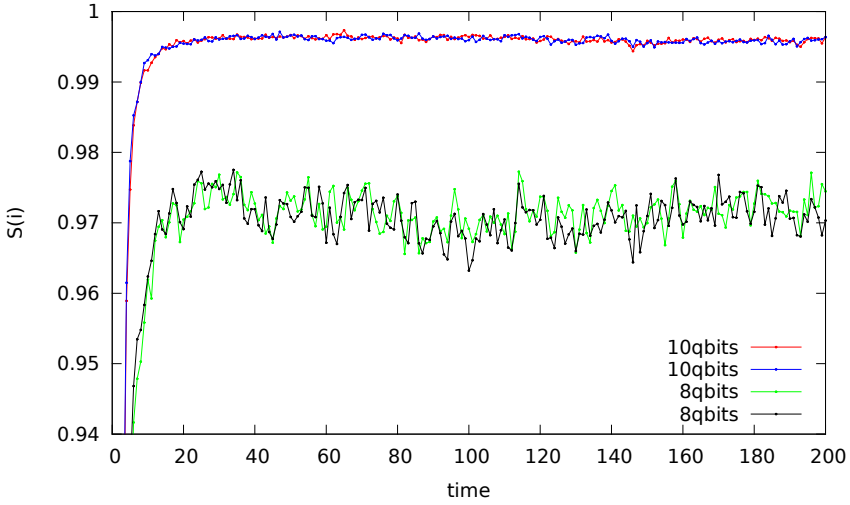


Figure 5.1: Mean Von Neumann reduced entropy $\langle S(\rho_i(t))\rangle$ on one site of a 1-dimensional PQCA of 8 and 10 qubits. Each line refers to an average over an ensemble of 250 different evolutions, each of which given by a different local unitary drawn at random according to the Haar measure. Even for such small size systems the reduced entropy is very close to the maximum value.

Chapter 6

Quantum random scattering interactions

In this chapter we present a modelization of scattering-like processes for discrete quantum systems. Typical properties – i.e. mean values accompanied by bounds on their fluctuations – of the state resulting from the interaction will be estimated through the evaluation of integrals over the Haar measure of the scattering unitaries, together with the use of Levy's lemma. Unlike the case of a usual system-environment bipartition, all expectatation values one can compute within the model turn out to be dependent on the initial global state.

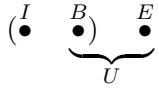
We will first define the model in Sec.(6.1). Results concerning the purity of the typical resulting scattered state will be discussed in Sec.(6.2), followed in Sec.(6.3) by the details of the calculation leading to the equation of the average purity (Eq.(6.4)). The last section of the chapter will deal with the properties of the mean state arising from the interaction.

6.1 The model

Typicality-based arguments, such as in [45], often rely on estimations of relevant quantities through averaging over the Haar measure on the Hilbert space $\mathcal{H}_{\sigma\epsilon} = \mathcal{H}_\sigma \otimes \mathcal{H}_\epsilon$ pertaining to a physical system σ interacting with an environment ϵ. However, as anticipated at the end of Sec.(1.9), although allowing to shed light on general properties and behaviours of quantum systems which otherwise would be lost in either too demanding mathematical formulations or too specific physical

modelizations, actual physical interactions cannot be accurately described by such averaging procedures, as those interactions do not extend over the whole system-*plus*-environment Hilbert space.

Building on the above consideration, a possible step towards a picture in which a certain level of abstraction is retained and a slightly more realistic description of physical interactions is provided may be achieved by restricting the Hilbert space associated to the interaction through making a partitioning of the system into two dynamically-wise distinct components: The main characteristic of the model presented here lies on the fact that only a part of the system interacts with the environment. The global state is tripartite, the system (S) being divided into an inner part I which is sheltered from the environment E and a boundary B that interacts with E. The dimensions of the Hilbert spaces $\mathcal{H}_I$, $\mathcal{H}_B$ and $\mathcal{H}_E$ need not and will not in general be the same. The global state ρ_{IBE} supported on $\mathcal{H}_I \otimes \mathcal{H}_B \otimes \mathcal{H}_E$ undergoes a closed evolution and the scattering interaction between B and E is unitary (see the sketch below).



For any given known initial pure global state, what can be said about the state of the composite system IB after a random, unknown, scattering interaction? In order to answer this question, we define the map:

$$\Phi(\rho_{IBE}) \mapsto \mathrm{Tr}_E \left[\int_{Haar} \mathrm{dU} \left(\mathbb{I}_I \otimes U_{BE} \right) \rho_{IBE} \left(\mathbb{I}_I \otimes U_{BE} \right)^\dagger \right] =: \langle \rho_{IB} \rangle \,, \tag{6.1}$$

where the Haar average over the unitary group takes into account the lack of information about the boundary-environment interaction. Indeed, Eq.(6.1) represents the expectation value over the Haar measure of the reduced IB state after the scattering process. We can also define the expectation value of the purity of the state:

$$\langle \pi(\rho_{IB}) \rangle := \mathrm{Tr}_{IB} \left\{ \int_{Haar} \mathrm{dU} \left[\mathrm{Tr}_E \left(\left(\mathbb{I}_I \otimes U_{BE} \right) \rho_{IBE} \left(\mathbb{I}_I \otimes U_{BE} \right)^\dagger \right) \right]^2 \right\} . \tag{6.2}$$

Both $\langle \rho_{IB} \rangle$ and $\langle \pi(\rho_{IB}) \rangle$ can be calculated and, as we will see in the next sections, the fluctuations around them can be bound by means of Levy's lemma.

6.2 Purity of the reduced scattered state

A remark on notation before starting to present the results of the model. In this section, as well as throughout the rest of the chapter, we will use a convention such that the indices of all matrices and coefficients will always follow the order: inner system-boundary-environment. Also, δ will always represent the Kroneker symbol.

Given the general expression of the initial global (pure) state,

$$\rho_{IBE} = |\Psi\rangle\langle\Psi| = \sum_{ii'bb'ee'} \psi_{ibe}\psi^*_{i'b'e'}|ibe\rangle\langle i'b'e'|\,, \tag{6.3}$$

we obtain:

$$\langle\pi(\rho_{IB})\rangle = \frac{d_B + d_E}{d_B d_E + 1} + \frac{d_B(1 - d_E^2)}{(d_B d_E)^2 - 1}\left(\Delta - \Gamma\right)\,, \tag{6.4}$$

where $d_X := \dim(\mathcal{H}_X)$ and we have defined

$$\Delta := \sum_{\substack{i,i',(be),(be)' \\ i\neq i',(be)\neq(be)'}} |\psi_{i(be)}|^2|\psi_{i'(be)'}|^2 \tag{6.5}$$

$$\Gamma := \sum_{\substack{i,i',(be),(be)' \\ i\neq i',(be)\neq(be)'}} \psi_{i(be)}\psi^*_{i'(be)}\psi_{i'(be)'}\psi^*_{i(be)'} \tag{6.6}$$

The details of the (rather long) calculation can be found in Section (6.3).

Proposition 5 *When the initial system-environment state is separable, the mean purity $\langle\pi(\rho_{IB})\rangle$ only depends on the Schmidt coefficients of the IB bipartition.*

Proof: The initial state $\rho_{IBE} = |\Psi\rangle\langle\Psi|$ is such that

$$|\Psi\rangle = |\Psi_{IB}\rangle \otimes |\Psi_E\rangle = \left(\sum_i^{M_{IB}} c_i|I_i\rangle \otimes |B_i\rangle\right) \otimes \left(\sum_j \xi_j|E_j\rangle\right)\,, \tag{6.7}$$

where $M_{IB} = \min((\dim(\mathcal{H}_I), \dim(\mathcal{H}_B))$. By plugging the coefficients of the above equation into Eq.(6.4) we have that the last term in the sum must (Γ) be null. In fact, by fixing the index "e" and upon recalling that the sum in Eq.(6.4) is over $i \neq i'$, for the last term to be non-zero we should have $ib \neq i'b$, which would imply the existence of more than one Schmidt coefficient for each basis state in the Schmidt

decomposition. So we have:

$$\begin{aligned}
\Delta - \Gamma &= \sum_{\substack{i,i',(be),(be)' \\ i\neq i',(be)\neq(be)'}} \left[|\psi_{i(be)}|^2 |\psi_{i'(be)'}|^2 - \psi_{i(be)}\psi^*_{i'(be)}\psi_{i'(be)'}\psi^*_{i(be)'} \right] \\
&= \sum_{\substack{jklm \\ j\neq l}} |c_j\xi_k|^2 |c_l\xi_m|^2 \\
&= \sum_{\substack{jl \\ j\neq l}} |c_j|^2 |c_l|^2 \sum_k |\xi_k|^2 \sum_m |\xi_m|^2 \\
&= \sum_{\substack{jl \\ j\neq l}} |c_j|^2 |c_l|^2 \,, \qquad (6.8)
\end{aligned}$$

where the last equality follows from the fact that the reduced state of the environment is trace-one. Hence when the initial state is separable such as is Eq.(6.7), the resulting purity is:

$$\langle \pi(\rho_{IB}) \rangle = \frac{d_B + d_E}{d_B d_E + 1} + \frac{d_B(1-d_E^2)}{(d_B d_E)^2 - 1} \sum_{\substack{jl \\ j\neq l}} |c_j|^2 |c_l|^2 \,. \qquad (6.9)$$

□

A direct consequence of Proposition (5) and Eq.(6.9) is that when the initial state of the IB system is also separable, i.e. $|\Psi\rangle = |I\rangle \otimes |B\rangle \otimes |E\rangle$, $M = 1$, we get:

$$\langle \pi(\rho_{IB}) \rangle = \frac{d_B + d_E}{d_B d_E + 1} \,, \qquad (6.10)$$

which is the – well known (see for instance [109]) – result one would get if dealing with a canonical bipartition of the global state between system (with dimension d_B) and environment only. This is actually true regardless the initial correlations between boundary and environment. Indeed, when $|\Psi\rangle = |I\rangle \otimes |BE\rangle = \sum_{i=1}^{d_I} \sum_{j=1}^{M_{BE}} \gamma_i \tau_j |\Gamma_i\rangle |T_j\rangle$:

$$\begin{aligned}
\Delta - \Gamma &= \sum_{ii'jj'} \left[|\gamma_i\tau_j|^2 |\gamma_{i'}\tau_{j'}|^2 - \gamma_i\tau_j\gamma^*_{i'}\tau^*_j\gamma_{i'}\tau_{j'}\gamma^*_i\tau^*_{j'} \right] \\
&= \sum_{ii'jj'} \left[|\gamma_i\tau_j|^2 |\gamma_{i'}\tau_{j'}|^2 - |\gamma_i\tau_j|^2 |\gamma_{i'}\tau_{j'}|^2 \right] \\
&= 0 \,. \qquad (6.11)
\end{aligned}$$

The fundamental difference between our scattering model and the conventional scenario in which the whole system interacts with an environment lies in the fact that in the latter case the expectation value of the purity is independent of the initial state, whilst in the former case, in general, this is clearly not true.[1]

Of course, in order to provide one with insight, the expectation value must be accompanied by an estimate of its variance. In order to bound the fluctuations around the average value of the purity, we will make use of Levy's lemma (a partial derivation of which can be found in Appendix B):

Lemma 1 *(**Levy's lemma**) Given a function $f : S^d \to \mathbb{R}$ defined on the d-dimensional hypersphere $\mathbb{S}^d$, and a point $\phi \in \mathbb{S}^d$ chosen at random,*

$$Prob\left[|f(\phi) - \langle f\rangle| \geq \epsilon\right] \leq 2exp\left(-\frac{(d+1)\epsilon^2}{9\pi^3\eta^2}\right), \tag{6.13}$$

where ϵ is an arbitrarily small positive constant and η is the Lipshitz constant of f, i.e. $\eta : |f(\phi_1) - f(\phi_2)| \leq \eta|\phi_1 - \phi_2|$, $\forall(\phi_1, \phi_2) \in \mathbb{S}^d$.

The above lemma can be applied anytime one deals with pure quantum states, as, for a Hilbert space of dimension d, they live on the surface of a $(2d-1)$ dimensional hypersphere. In our case though, we cannot apply the lemma to the whole Hilbert space, where the global state lives, because initial states will lead in general to different expectation values. We thus have to bound the fluctuations around each of them, meaning that *for each initial state* Levy's lemma is intended to be applied to the surface of the $(2d_Bd_E-1)$-dimensional hypersphere generated by the non-trivial part of the system-environment interaction $\{\mathbb{I}_I \otimes U_{BE}\}$. Therefore, for the purity of each initial state $\rho^\phi = |\phi\rangle\langle\phi|$, Eq.(6.13) reads:

$$\text{Prob}\left[|\pi(\rho^\phi_{IB}) - \langle\pi(\rho^\phi_{IB})\rangle| \geq \epsilon\right] \leq 2\text{exp}\left(-\frac{2d_Bd_E\epsilon^2}{9\eta^2\pi^3}\right), \tag{6.14}$$

where $\pi(\rho^\phi_{IB}) = \text{Tr}_{IB}\left[\text{Tr}_E\left(\left(\mathbb{I}_I \otimes U_{BE}\right)\rho^\phi\left(\mathbb{I}_I \otimes U_{BE}\right)^\dagger\right)^2\right]$. For the Lipschitz constant of the purity, we have the following lemma:

[1] Not even in the limit of infinite dimension of the environment:

$$\lim_{d_E\to\infty}\langle\pi(\rho_{IB})\rangle = \frac{1}{d_B}\left(1 - \Delta + \Gamma\right). \tag{6.12}$$

Lemma 2 *The Lipschitz constant η of the function $f(\phi) = Tr_S\left(\rho_S^2\right)$ satisfies $\eta \leq 4$.*

Proof: Defining the reduced states $\rho_1 = \mathrm{Tr}_E(|\phi_1\rangle\langle\phi_1|)$ and $\rho_2 = \mathrm{Tr}_E(|\phi_2\rangle\langle\phi_2|)$, where in light of the consideration above, for any fixed state $\rho = |\phi\rangle\langle\phi|$ defined in $\mathcal{H}_I \otimes \mathcal{H}_B \otimes \mathcal{H}_E$, $|\phi_1\rangle\langle\phi_1|$ and $|\phi_2\rangle\langle\phi_2|$ are given by any two partial rotations

$$|\phi_1\rangle\langle\phi_1| = \left(\mathbb{I}_I \otimes U_{BE}^{(1)}\right) |\phi\rangle\langle\phi| \left(\mathbb{I}_I \otimes U_{BE}^{(1)}\right)^\dagger, \quad |\phi_2\rangle\langle\phi_2| = \left(\mathbb{I}_I \otimes U_{BE}^{(2)}\right) |\phi\rangle\langle\phi| \left(\mathbb{I}_I \otimes U_{BE}^{(2)}\right)^\dagger, \tag{6.15}$$

one has:

$$\begin{aligned} |f(\phi_1) - f(\phi_2)| &= |\mathrm{Tr}_S(\rho_1^2) - \mathrm{Tr}_S(\rho_2^2)| \\ &= |\mathrm{Tr}_S\left[(\rho_1 - \rho_2)\rho_2\right] + \mathrm{Tr}_S\left[\rho_1(\rho_1 - \rho_2)\right]| \\ &\leq 2\|\rho_1 - \rho_2\|_1 \\ &\leq 2\||\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|\|_1 \\ &= 4\sqrt{1 - |\langle\phi_1|\phi_2\rangle|^2} \\ &\leq 4||\phi_1\rangle - |\phi_2\rangle|, \end{aligned} \tag{6.16}$$

where in the first inequality we have used $|\mathrm{Tr}(CD)| \leq \|C\|_1 \cdot \|D\|_{op}$ (with $\|\cdot\|_{op}$ the operator norm), while the second inequality follows from the monotonicity of the trace norm under partial trace.

□

Therefore, when the dimension of the Hilbert space is large, the fluctuations around the average value of the purity will be small. That of course includes the physically relevant case in which a small quantum system interacts with a large environment, such as spins interacting with harmonic oscillators.

We have checked numerically the validity of Eqs.(6.4,6.14) when the initial state is prepared as a GHZ and a W state. For N qubits, these two states, which are important for the study of multipartite entanglement [64], are defined as:

$$|GHZ\rangle_N = \frac{1}{\sqrt{2}}\left(|0\rangle^{\otimes N} + |1\rangle^{\otimes N}\right), \tag{6.17}$$

$$|W\rangle_N = \frac{1}{\sqrt{N}}\left(|100\ldots0\rangle + |01\ldots0\rangle + \cdots + |00\ldots1\rangle\right) \tag{6.18}$$

Defining $\rho^{GHZ} = |GHZ\rangle\langle GHZ|_N$ and $\rho^{W} = |W\rangle\langle W|_N$, a direct calculation leads to:

$$\begin{aligned} \langle \pi(\rho_{IB}^{GHZ}) \rangle &= \frac{d_B + d_E}{d_B d_E + 1} + \frac{d_B(1-d_E^2)}{(d_B d_E)^2 - 1} \cdot \frac{1}{2} \\ \langle \pi(\rho_{IB}^{W}) \rangle &= \frac{d_B + d_E}{d_B d_E + 1} + \frac{d_B(1-d_E^2)}{(d_B d_E)^2 - 1} \cdot \frac{2\left[\log_2 D - 1\right]}{(\log_2 D)^2} \,, \end{aligned} \tag{6.19}$$

where $D = d_I d_B d_E = 2^N$.

We have also considered the case where three-qubit GHZ and W states interact with an $N_E = N - 3$ qubit environment prepared in a fiducial state: $\tilde{\rho}^{GHZ} := |GHZ\rangle\langle GHZ|_3 \otimes |0\rangle\langle 0|_E^{\otimes(N-3)}$, $\tilde{\rho}^{W} := |W\rangle\langle W|_3 \otimes |0\rangle\langle 0|_E^{\otimes(N-3)}$, finding

$$\langle \pi(\tilde{\rho}_{IB}^{GHZ}) \rangle = \langle \pi(\rho_{IB}^{GHZ}) \rangle \,, \quad \langle \pi(\tilde{\rho}_{IB}^{W}) \rangle = \frac{d_B + d_E}{d_B d_E + 1} + \frac{d_B(1-d_E^2)}{(d_B d_E)^2 - 1} \cdot \frac{4}{9} \,. \tag{6.20}$$

As can be appreciated in Fig.(6.1), the fluctuations around the expected value of

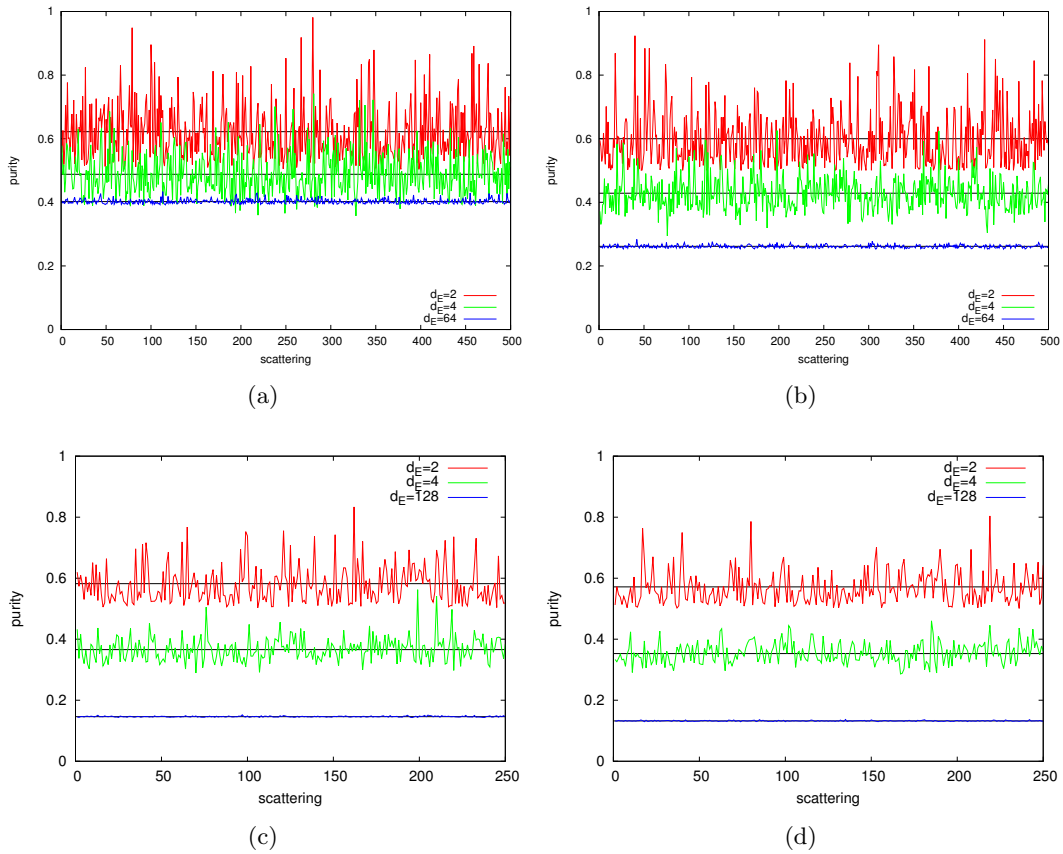


Figure 6.1: Purity of the state resulting from a random scattering boundary-environment interaction for (see Eqs.(6.19,6.20)) (a) ρ^{W}, (b) ρ^{GHZ}, (c) $\tilde{\rho}^{W}$, (d) $\tilde{\rho}^{GHZ}$ initial states. Each value on the x axis labels a different U_{BE} random extraction. The straight horizontal lines in the plots represent the expected values of the purity, computed with Eqs.(6.19), 6.20, where in (a),(b) $d_I = d_B = 2$, whereas in (c),(d) $d_I = 2$, $d_B = 4$.

π are quite large for an environment composed of $N_E = 1$, $N_E = 2$ qubits, but are almost completely damped already for $N_E = 6$.

6.3 Computing the expectation value of the purity

Here we explicitely show how to get to Eq.(6.4). Substituting Eq.(6.3) into Eq.(6.2) and expressing the scattering unitaries in terms of their components in the BE basis, $U_{BE} = \sum_{i,k=1}^{d_B} \sum_{j,l=1}^{d_E} U_{(ij)(kl)} |ij\rangle\langle kl|$:

$$\begin{aligned}
\langle \pi(\rho_{IB}) \rangle &= \mathrm{Tr}_{IB} \left\{ \int_H \mathrm{dU} \left[\mathrm{Tr}_E \left((\mathbb{I}_I \otimes U_{BE}) \, \rho_{IBE} \, (\mathbb{I}_I \otimes U_{BE})^\dagger \right) \right]^2 \right\} \\
&= \int_H \mathrm{dU} \sum_{\gamma\gamma'\beta\beta'\xi\xi'} \langle (\gamma\beta)\xi | \sum_{\substack{ibe \\ i'b'e'}} \sum_{\substack{jklm \\ nopq}} \psi_{ibe} \psi^*_{i'b'e'} U_{(jk)(lm)} U^*_{(pq)(no)} |jk\rangle\langle lm| \\
&\cdot \quad |ibe\rangle\langle i'b'e'| \cdot |no\rangle\langle pq| \cdot |(\gamma'\beta')\xi\rangle\langle(\gamma'\beta')\xi'| \sum_{\substack{i^2b^2e^2 \\ i^3b^3e^3}} \sum_{\substack{rstu \\ vwxy}} \psi_{i^2b^2e^2} \psi^*_{i^3b^3e^3} \\
&\cdot \quad U_{(rs)(tu)} U^*_{(xy)(vw)} |rs\rangle\langle tu| \cdot |i^2b^2e^2\rangle\langle i^3b^3e^3| \cdot |vw\rangle\langle xy| \cdot |(\gamma'\beta')\xi\rangle\langle(\gamma\beta)\xi'| \\
&= \sum_{\gamma\gamma'\beta\beta'\xi\xi'} \sum_{\substack{be b'e' \\ b^2e^2b^3e^3}} \psi_{\gamma be} \psi^*_{\gamma b'e'} \psi_{\gamma' b^2e^2} \psi^*_{\gamma b^3e^3} \\
&\cdot \quad \int_H \mathrm{dU} \left[U^*_{(\beta'\xi)(b'e')} U^*_{(\beta\xi')(b^3e^3)} U_{(\beta\xi)(be)} U_{(\beta'\xi')(b^2e^2)} \right] \\
&\equiv I + J \,, \qquad (6.21)
\end{aligned}$$

where we have split the sum into two components

$$\begin{aligned}
I &:= \sum_{\gamma\beta\beta'\xi\xi'} \sum_{n_0n_1n_2n_3} \psi_{\gamma n_0} \psi^*_{\gamma n_1} \psi_{\gamma n_2} \psi^*_{\gamma n_3} \int_H \mathrm{dU} \left[U^*_{(\beta'\xi)n_1} U^*_{(\beta\xi')n_3} U_{(\beta\xi)n_0} U_{(\beta'\xi')n_2} \right] \\
J &:= \sum_{\substack{\gamma\gamma'\beta\beta'\xi\xi' \\ (\gamma\neq\gamma')}} \sum_{n_0n_1n_2n_3} \psi_{\gamma n_0} \psi^*_{\gamma' n_1} \psi_{\gamma' n_2} \psi^*_{\gamma n_3} \int_H \mathrm{dU} \left[U^*_{(\beta'\xi)n_1} U^*_{(\beta\xi')n_3} U_{(\beta\xi)n_0} U_{(\beta'\xi')n_2} \right] . \qquad (6.22)
\end{aligned}$$

In the above equalities we have also shortened the notation, merging the boundary and environment indices pertaining to both the coefficients of $|\Psi\rangle$ and U into a single

$\sum_{n_0n_1n_2n_3}$	$\mathbf{I}(\xi \neq \xi')$	$\mathbf{II}(\beta \neq \beta')$	$\mathbf{III}(\beta\xi = \beta'\xi')$
$n_0 = n_1 \neq n_2 = n_3$	$d_B d_E(d_E - 1)\cdot$(B.5)	$d_B d_E(d_B - 1)\cdot$(B.5)	$d_B d_E\cdot$(B.7)
$n_0 = n_3 \neq n_1 = n_2$	$d_B d_E(d_E - 1)\cdot$(B.6)	$d_B d_E(d_B - 1)\cdot$(B.6)	$d_B d_E\cdot$(B.7)
$n_0 = n_1 = n_2 = n_2$	$d_B d_E(d_E - 1)\cdot$(B.8)	$d_B d_E(d_B - 1)\cdot$(B.8)	$d_B d_E\cdot$(B.9)

Table 6.1: Decomposition of I into a sum of the non-zero integrals Eqs.(B.5-B.9). In the second to fourth columns, each of these factors is multiplied by their multiplicity.

one. Let us take care of I first.

$$
\begin{aligned}
I \;=\; & \underbrace{\sum_{\substack{\gamma\beta\xi\xi' \\ \xi\neq\xi'}} \sum_{n_0n_1n_2n_3} \psi_{\gamma n_0}\psi^*_{\gamma n_1}\psi_{\gamma n_2}\psi^*_{\gamma n_3} \int_H \mathrm{dU}\left[U^*_{(\beta\xi)n_1}U^*_{(\beta\xi')n_3}U_{(\beta\xi)n_0}U_{(\beta\xi')n_2}\right]}_{=:\mathbf{I}(\xi\neq\xi')} + \\
& \underbrace{\sum_{\substack{\gamma\beta\beta'\xi \\ \beta\neq\beta'}} \sum_{n_0n_1n_2n_3} \psi_{\gamma n_0}\psi^*_{\gamma n_1}\psi_{\gamma n_2}\psi^*_{\gamma n_3} \int_H \mathrm{dU}\left[U^*_{(\beta'\xi)n_1}U^*_{(\beta\xi)n_3}U_{(\beta\xi)n_0}U_{(\beta'\xi)n_2}\right]}_{=:\mathbf{II}(\beta\neq\beta')} + \\
& \underbrace{\sum_{\gamma\beta\xi} \sum_{n_0n_1n_2n_3} \psi_{\gamma n_0}\psi^*_{\gamma n_1}\psi_{\gamma n_2}\psi^*_{\gamma n_3} \int_H \mathrm{dU}\left[U^*_{(\beta\xi)n_1}U^*_{(\beta\xi)n_3}U_{(\beta\xi)n_0}U_{(\beta\xi)n_2}\right]}_{=:\mathbf{III}(\beta\xi=\beta'\xi')} .
\end{aligned}
\tag{6.23}
$$

We should now further decompose the sums above to get to a sum of integrals like Eq.s(B.5-B.9) of Appendix B. Writing it down explicitly would be rather unmanageable, though. Arguably the best way to work it out is to group the decomposition into a table. Using Tab.(6.1), after a little bookkeeping we obtain

$$
\begin{aligned}
I \;&=\; (d(d_E-1)+d(d_B-1))\left(\sum_{\substack{n_0n_2\gamma \\ n_0\neq n_2}} \frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma n_2}|^2}{d(d+1)} + \sum_{n_0\gamma}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma n_0}|^2}{d(d+1)}\right) \\
&+\; 2d\left(\sum_{\substack{n_0n_2\gamma \\ n_0\neq n_2}} \frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma n_2}|^2}{d(d+1)} + \sum_{n_0\gamma}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma n_0}|^2}{d(d+1)}\right) \\
&=\; d(d_E+d_B)\left(\sum_{\substack{n_0n_2\gamma \\ n_0\neq n_2}} \frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma n_2}|^2}{d(d+1)} + \sum_{n_0\gamma}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma n_0}|^2}{d(d+1)}\right),
\end{aligned}
\tag{6.24}
$$

with $d = d_E d_B$.

We can do exactly the same thing with J. First, decompose the sum as in

Eq.(6.23)

$$
\begin{aligned}
J \;=\; & \underbrace{\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{\beta\xi\xi'\\ \xi\neq\xi'}}\sum_{n_0n_1n_2n_3}\psi_{\gamma n_0}\psi^*_{\gamma' n_1}\psi_{\gamma' n_2}\psi^*_{\gamma n_3}\int_H \mathrm{dU}\left[U^*_{(\beta\xi)n_1}U^*_{(\beta\xi')n_3}U_{(\beta\xi)n_0}U_{(\beta\xi')n_2}\right]+}_{\mathbf{I}(\xi\neq\xi')}\\
& \underbrace{\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{\beta\beta'\xi\\ \beta\neq\beta'}}\sum_{n_0n_1n_2n_3}\psi_{\gamma n_0}\psi^*_{\gamma' n_1}\psi_{\gamma' n_2}\psi^*_{\gamma n_3}\int_H \mathrm{dU}\left[U^*_{(\beta'\xi)n_1}U^*_{(\beta\xi)n_3}U_{(\beta\xi)n_0}U_{(\beta'\xi)n_2}\right]+}_{\mathbf{II}(\beta\neq\beta')}\\
& \underbrace{\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\beta\xi}\sum_{n_0n_1n_2n_3}\psi_{\gamma n_0}\psi^*_{\gamma' n_1}\psi_{\gamma' n_2}\psi^*_{\gamma n_3}\int_H \mathrm{dU}\left[U^*_{(\beta\xi)n_1}U^*_{(\beta\xi)n_3}U_{(\beta\xi)n_0}U_{(\beta\xi)n_2}\right],}_{\mathbf{III}(\beta\xi=\beta'\xi')}
\end{aligned}
\tag{6.25}
$$

and then use Tab.(6.1) (the integrals are the same of Eq.(6.23)) to obtain, after some algebra,

$$
\begin{aligned}
J \;=\; & dd_B\left(\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{n_0n_2\\ n_0\neq n_2}}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_2}|^2}{d^2-1}-\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{n_0n_2\\ n_0\neq n_2}}\frac{\psi_{\gamma n_0}\psi^*_{\gamma' n_0}\psi_{\gamma' n_2}\psi^*_{\gamma n_2}}{d(d^2-1)}+\sum_{\substack{n_0\gamma\gamma'\\ \gamma\neq\gamma'}}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_0}|^2}{d(d+1)}\right)\\
+\; & dd_E\left(\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{n_0n_2\\ n_0\neq n_2}}\frac{\psi_{\gamma n_0}\psi^*_{\gamma' n_0}\psi_{\gamma' n_2}\psi^*_{\gamma n_2}}{d^2-1}-\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{n_0n_2\\ n_0\neq n_2}}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_2}|^2}{d(d^2-1)}+\sum_{\substack{n_0\gamma\gamma'\\ \gamma\neq\gamma'}}\frac{|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_0}|^2}{d(d+1)}\right).
\end{aligned}
\tag{6.26}
$$

Now, putting it all together and rearranging a bit:

$$
\begin{aligned}
I+J \;=\; & \left(\sum_{\substack{\gamma n_0n_2\\ n_0\neq n_2}}|\psi_{\gamma n_0}|^2|\psi_{\gamma n_2}|^2+\sum_{\gamma n_0}|\psi_{\gamma n_0}|^2|\psi_{\gamma n_0}|^2+\sum_{\substack{\gamma\gamma' n_0\\ \gamma\neq\gamma'}}|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_0}|^2\right.\\
& \left.+\;\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{n_0n_2\\ n_0\neq n_2}}|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_2}|^2\right)\frac{d_B+d_E}{d+1}\\
& +\;\frac{d_B-dd_E}{d^2-1}\sum_{\substack{\gamma\gamma'\\ \gamma\neq\gamma'}}\sum_{\substack{n_0n_2\\ n_0\neq n_2}}\left(|\psi_{\gamma n_0}|^2|\psi_{\gamma' n_2}|^2-\psi_{\gamma n_0}\psi^*_{\gamma' n_0}\psi_{\gamma' n_2}\psi^*_{\gamma n_2}\right).
\end{aligned}
\tag{6.27}
$$

Notice that what is inside the brakets in the first and second line of the above

equation is the trace of the global state, so we finally have

$$\langle \pi(\rho_{IB}) \rangle = \frac{d_B + d_E}{d_E d_B + 1} + \frac{d_B(1+d_E^2)}{(d_E d_B)^2 - 1} \sum_{\substack{\gamma\gamma' \\ \gamma \neq \gamma'}} \sum_{\substack{n_0 n_2 \\ n_0 \neq n_2}} \left(|\psi_{\gamma n_0}|^2 |\psi_{\gamma' n_2}|^2 - \psi_{\gamma n_0} \psi^*_{\gamma' n_0} \psi_{\gamma' n_2} \psi^*_{\gamma n_2} \right) . \tag{6.28}$$

6.4 The scattering map

The scattering map Eq.(6.1) has the effect of totally suppressing any initial correlation between the boundary and the inner part of the system.

Proposition 6 *For any given initial state ρ_{IBE}, the expectation value over the Haar measure of the reduced IB state after the scattering interaction defined in Eq.(6.1) is a separable state such that:*

$$\langle \rho_{IB} \rangle = \rho_I \otimes \overline{\rho}_B \, , \tag{6.29}$$

with

$$\rho_I = Tr_{BE}(\rho_{IBE}) \quad and \quad \overline{\rho}_B = \frac{1}{d_B} \sum_{\beta=1}^{d_B} |\beta\rangle\langle\beta| \, . \tag{6.30}$$

Proof: Substituting Eq.(6.3) into Eq.(6.1) and expressing the scattering unitaries in terms of their components in the BE basis, $U_{BE} = \sum_{i,k=1}^{d_B} \sum_{j,l=1}^{d_E} U_{(ij)(kl)} |ij\rangle\langle kl|$:

$$\begin{aligned}
\Phi(\rho_{IBE}) \;\; \mapsto \;\; & \mathrm{Tr}_E \left[\int_H \mathrm{dU} \, (\mathbb{I}_I \otimes U_{BE}) \, \rho_{IBE} \, (\mathbb{I}_I \otimes U_{BE})^\dagger \right] \\
= \;\; & \sum_{\xi=1}^{d_E} \langle \xi | \int_H \mathrm{dU} \sum_{\substack{jklm \\ mnop}} \sum_{\substack{sbe \\ s'b'e'}} U_{(ij)(kl)} \psi_{sbe} |ij\rangle\langle kl| \cdot |sbe\rangle\langle s'b'e'| \\
\cdot \;\; & |mn\rangle\langle op| \psi^*_{s'b'e'} U^*_{(op)(mn)} |\xi\rangle \\
= \;\; & \sum_{\xi=1}^{d_E} \sum_{\substack{jklm \\ mnop}} \sum_{\substack{sbe \\ s'b'e'}} \psi_{sbe} \psi^*_{s'b'e'} \underbrace{\langle \xi | \cdot |ij\rangle\langle kl| \cdot |sbe\rangle\langle s'b'e'| \cdot |mn\rangle\langle op| \cdot |\xi\rangle}_{\delta^\xi_j \delta^k_b \delta^l_e \delta^m_{b'} \delta^m_{e'} \delta^\xi_o} \\
\cdot \;\; & \int_H \mathrm{dU} \left[U^*_{(op)(mn)} U_{(ij)(kl)} \right] \\
= \;\; & \sum_{\xi=1}^{d_E} \sum_{\substack{sbe \\ s'b'e'}} \sum_{io} \psi_{sbe} \psi^*_{s'b'e'} |si\rangle\langle s'o| \int_H \mathrm{dU} \left[U^*_{(o\xi)(b'e')} U_{(i\xi)(be)} \right] \\
= \;\; & \sum_{\xi=1}^{d_E} \sum_{\substack{sbe \\ s'b'e'}} \sum_{io} \psi_{sbe} \psi^*_{s'b'e'} |si\rangle\langle s'o| \frac{1}{d_B d_E} \delta^o_i \delta^{be}_{b'e'}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{d_B d_E} \sum_{\xi ss'bei} \psi_{sbe}\psi^*_{s'be}|si\rangle\langle s'i| \\
&= \sum_{ss'be} \psi_{sbe}\psi^*_{s'be}|s\rangle\langle s'| \otimes \frac{1}{d_B}\sum_{i=1}^{d_B}|i\rangle\langle i| \\
&= \rho_I \otimes \overline{\rho}_B \,, \qquad (6.31)
\end{aligned}
$$

where for the fourth equality we have used the results of Appendix B.

□

The Haar-averaged state is thus such that: $\mathrm{Tr}_B\left(\langle\rho_{IB}\rangle\right) = \mathrm{Tr}_{BE}\left(\rho_{IBE}\right)$ and $\mathrm{Tr}_I\left(\langle\rho_{IB}\rangle\right) = \overline{\rho}_B$, where $\overline{\rho}_B$ is maximally mixed. Both results were expected. The first one following from the fact that the interaction does not involve the inner part of the system and therefore cannot change its reduced state; the second one is equivalent to what one would get if we were calculating the Haar-averaged reduced state of the system within the usual, non-tripartite, system-environment interaction framework (see Appendix B). However, notice that these two conditions alone do not imply complete absence of entanglement and classical correlations between the inner and boundary parts of the system.

As for the purity, we need to bound the fluctuations around the mean state $\langle\rho_{IB}\rangle$. To this aim, analogously to what Popescu *et al.* do in Ref.[45], we can apply Levy's lemma to the trace distance $f(\phi) = \|\mathrm{Tr}_E\left[\left(\left(\mathbb{I}_I \otimes U_{BE}\right)\rho_\phi\left(\mathbb{I}_I \otimes U_{BE}\right)^\dagger\right] - \Phi\left(\rho_\phi\right)\|_1 \equiv \|R(\rho_\phi) - \Phi\left(\rho_\phi\right)\|_1$, with $\rho_\phi = |\phi\rangle\langle\phi|$ defined in $\mathcal{H}_I \otimes \mathcal{H}_B \otimes \mathcal{H}_E$ and Φ the scattering map of Eq.(6.1). Levy's lemma applied to $f(\phi)$ then reads:

$$
\mathrm{Prob}\left[\left|\|R(\rho_\phi) - \Phi\left(\rho_\phi\right)\|_1 - \langle\|R(\rho_\phi) - \Phi\left(\rho_\phi\right)\|_1\rangle\right| \geq \epsilon\right] \leq 2\mathrm{exp}\left(-\frac{2d_B d_E \epsilon^2}{9\pi^3\eta}\right). \qquad (6.32)
$$

It is convenient to rearrange Eq.(6.32) such that we get to an expression of the form:

$$
\mathrm{Prob}\left[\|R(\rho_\phi) - \Phi\left(\rho_\phi\right)\|_1 \geq \gamma\right] \leq \gamma' \,, \qquad (6.33)
$$

where

$$
\gamma = \epsilon + \langle\|R(\rho_\phi) - \Phi\left(\rho_\phi\right)\|_1\rangle \,, \quad \gamma' = 2\mathrm{exp}\left(-\frac{2d_B d_E \epsilon^2}{9\pi^3\eta}\right). \qquad (6.34)
$$

So in order to estimate the fluctuations around the mean state we need to bound $\langle \| R(\rho_\phi) - \Phi(\rho_\phi) \|_1 \rangle$. As shown in Sec.(1.8.2), the Hilbert-Schmidt norm $\|M\|_2 = \sqrt{\mathrm{Tr}(M^\dagger M)}$ and the trace norm $\|M\|_1 = \mathrm{Tr}\sqrt{M^\dagger M}$ satisfy, for any $n \times n$ matrix M, the relation: $\|M\|_1^2 \leq n \|M\|_2^2$. That is extremely helpful, as we can now switch to the much more mathematically-gentle HS norm and go back to the trace norm just at the end of the calculation. We thus have:

$$\begin{aligned}
\langle \| R(\rho_\phi) - \Phi(\rho_\phi) \|_2 \rangle &\leq \sqrt{\langle \| R(\rho_\phi) - \Phi(\rho_\phi) \|_2^2 \rangle} \\
&= \sqrt{\langle \mathrm{Tr}_{IB} \left[(R(\rho_\phi) - \Phi(\rho_\phi))^2 \right] \rangle} \\
&= \sqrt{\langle \mathrm{Tr}_{IB} (R(\rho_\phi)^2) \rangle + \langle \mathrm{Tr}_{IB} (\Phi(\rho_\phi)^2) \rangle - 2\mathrm{Tr}_{IB} (\langle R(\rho_\phi) \rangle \Phi(\rho_\phi))} \\
&= \sqrt{\langle \mathrm{Tr}_{IB} (R(\rho_\phi)^2) \rangle - \mathrm{Tr}_{IB} (\Phi(\rho_\phi)^2)} \,.
\end{aligned} \tag{6.35}$$

That is, the desired bound is given by (the square root of) the difference between the mean purity and the purity of the Haar-averaged state. Writing the average state as in the second to last line of Eq.(6.31), the latter is:

$$\begin{aligned}
\mathrm{Tr}_{IB} \left(\Phi(\rho)^2 \right) &= \frac{1}{d_B^2} \sum_{\sigma\sigma'\beta\beta'} \langle \sigma\beta | \sum_{\substack{ii'i^2i^3ee^2 \\ bb'b^2b^3}} \psi_{ibe} \psi^*_{i'be} |ib'\rangle\langle i'b'| \cdot |\sigma'\beta'\rangle\langle\sigma'\beta'| \\
&\cdot \quad \psi_{i^2b^2e^2} \psi^*_{i^3b^2e^2} |i^2b^3\rangle\langle i^3b^3| \cdot |\sigma\beta\rangle \\
&= \frac{1}{d_B^2} \sum_{\sigma\sigma' bb^2ee^2\beta} \psi_{\sigma be} \psi^*_{\sigma' be} \psi_{\sigma' b^2e^2} \psi^*_{\sigma b^2 e^2} \\
&= \frac{1}{d_B} \sum_{ii'(be)(be)'} \psi_{i(be)} \psi^*_{i'(be)} \psi_{i'(be)'} \psi^*_{i(be)'}
\end{aligned} \tag{6.36}$$

On the other hand, looking at the last term of the average purity, by decomposing the sum and using $\mathrm{Tr}(\rho) = 1$ we have:

$$\Delta - \Gamma = 1 - \sum_{ii'(be)(be)'} \psi_{i(be)} \psi^*_{i'(be)} \psi_{i'(be)'} \psi^*_{i(be)'} \,, \tag{6.37}$$

hence, defining $A = \sum_{ii'(be)(be)'} \psi_{i(be)} \psi^*_{i'(be)} \psi_{i'(be)'} \psi^*_{i(be)'}$[2],

$$\langle \mathrm{Tr}_{IB} \left(R(\rho_\phi)^2 \right) \rangle - \mathrm{Tr}_{IB} \left(\Phi(\rho_\phi)^2 \right) = \frac{d_B + d_E}{d_B d_E + 1} + \frac{d_B (1 - d_E^2)}{(d_B d_E)^2 - 1}$$

[2]Notice that $A \in \left[\frac{1}{d_I}, d_B \right]$ (cf. Eq.(6.36)).

$$
\begin{aligned}
&- \left[\frac{d_B(1-d_E^2)}{(d_B d_E)^2-1}+\frac{1}{d_B}\right] A \\
&= \frac{(d_B^2-1)(d_E+A)}{d_B\left[(d_B d_E)^2-1\right]}\,. \qquad (6.38)
\end{aligned}
$$

Therefore, finally, switching back to the trace norm:

$$
\begin{aligned}
\langle \| R(\rho_\phi) - \Phi\left(\rho_\phi\right) \|_1 \rangle &\leq d_I d_B \langle \| R(\rho_\phi) - \Phi\left(\rho_\phi\right) \|_2 \rangle \\
&\leq \sqrt{\frac{d_I(d_B^2-1)(d_E+A)}{(d_B d_E)^2-1}}\,. \qquad (6.39)
\end{aligned}
$$

We have then that when $d_E \gg d_I d_B$:

$$
\langle \| R(\rho_\phi) - \Phi\left(\rho_\phi\right) \|_1 \rangle \leq \sqrt{\frac{d_I}{d_E}}\,. \qquad (6.40)
$$

To complete the Levy's bound we are looking for, we make use of the following lemma:

Lemma 3 *For any given $\rho = |\phi\rangle\langle\phi|$ and for any unitary U_{BE}, the Lipschitz constant η of the function $f(\phi) = \| Tr_E \left[\left(\left(\mathbb{I}_I \otimes U_{BE}\right) \rho_\phi \left(\mathbb{I}_I \otimes U_{BE}\right)^\dagger \right] - \Phi\left(\rho_\phi\right) \|_1 \equiv \| R(\rho_\phi) - \Phi\left(\rho_\phi\right) \|_1$ satisfies $\eta \leq 2$.*

Proof: Let us use a notation such that ϕ_x identifies the state obtained through rotating by $U_{BE}^{(x)}$, i.e. $|\phi_x\rangle\langle\phi_x| = (\mathbb{I} \otimes U_{BE}^{(x)})|\phi\rangle\langle\phi|(\mathbb{I} \otimes U_{BE}^{(x)})^\dagger$, then

$$
\begin{aligned}
\left| f(\phi_1) - f(\phi_2) \right|^2 &= \left| \|R(\rho_{\phi_1}) - \Phi(\rho_\phi)\|_1 - \|R(\rho_{\phi_2}) - \Phi(\rho_\phi)\|_1 \right|^2 \\
&\leq \|R(\rho_{\phi_1}) - R(\rho_{\phi_2})\|_1^2 \\
&\leq \|\rho_{\phi_1} - \rho_{\phi_2}\|_1^2 \\
&= 4\left(1 - |\langle\phi_1|\phi_2\rangle|^2\right) \\
&\leq 4\||\phi_1\rangle - |\phi_2\rangle\|^2\,, \qquad (6.41)
\end{aligned}
$$

where the first inequality follows from the fact that $\left| \|\sigma_1 - \sigma_0\|_1 - \|\sigma_2 - \sigma_0\|_1 \right|^2 \leq \|\sigma_1 - \sigma_2\|_1^2$, while the second inequality is due to the monotonicity of the trace norm under partial tracing and its invariance under unitary transformations.

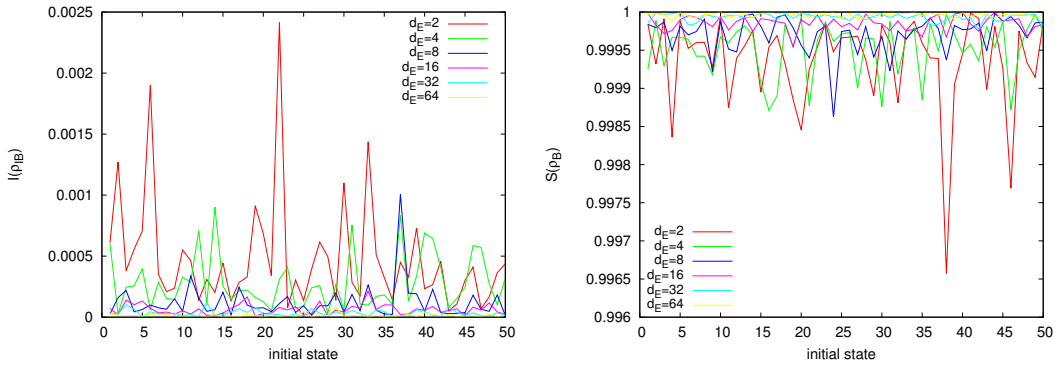
□

Substituting the result of the above Lemma and the inequality Eq.(6.40) in Eq.(6.33) we obtain:

$$\text{Prob}\left[\|R(\rho_\phi)) - \Phi\left(\rho_\phi\right)\|_1 \geq \epsilon + \sqrt{\frac{d_I}{d_E}}\right] \leq 2\text{exp}\left(-\frac{d_B d_E \epsilon^2}{18\pi^3}\right), \tag{6.42}$$

which, in the limit of large environment dimension, bounds the fluctuations around the average state Eq.(6.29).

We have run several simulations to corroborate the validity of Prop.(6). The absence of correlations between the reduced states ρ_I and ρ_B can be checked by computing the mutual information (Eq.(1.29)) $I(\rho_{IB})$, whereas if the reduced state ρ_B is actually maximally mixed as in Eq.(6.30) can be verified by calculating its Von Neumann reduced entropy (Eq.(1.23)) $S(\rho_B)$. As can be appreciated in Fig.(6.2), our numerical results are in very good agreement with Prop.(6).



(a) (b)

Figure 6.2: Average values of (a) mutual information and (b) Von Neumann entropy of the reduced inner-boundary state. For each one of the 50 random initial states (with $d_I = d_B = 2$), the average is taken over 250 random drawings of a scattering interaction U_{BE}.

Summary and outlook

The work presented in this thesis was aimed at addressing several different problems, drawn from the contexts of quantum biology, quantum communication and typicality approaches to interactions in closed quantum systems, within the framework of discrete quantum systems governed by discrete-time evolutions.

Inspired by the recent years' growing interest in understanding whether some biological systems may or may not be affected by quantum effects, we began by introducing a strictly local model of energy transfer via a noisy quantum cellular automaton construction on a qubit lattice. To do so, we first considered the problem of constructing a class of one-qubit completely positive maps that, in a certain limit, reproduce all classical Markov transition matrices on dichotomic probability distributions. We then applied our construction to the first excitation subspace of a partitioned quantum cellular automaton structure, where one-qubit maps can be applied to the two-dimensional space spanned by excitations at neighboring sites, obtaining a global dynamics on a lattice which is capable of describing excitation transfer. Tuning one real parameter of such a model – the dephasing strength parameter, which arguably represents the most natural decoherence mechanism in several practical cases – allows one to range from a classical Markov chain, where quantum coherence is systematically suppressed at each time step of the automaton, to dynamics where quantum coherence is allowed to build up over time, while keeping, by construction, the local transition probabilities constant. Thus, a "fair" comparison between classical and quantum energy transfer may be carried out, where the effect of quantum interference is singled out with no ambiguity. We have then presented a study of the performance of classical versus quantum maps, showing by how much and under what conditions does quantum coherence improve the probability of excitation transfer through the lattice. The model is capable of highlighting coherent effects, such as noise-assistance, can be applied to very large systems and allows one

to treat conditional quantum dynamics exactly.

Next, we addressed the problem of quantum state transfer. Keeping the same QCA dynamics used for excitation transport, we enlarged the Hilbert space to allow for transport of initial coherences as well, finding the conditions selecting the class of proper – causal and translational invariant – noisy QCA out of all possible dynamics in the $0 \oplus 1$ sector. The extension of the automata to the vacuum state grants the possibility to consider the effect of the quantum to classical transition on on-site coherences. As shown through numerical simulations, there are instances of the dynamics in which a transfer fidelity larger than the classical threshold is achievable. We have then discussed the role played by the different parameters characterizing the dynamics. In particular we show the existence of an optimal choice of the free phases (ϕ_1, ϕ_2) parametrizing the local evolution, that allows for perfect state transfer. We then highlighted the different impact of the sources of noise taken into account, in particular amplitude damping and dephasing, on excitation transfer and quantum state transfer: while in the first case noise can sometimes be beneficial, for the latter it proves always detrimental. Note that the capability of transferring a quantum state with high fidelity mirrors the ability to transmit quantum entanglement, so that the possibility to distribute entanglement between different lattice sites is implied in this study.

It is reasonable to expect that the application of the framework developed here may be extended to other general communication problems, such as quantum and classical capacities [110]. Indeed, from a more general perspective, the results shown suggest that QCA are a new and potentially interesting alternative scheme to model relevant processes for quantum communication.

Back to the full 2^N Hilbert space, we have then presented another possible application of the QCA framework, namely the investigation of thermalization in closed quantum systems. Numerical results – obtained by computing the mean reduced Von Neumann entropy of small parts of one-dimensional quantum cellular automata over an ensemble of evolutions drawn at random according to the Haar measure – point towards conjecturing local thermalization in those systems, and in the future it would be desirable to find analytical proof that would reinforce the results of [50].

Finally, abandoning QCA, we have introduced a modelization of random scattering-

like processes for discrete quantum systems. In the model, a global pure state is tripartite and the system-environment (unitary) interaction involves only a part – which can be regarded as the "boundary" – of the system. For each initial state, although the interaction is unknown, the purity of the scattered reduced state (where the environment is traced out), as well as the form of the state itself can be analytically evaluated by exploiting properties of the Haar measure over the unitary group, while the fluctuations around the calculated mean values can be bound by means of the Levy's lemma. Among other results, arguably the most interesting one states that random scattering interactions – as those considered in the model – lead to total suppression of any initial correlation between the boundary and the inner part of the system.

Possible foreseeable extensions of the model could imply adding further structure to the system, e.g. by making either (or both) the boundary and the inner part of it linear chains of qubits; that way it would be possible to estimate the effect of unknown scattering interactions on more realistic physical systems.

Appendix A

Partial trace in the $0 \bigoplus 1$ sector

Here we show how to calculate a partial trace in the $\mathcal{H}_0 \oplus \mathcal{H}_1$ sector of the Hilbert space, assuming that no other sectors are populated. The Hilbert space is spanned by the basis $\{|n\rangle, 0 \leq n \leq N\}$, where $|0\rangle$ is the global vacuum and $|n > 0\rangle$ represents the state with the n^{th} qubit in the excited state and all the other qubits in the ground state. In order to obtain the reduced state of qubit x, a generic state of the global system $\tilde{\rho} = \sum_{j,k=0}^{N} \psi_j \psi_k^* |j\rangle\langle k|$ can be rewritten in a convenient way bearing in mind that whenever the excitation is at site x it cannot be anywhere else $(\mathcal{L} \setminus x)$, and vice versa:

$$\begin{aligned}
\sum_{j,k=0}^{N} \psi_j \psi_k^* |j\rangle\langle k| &= \sum_{j,k=0} \psi_j \psi_k^* |j\rangle\langle k|_{\mathcal{L}\setminus x} \otimes |0\rangle\langle 0|_x + \psi_x \psi_k^* |0\rangle\langle k|_{\mathcal{L}\setminus x} \otimes |1\rangle\langle 0|_x \\
&+ \psi_j \psi_x^* |j\rangle\langle 0|_{\mathcal{L}\setminus x} \otimes |0\rangle\langle 1|_x + |\psi_x|^2 |0\rangle\langle 0|_{\mathcal{L}\setminus x} \otimes |1\rangle\langle 1|_x \\
&+ \psi_x \psi_0^* |0\rangle\langle 0|_{\mathcal{L}\setminus x} \otimes |1\rangle\langle 0|_x + \psi_0 \psi_x^* |0\rangle\langle 0|_{\mathcal{L}\setminus x} \otimes |0\rangle\langle 1|_x \, . \qquad \text{(A.1)}
\end{aligned}$$

It is now easy to see that a partial trace over the lattice $\mathcal{L} \setminus x$ gives:

$$\rho_x = \sum_{l \neq x} |\psi_l|^2 |0\rangle\langle 0| + |\psi_x|^2 |1\rangle\langle 1| + \psi_x \psi_0^* |1\rangle\langle 0| + \psi_0 \psi_x^* |0\rangle\langle 1| \, , \qquad \text{(A.2)}$$

which is a well defined, trace-one reduced state.

Appendix B

Integrals over the unitary group

Here we just summarize the results of [111] which are relevant for the purposes of our model.

The maps Eqs.(6.1,6.2) involve the calculation of integrals of the form

$$\int_H \mathrm{dU}\left[U^*_{i,j}U_{k,l}\right]\,, \quad \int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_2,j_2}U_{k_1,l_1}U_{k_2,l_2}\right]\,, \tag{B.1}$$

where $\int_H$ means integrating over the Haar measure. Integrals of this kind can be tackled using Schur's lemma (see e.g. [112, 109]), but here we follow the, somewhat easier, approach described in [111].

In general, for some degrees of the polynomials p, q in U^* and U, one wants to compute

$$\begin{aligned}\int_H \mathrm{dU}\left[U^*_{i_1,j_1}\dots U^*_{i_p,j_p}U_{k_1,l_1}\dots U_{k_q,l_q}\right] &= \int_H \mathrm{dU}\left[\prod_{a=1}^{p}U^*_{i_a,j_a}\prod_{b=1}^{q}U_{k_b,l_b}\right]\\ &\equiv \int_H \mathrm{dU}\left[U^*_{I_pJ_p}U_{K_qL_q}\right]\\ &\equiv \langle I_p,J_p|K_q,L_q\rangle\,,\end{aligned} \tag{B.2}$$

where we have defined $X_p=(x_1,x_2,\dots x_p)$. It is shown in [111] that the only non-zero integrals are the ones in which the degrees are such that $p=q$ (thus we will drop this index), $K=I$ and $L=J_Q$, where J_Q is any permutation of the indices in the set J:

$$\langle I_p,J_p|K_q,L_q\rangle=\langle I,J|I,J_Q\rangle\,. \tag{B.3}$$

When $p = 1$

$$\int_H \mathrm{dU}\left[U^*_{i,j}U_{k,l}\right] = \int_H \mathrm{dU}\left[U^*_{i,j}U_{i,j}\right] = \langle i,j|i,j\rangle = \frac{1}{d}\,, \tag{B.4}$$

where d is the dimension of U.

When $p = 2$, the non-zero integrals are:

$$\bullet\,(i_1 \neq i_2, j_1 \neq j_2) \quad : \quad \int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_2,j_2}U_{i_1,j_1}U_{i_2,j_2}\right] = \frac{1}{d^2-1}\,; \tag{B.5}$$

$$\bullet\,(i_1 \neq i_2, j_1 \neq j_2) \quad : \quad \int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_2,j_2}U_{i_1,j_2}U_{i_2,j_1}\right] = -\frac{1}{d(d^2-1)}\,; \tag{B.6}$$

$$\bullet\,(i_1 = i_2, j_1 \neq j_2) \quad : \quad \int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_1,j_2}U_{i_1,j_1}U_{i_1,j_2}\right] = \frac{1}{d(d+1)}\,,$$

$$\int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_1,j_2}U_{i_1,j_2}U_{i_1,j_1}\right] = \frac{1}{d(d+1)}\,; \tag{B.7}$$

$$\bullet\,(i_1 \neq i_2, j_1 = j_2) \quad : \quad \int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_2,j_1}U_{i_1,j_1}U_{i_2,j_1}\right] = \frac{1}{d(d+1)}\,; \tag{B.8}$$

$$\bullet\,(i_1 = i_2, j_1 = j_2) \quad : \quad \int_H \mathrm{dU}\left[U^*_{i_1,j_1}U^*_{i_1,j_1}U_{i_1,j_1}U_{i_1,j_1}\right] = \frac{2}{d(d+1)}\,. \tag{B.9}$$

Knowing how to deal with this kind of integrals allows one to compute relevant quantities such as the mean reduced state $\overline{\rho_S}$ of a bipartite system-environment (SE) density matrix:

$$\begin{aligned}
\overline{\rho_S} &= \mathrm{Tr}_E(\langle\rho_{SE}\rangle_H) \\
&= \mathrm{Tr}_E\left\{\int_H \mathrm{dU}\left[U\rho_{SE}U^\dagger\right]\right\} \\
&= \mathrm{Tr}_E\left\{\int_H \mathrm{dU} \sum_{acgh=1}^{d_S}\sum_{ik=1}^{d_S}\sum_{bdhf=1}^{d_E}\sum_{jl=1}^{d_E} U_{(ab)(cd)}U^*_{(ef)(gh)}\psi_{ij}\psi^*_{kl}|ab\rangle\langle cd|\cdot|ij\rangle\langle kl|\cdot|gh\rangle\langle ef|\right\} \\
&= \mathrm{Tr}_E\left\{\sum_{ikae=1}^{d_S}\sum_{jlbf=1}^{d_E}\psi_{ij}\psi^*_{kl}\underbrace{\int_H \mathrm{dU}\left[U_{(ab)(ij)}U^*_{(ef)(kl)}\right]}_{=\frac{1}{d_S d_E}\delta^{ab}_{ef}\delta^{ij}_{kl}}\right\} \\
&= \mathrm{Tr}_E\left\{\frac{1}{d_S d_E}\sum_{ij}|\psi_{ij}|^2\sum_{a=1}^{d_S}\sum_{b=1}^{d_E}|ab\rangle\langle ab|\right\} \\
&= \frac{1}{d_S d_E}\sum_{\xi=1}^{d_E}\langle\xi|\sum_{a=1}^{d_S}\sum_{b=1}^{d_E}|ab\rangle\langle ab|\cdot|\xi\rangle \\
&= \frac{1}{d_S}\sum_{a=1}^{d_S}|a\rangle\langle a|\,.
\end{aligned} \tag{B.10}$$

Appendix C

Measure concentration and Levy's lemma

d-dimensional pure quantum states can be described as points on the surface of a (2d-1)-dimensional unit sphere. This can be realized by expressing a generic state in complex coordinates $|\psi\rangle = (z_1, z_2, \ldots, z_d)$, where $z_j \in \mathbb{C}$, for $j = 1, 2, \ldots, d$, with $\sum_j^d |z_j|^2 = 1$ and writing the coordinates in real components $z_j = x_j + iy_j$, so that $\sum_j^d x_j^2 + \sum_j^d y_j^2 = 1$.

Heuristically, the phenomenon of measure concentration on a unit sphere $S^{(2d-1)}$ in $\mathbb{R}^{2d}$ translates to the fact that almost all surface measure of the sphere is concentrated around the equator, for *any* equator. That is, for any random choice of a coordinate x_j, consider an equator of width ϵ

$$E_\epsilon := \{x \in S^{(2d-1)} \,|\, d(x_j, 0) \leq \frac{\epsilon}{2}\}\,, \tag{C.1}$$

where $d(x, y) = \arccos\langle x, y\rangle \ \forall x, y \in S^{(2d-1)}$ is the angular distance. Provided a normalized surface measure $\mu(S^{(2d-1)}) = 1$, it can be shown that

$$\mu(E_\epsilon) \geq 1 - e^{(-kd\epsilon^2)}\,, \tag{C.2}$$

where $k > 0$ is some constant.

Measure concentration is at the basis of Levy's lemma (Sec.(6.2)), as we show in the following. The kind of Levy's lemma we will sketch the derivation of here is slightly different from the one used in the third part of the thesis, but the two formu-

lations are strictly related. For space reasons, not all the details of the calculations will be shown; the interested reader can find them in [113].

To proceed, we first need to define two quantities:

Definition 7 *(Median): Let X be a metric space and $f : X \to \mathbb{R}$ a continuous function. A median M_f is defined by:*

$$\mu\{x \in X \,|\, f(x) \leq M_f\} = \frac{1}{2}\,. \tag{C.3}$$

Definition 8 *(Concentration function): Let X be a metric space and S a subset of it, with $\mu(S) = \frac{1}{2}$. For any $\epsilon > 0$, the concentration function is defined as:*

$$\alpha_X(\epsilon) := sup\{\mu(X \setminus N_\epsilon(S))\}\,, \tag{C.4}$$

where $N_\epsilon(S)$ is the ϵ-neighborhood of S:

$$N_\epsilon(S) := \{x \in X \,|\, \exists s \in S \,:\, d(s,x) < \epsilon\}\,. \tag{C.5}$$

These definitions allow to formulate the following lemma:

Lemma 4 *Let X be a metric space and $f : X \to \mathbb{R}$ a Lipschitz-continuous function with constant 1, then*

$$\mu\{x \in X \,|\, f(x) \geq M_f + \epsilon\} \leq \alpha_X(\epsilon) \tag{C.6}$$

Proof: Take $S : \{x \,|\, f(x) \leq M_f\}$ so that $\mu(S) = 1/2$ and consider a subset $B \subseteq X$ such that $f(b) \geq M_f + \epsilon$, $\forall b \in B$. Because f is Lipschitz continuous, all points $x \in N_\epsilon(S)$ satisfy $f(x) < M_f + \epsilon$, so it must be $b \notin N_\epsilon(S)$, $\forall b \in B$. That means B is a subset of X: $\{b \in X \,|\, f(b) \geq M_f + \epsilon\} \subseteq X \setminus N_\epsilon(S)$ and thus $\mu\{x \in X \,|\, f(x) \geq M_f + \epsilon\} \leq \mu(X \setminus N_\epsilon(S)) \leq \alpha_X(\epsilon)$.

□

In terms of probabilities, and by rescaling of the ϵ to $\epsilon \to \epsilon' = \eta\epsilon$ for Lipschitz functions such that $|f(x) - f(y)| \leq \eta\|x - y\| \leq \eta\epsilon$, the above lemma reads:

$$\text{Prob}(f(x) \geq M_f + \epsilon') \leq \alpha_X(\frac{\epsilon'}{\eta})\,. \tag{C.7}$$

In order to calculate the value of the concentration function $\alpha_{S^{(2d-1)}}$, one needs to invoke the isoperimetric inequality for the sphere (see e.g. [113]):

Lemma 5 *(Isoperimetric inequality for the sphere): Let $A \subseteq S^{(2d-1)}$ be a closed subset of the sphere and let $C(a,r) := \{x \in X \,|\, d(a,x) \leq r\} \subset S^{(2d-1)}$ a spherical cap around any point $a \in S^{(2d-1)}$, with the radius r chosen such that $\mu(C(a,r)) = \mu(A)$. Then*

$$\mu(N_\epsilon(A)) \geq \mu(N_\epsilon(C(a,r)))\,. \tag{C.8}$$

Therefore we have

$$\begin{aligned}
\alpha_{S^{(2d-1)}}(\epsilon) &= sup\{\mu(S^{(2d-1)} \setminus N_\epsilon(S))\} \\
&= \mu(S^{(2d-1)}) - \inf\{\mu(N_\epsilon(S))\} \\
&= 1 - \inf\{\mu(N_\epsilon(S))\} \\
&= 1 - \mu(C(a, \frac{\pi}{2} + \epsilon)) \\
&\leq e^{-d\epsilon^2}\,,
\end{aligned} \tag{C.9}$$

where the details of the calculation leading to the last inequality can be found in [114].

So far then, for functions f with Lipschitz constant $\eta \leq 1$:

$$\mu\{f(x) \geq M_f + \epsilon\} \leq \alpha_{S^{(2d-1)}}(\epsilon) \leq e^{-d\epsilon^2}\,. \tag{C.10}$$

Applying Lemma 4 to the function $g(x) = -f(x)$, one gets $\mu\{g(x) \geq M_f - \epsilon\} \leq \alpha_{S^{(2d-1)}}(\epsilon)$, thus

$$\mu\{|f(x) - M_f| \geq \epsilon\} \leq 2\alpha_{S^{(2d-1)}}(\epsilon)\,. \tag{C.11}$$

By rescaling $\epsilon \to \epsilon\eta$ for functions with $\eta \geq 1$ and interpreting the relative measure above as a probability, we get to

$$\text{Prob}\{|f(x) - M_f| \geq \epsilon\} \leq 2\text{exp}(-d\frac{\epsilon^2}{\eta^2})\,. \tag{C.12}$$

Finally, an inequality can be shown which relates median and expectation value of f, bringing the missing factors in the exponential which appear in the version of the Levy's lemma we made use of in the thesis (Eq.(6.13)).

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