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Dynamics of Initially Entangled Open Quantum Systems

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Dynamics of Initially Entangled Open Quantum Systems

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Dedicated

to

Babumaman.

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Preface

The need for a satisfying resolution of the conceptual debates that have accompanied the development of quantum mechanics over the past century is being progressively made immediate by advances in experimental science. Quantum superposition, entanglement and measurement are no longer theoretical and philosophical constructs that provide an understanding of the microscopic world. They are now resources created, controlled, and used up at will, and actions performed on demand. Understanding, generating and harnessing the essentially quantum characteristics of microscopic systems with the aim of performing computations is at the center of the novel paradigm of quantum information theory.

Information processing of any practical use, by its very nature, cannot be performed in isolation. Effective quantum computations therefore demand a clear understanding of quantum systems interacting with their surroundings. In this dissertation I study the dynamics of open quantum systems that are entangled to other quantum systems in its surroundings. The bulk of the theory of open quantum systems in its current form is concerned with systems interacting with an environment that has a large number of degrees of freedom. This approach can be successfully applied to understand several aspects of open quantum evolution including, to a certain extent, the unresolved issues

in quantum-classical correspondence. In fact more is known about quantum systems interacting with large environments, thanks to powerful statistical methods, than about a system in contact with an environment of comparable size. The scope of the open quantum evolution considered in what follows is therefore kept more modest. I investigate quantum mechanical systems with finite dimensional Hilbert spaces coupled through well defined interactions to an environment, also with a finite dimensional Hilbert space and itself quantum in nature. The emphasis being on the effect of initial entanglement between the system and the environment on the transformations that the system undergoes. Incidentally, it turns out that several of the effects of a quantum system interacting with a large environment (reservoir) are reproduced even when the environment has only a few degrees of freedom. Stochastic evolution does not always demand a 'reservoir' that is arbitrarily large. Entanglement adds previously unexpected dimensions to the reduced evolution of the system of interest.

The question of reduced dynamics in the presence of initial entanglement has been raised, albeit briefly in the past. I believe that the discussion was cut short prematurely for reasons that do not seem to hold up on closer scrutiny. A discussion of the previous work on the topic is included to put this dissertation in context and to identify potential points of contention and confusion.

The extension of the Church-Turing theorem to quantum systems shows that any such system with finite dimensional Hilbert space and its dynamics

can be represented equivalently using two state quantum systems (qubits[1]) and the transformations on them. The discussion here is therefore phrased, for the most part, in terms of qubits interacting with each other and with their environment. This has the added advantage of keeping the language that is used close to the terminology used in quantum information theory.

The starting point of the discussion presented here is an introduction to some of the relevant terminology and concepts followed by a summary of the established results in the field. This sets the stage for the new features that appear when entanglement is thrown into the mix. With entanglement between a system and its environment, the mathematical nature of the dynamics that the system undergoes poses certain questions regarding its interpretation. These issues and their resolution are presented in terms of a concrete example rather than in generality. It is only after discussing the features of the specific example that an attempt is made at generalizing the results. Some speculations about the new possibilities that are opened up by allowing a wider class of dynamics for open systems than was previously considered physically reasonable are also included as an invitation to further investigations into the problems that are discussed here.

[1]See Appendix A.1

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Linear, trace and hermiticity preserving, maps of density matrices that describe the evolution of open quantum systems initially entangled to parts of their environment are studied. Complete positivity is an additional property that is often attributed to maps describing the evolution of open quantum dynamics. If there is initial entanglement the dynamical maps are found to be not completely positive. They are not even positive unless the domain of action of the maps is restricted. The initial entanglement of the system means that only subset of states, called the compatibility domain, are allowed and it gives a physical reason for restricting the domain of action of the map. The maps we obtain are shown to be positive on the compatibility domain. An example for two initially entangled qubits is worked out in detail. The maps are obtained first as maps between expectation values of observables

of the system and then generalized to maps between basis matrices. The maps are also studied as affine transformations on the space of states of the system. An operator sum representation similar to that of completely positive maps is constructed for the maps obtained here and a parameterization of the maps given. The reasons commonly cited for stipulating that open quantum dynamics be described exclusively in terms of completely positive maps are analyzed and found inconclusive in light of the understanding gained here. We find that positive as well as not positive maps are good candidates for describing open quantum evolution.

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Chapter 1

Introduction

The dynamics of simple quantum systems open to influences from its environment is the focus of this work. Of particular interest is how the dynamics is modified when the external influences includes entanglement of the system of interest to its environment.

An isolated quantum system is in itself an infinitely fascinating entity. Quantum superposition, entanglement and even the notion of measurement being of a character that does not fall within the boundaries of normal human experiences, perception and imagination. Real quantum systems however can very rarely be treated as evolving in isolation. Furthermore, if we seek not only to understand how a system behaves but also to control it then we have to know how it responds to the influences we exert on it as well as its interaction with the environment to correct for undesirable effects.

Quantum information theory [1, 2] concerns itself with the avenues that are opened up when it is possible to manipulate at will the state and evolution of individual quantum systems. It took almost a hundred years after the inception of quantum mechanics to acquire the ability to exert precise control over real quantum systems; albeit very simple ones. With this ability comes

the capacity to manipulate information in ways that are not conceivable using classical information processing devices. The ability to build quantum computers that can perform computations that are beyond the capacities of any imaginable classical computer [3]. The fragility of quantum information under the influence of the environment on the physical system that encodes the information is added motivation to push the limits of our understanding of open quantum dynamics.

Understanding open quantum evolution is a challenging problem that has led to the development of several approaches that are useful in different contexts. In close analogy with the familiar Schrödinger equation in standard quantum mechanics, quantum master equations may be constructed for open systems that keeps continuous track of the state of the system. The unitary transformations that describe the development of a closed system through a finite interval in time is the starting point for considering more general transformations that connect the states of open quantum systems at different times. A third approach is to condense the effect of the environment into an 'influence functional' using the path integral formulation of quantum mechanics. These are just a few of the possible methods of dealing with open quantum systems (for detailed discussions on the various methods see [4]). In this work we limit our considerations to the first two ways of dealing with the evolution of open quantum systems.

1.1 Organization of this dissertation

We review the description of open quantum evolution in terms of dynamical maps on density matrices in Chapter 2. The sub-class of such maps called completely positive maps are introduced. The reasons that are often put forward to justify considering only completely positive maps as reasonable descriptions of open quantum systems are examined. We find that these arguments are not conclusive and that any entanglement[1] or other correlations that may exist between the system and environment forces us to consider other types of maps as well [5, 6].

In Chapter 3 we examine in detail the simplest possible model of a system and and environment looking at only the reduced dynamics of the system. In this model both the system and the environment are single qubits couped through a simple interaction. The focus will be on the modifications made to the open dynamics of the system qubit by the introduction of pre-existing entanglement between the system and environment qubits. The nature of the dynamical maps induced on the system due to such coupled evolution is studied.

Chapter 4 is about the physical interpretation of the reduced dynamics induced on the system when there is initial entanglement with the environment. We show that dynamics is not necessarily completely positive in nature. In fact, it is not even positivity preserving in general. This introduces a certain

[1] See Appendix A.2

amount of subtlety in coming up with a consistent physical interpretation of such open dynamics. A few new ideas like the "compatibility domain" and the "positivity domain" of the maps have to be defined to make sense of its action on states of the system.

In Chapter 5 we generalize the discussion in the previous chapters to open quantum systems having Hilbert spaces with larger (but finite) dimensions. Chapter 6 contains a discussion on how the dynamical maps acting on quantum systems may be reconstructed from experimental data and the different ways of looking at the maps thus obtained. Our main results, conclusions and a discussion of future work are included in Chapter 7.

Chapter 2

Completely positive reduced dynamics

A quantum system with a finitely many dimensional state space may be represented by a $N \times N$ quantum density matrix ρ. The density matrix must be of trace class and should satisfy the properties of hermiticity and positivity:

$$\mathrm{tr}(\rho) = 1 \quad ; \quad \rho^\dagger = \rho \quad ; \quad x_r^* \rho_{rs} x_s \geq 0. \tag{2.1}$$

Hermiticity of the density matrix means its eigenvalues are real. Positivity assures us that the eigenvalues are non-negative and the trace condition means that they add up to one. These three conditions allows for the interpretation of the diagonal elements of ρ as probabilities (Born's rule).

For pure quantum states there is an equivalent description in terms of rays in Hilbert space. This representation has the shortcoming that it cannot describe mixed states. If a quantum state remains pure under time evolution then that means that the evolution is unitary and the system is closed. Studying open quantum evolution almost always means having to deal with mixed states. Therefore we choose to represent the states of quantum systems exclusively using density matrices in our discussion.

2.1 Closed vs. open quantum dynamics

For a closed quantum system dynamical evolution is governed by the von-Neumann equation

$$\frac{\partial \rho}{\partial t} = \mathcal{L}(t)\rho = -\frac{i}{\hbar}[H(t)\,,\,\rho] \tag{2.2}$$

where $H(t)$ is the (possibly time dependent) Hamiltonian. If we are not interested in a differential equation like Eq. (2.2) that tracks the time evolution of the state at all times we can integrate the equation and find the time evolution operator that connects the states of the system at two different times. This finite time development is given for closed systems by the action of a time development operator $\mathcal{U}$.

$$\rho(t_2) = \mathcal{U}(t_2, t_1)\rho(t_1) = e^{\mathcal{L}(t_2, t_1)}\rho(t_1) = U(t_1, t_2)\rho(t_1)U^{\dagger}(t_1, t_2) \tag{2.3}$$

where

$$U(t_1, t_2) = \mathcal{T}\left\{\exp\left(-i\int_{t_1}^{t_2} H(t')dt'\right)\right\}. \tag{2.4}$$

The evolution is linear so that

$$e^{\mathcal{L}(t_2, t_1)}\sum_i p_i\rho^{(i)}(t_1) = \sum_i p_i\rho^{(i)}(t_2) \quad , \quad \sum_i p_i = 1\ ,\ p_i \geq 0.$$

The transparent relationship between the time development operator and the generator of infinitesimal time translations, $\mathcal{U}(t) = e^{\mathcal{L}(t)}$ (equivalently, between $H(t)$ and $U(t_1, t_2)$ in Eq. (2.4)), is one of the nice features of closed quantum systems.

In quantum information theory one is often interested in the unitary time development operator than the differential equation because $U(t_1, t_2)$ represent unitary *quantum logic gates* that perform specific operations on the state of a system. Only the finite transformation on the state is of interest in many contexts. How the transformation is achieved and the corresponding generators are not always of interest in information processing. For instance, the quantum *phase*-gate takes a state that is a superposition of two mutually orthogonal states and changes the relative phase between the components of the superposition by a fixed amount. Through what process the relative phase is changed is quite frequently not relevant when applying such gates to do an information processing operation.

For open quantum systems the situation is a bit more complicated. Very often it is not possible to write down a differential equation describing the evolution of just the state of the system of interest because of the influence of its environment. More precisely, if the environment is of such a nature that it is affected by the changes in the system and if it passes this influence back to the system at some point then the evolution becomes non Markovian[1]. Formally one might still be able to write down a differential equation for the state of the system but the non Markovian nature of the evolution will preclude any meaningful solutions. For a review of the restricted situations under which Markov approximation holds and a differential equation and its solutions can

[1]In a Markov process the state of the system at one time step depends *only* on its state in the previous step and not on the sequence of states the system has traversed to get to the current state

be written down for an open quantum system see [4, 7, 8]. Such difficulties are not too hard to understand in light of the fact that just from calling the system open we are conceding that all the details of the nature and the influence of the environment *cannot* be known. If all the details were known then we could just as well have treated the system and its environment together as one closed system.

One way out of these difficulties is to turn the problem on its head and ask a tractable question. Given that the details of the nature and influence of the environment is not known, what is the most general evolution that is allowed for the state of the system of interest. Rather than seeking a differential equation describing such general evolution if one is satisfied in knowing the finite time evolution of the system of interest then the answer is straightforward. One can extend the unitary evolution of closed systems to a general linear evolution of the form [9]:

$$\rho(t_2) = A(t_1, t_2)\rho(t_1). \tag{2.5}$$

The linearity of $A(t_1, t_2)$ follows from the linearity of quantum mechanics and for this reason we do not consider more complicated forms of maps on density matrices. The operator A can be written as a matrix if ρ is finite dimensional and the transformation can be written as

$$\rho_{rs} \longrightarrow A_{rs;r's'}\rho_{r's'} = (A\rho)_{rs}.$$

In the equation given above, the elements of the density matrix has been

suitably regrouped into a column vector so that A can be in the form of a $N^2 \times N^2$ matrix.

The only constraints on A stem from the fact that it has to map *density matrices* satisfying Eq. (2.1) to other *density matrices*. The properties of density matrices impose the following restrictions on A:

$$A_{sr;s'r'}(t) = [A_{rs;r's'}(t)]^* \quad \text{(Hermiticity preserving)} \tag{2.6}$$

$$A_{rr;r's'} = \delta_{r's'} \quad \text{(Trace preserving)} \tag{2.7}$$

$$x_r^* x_s A_{rs;r's'} y_{r'} y_{s'}^* \geq 0 \quad \text{(Positivity).} \tag{2.8}$$

It is instructive to first recast A into another dynamical matrix B [7, 10–15] such that

$$A_{rs;r's'}(t) = B_{rr';ss'}(t). \tag{2.9}$$

In the form B the restrictions in Eq. (2.6)-(2.8) on the map gets modified to the following relations:

$$B^*_{ss';rr'}(t) = B_{rr';ss'}(t) \quad \text{(Hermiticity)} \tag{2.10}$$

$$B_{nr';ns'} = \delta_{r's'} \quad \text{(Trace preserving)} \tag{2.11}$$

$$x_r^* y_{r'} B_{rr';ss'} x_s y_{s'}^* \geq 0 \quad \text{(Positivity).} \tag{2.12}$$

In terms of the pairs of indices rr' and $s's$, B is a hermitian matrix which gives non-negative expectation values for factorisable vectors.

$$u^\dagger B u \geq 0 \quad \text{if} \quad u_{rs} = x_r y_s^*.$$

This means that the action of the operator B on a positive matrix is to take it to another positive matrix. Positivity of the matrix, in turn, means that all

its eigenvalues are non-negative. We note here, as a taste of things to come, that the last condition on B can be relaxed to some extent when considering all possible varieties of open quantum evolution. For the time being though we adhere to the conventional treatment of maps on density matrices and go in the opposite direction to see the consequences of imposing an even stronger condition than positivity on B.

The operator B represents the most general transformation that a quantum system can undergo and so we refer to the action of B as a *dynamical map* and B itself is the *dynamical matrix*. It is not necessary that B itself be a positive matrix ($B \geq 0$) for maintaining the positivity of the density matrices under dynamical evolution even though it is a sufficient condition. If B is in itself a positive matrix ($B \geq 0$) we will call the map "completely positive" [10]. The terminology is slightly confusing unless one keeps in mind that positivity of the map is a statement about its action on density matrices while complete positivity can be regarded as a statement about the map itself, in addition to saying something about its action. For instance, the action of taking the transpose of a density matrix: $\rho \rightarrow \rho^T$ is a positive map but not a *completely positive* map.

2.2 Consequences of complete positivity

The requirement of complete positivity for the reduced dynamics places certain restrictions on the allowed behavior of an open quantum system. Let us explore some of these restrictions using a simple example which will also

serve as a means of introducing some of the notation that will be used in what follows. The operational definition of complete positivity in terms of the positivity of the matrix B is sufficient for looking at the example. We will go on to more formal definitions in the next section.

Let the system of interest S be a single qubit (See Appendix A.1 for a short discussion on qubits). The state of the system is represented by a 2×2, Hermitian, positive, complex matrix ρ of unit trace. We can write the density matrix in the form

$$\rho = \frac{1}{2}(1 + a_i \sigma_i) = \frac{1}{2} \begin{pmatrix} 1 + a_3 & a_1 - i a_2 \\ a_1 + i a_2 & 1 - a_3 \end{pmatrix} \tag{2.13}$$

where σ_i are the familiar Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad ; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad ; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The vector $\mathbf{a} = (a_1\,,\, a_2\,,\, a_3)$ is often called the Bloch vector and physical states of the qubit correspond to $|\mathbf{a}| \leq 1$. The space of all one qubit states can therefore be viewed as all the points on or inside the "Bloch sphere" which is the unit ball in the space spanned by a_1, a_2 and a_3.

We now consider a map on ρ that scales each of the three independent directions, deforming the Bloch sphere to an ellipsoid:

$$\rho' = A\rho = \frac{1}{2}(1 + x_i a_i \sigma_i) \quad \text{with} \quad 0 \leq x_1 \leq x_2 \leq x_3 \leq 1. \tag{2.14}$$

The particular ordering that we have chosen for the scaling parameters x_i is not at the expense of any generality because a different ordering corresponds to just

a re-labeling of the axes. Rearranging the matrices ρ and ρ' and constructing the following equation

$$\frac{1}{2}\begin{pmatrix} 1+x_3a_3 \\ x_1a_1 - ix_2a_2 \\ x_1a_1 + ix_2a_2 \\ 1-x_3a_3 \end{pmatrix} = A \cdot \frac{1}{2}\begin{pmatrix} 1+a_3 \\ a_1 - ia_2 \\ a_1 + ia_2 \\ 1-a_3 \end{pmatrix}, \tag{2.15}$$

the linear operator A may be written down by inspection to be

$$A = \frac{1}{2}\begin{pmatrix} 1+x_3 & 0 & 0 & 1-x_3 \\ 0 & x_1+x_2 & x_1-x_2 & 0 \\ 0 & x_1-x_2 & x_1+x_2 & 0 \\ 1-x_3 & 0 & 0 & 1+x_3 \end{pmatrix}. \tag{2.16}$$

From the A matrix we obtain the dynamical matrix as

$$B = \frac{1}{2}\begin{pmatrix} 1+x_3 & 0 & 0 & x_1+x_2 \\ 0 & 1-x_3 & x_1-x_2 & 0 \\ 0 & x_1-x_2 & 1-x_3 & 0 \\ x_1+x_2 & 0 & 0 & 1+x_3 \end{pmatrix}. \tag{2.17}$$

The eigenvalues of B are

$$\begin{aligned} \lambda_1 &= \frac{1}{2}(1+x_1-x_2-x_3) \\ \lambda_2 &= \frac{1}{2}(1-x_1+x_2-x_3) \\ \lambda_3 &= \frac{1}{2}(1-x_1-x_2+x_3) \\ \lambda_4 &= \frac{1}{2}(1+x_1+x_2+x_3). \end{aligned} \tag{2.18}$$

If B has to be completely positive then all λ_i must be positive semi-definite. This means that the scaling parameters x_i have to be such that

$$x_3 \leq 1-(x_2-x_1) \quad \text{given that} \quad x_1 \leq x_2. \tag{2.19}$$

From Eq. (2.19) we see the if we require complete positivity of the dynamical map then certain transformations of the Bloch sphere are not allowed. For instance the map cannot take the unit ball into the unit disk because this would correspond to the choice $x_1 = 0$ and $x_2 = x_3 = 1$ which violates (2.19). For a qubit represented by the spin of a spin 1/2 particle complete positivity means that open dynamics cannot produce relaxation of the spin along just one of the three orthogonal directions. If there is relaxation along one direction keeping the polarization along another orthogonal direction constant then the third direction necessarily has to relax too. In other words the best one can do is to reduce the Bloch sphere to a spindle shaped object if the polarization along one of the three directions is to be kept constant. The transpose operation corresponds to $x_1 = x_3 = 1$ and $x_2 = -1$ which is not completely positive. In general, any one of x_1, x_2, x_3 being negative while the other two are positive is not completely positive but $x_3 = 1$, $x_1 = x_2 = -1$ is a pure rotation of the Bloch sphere and is allowed.

The scaling of a_i through x_i is not the only kind of completely positive transformation allowed on the space of single qubit states. We can also have dynamical maps with inhomogeneous parts that not only squeezes and rotates the Bloch sphere but moves the center too. Transformations that do not move the center are called *unital*. Even for non unital transformations it turns out that the requirement of complete positivity puts restrictions on the allowed forms. The transformations that are allowed are summarized graphically in figure 2.1.

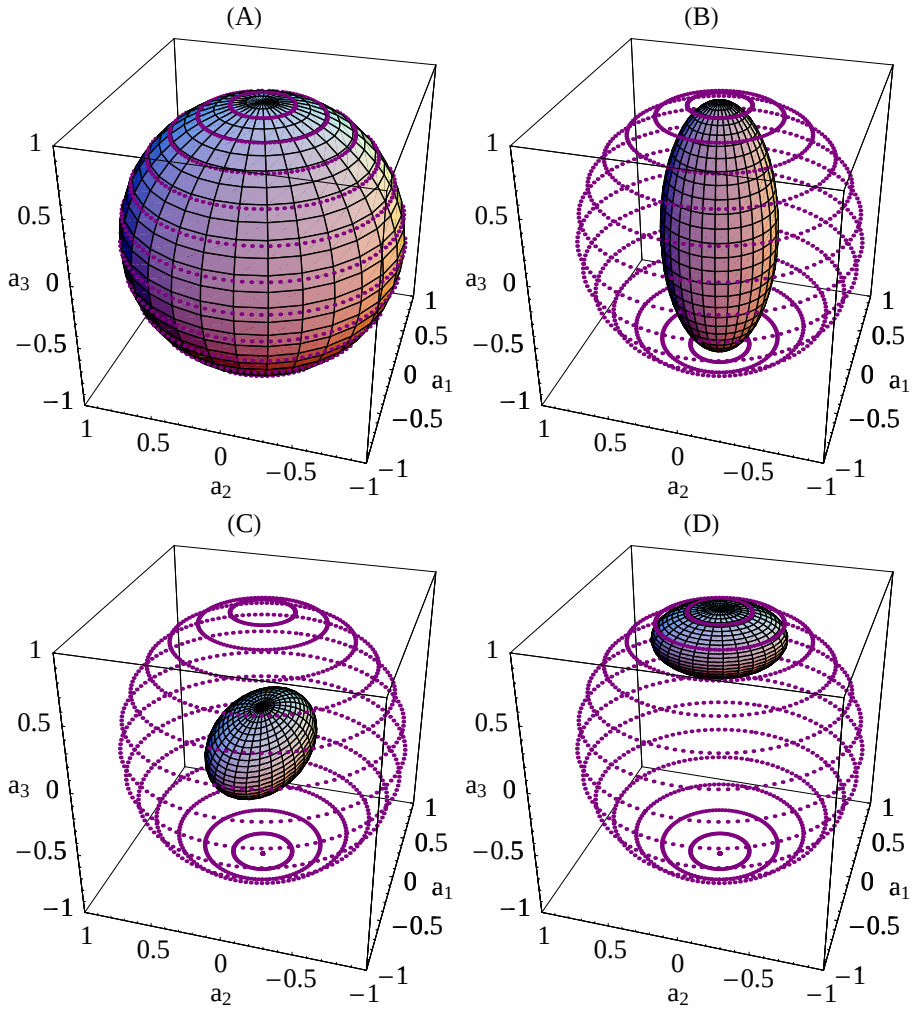

Figure 2.1: The allowed completely positive single qubit transformations: (A) Unitary rotation, (B) pure dephasing (off diagonal elements of the density matrix go to zero) with $x_1 = x_2$ and $x_3 = 1$, (C) Depolarizing map with $x_1, x_2, x_3 < 1$, (D) A completely positive map involving an inhomogeneous shift in addition to scaling of the Bloch sphere (sometimes called the pin map or decaying map). The dotted lines show the unit sphere.

The question is whether the restrictions on the allowed forms of open quantum dynamics are actually justified or observed in experiments. Experimental investigations of the nature of the dynamics that an open quantum system undergoes is called quantum process tomography [16]. At present only very rudimentary forms of quantum process tomography are possible due to the limitations in measuring and controlling individual quantum systems but preliminary data seems to suggest that observed dynamics can take on forms that are not allowed by the requirement of complete positivity [17]. We will return to the question whether the requirement of complete positivity is too restrictive in Chapter 7.

2.3 Choi's definition of completely positive maps

M-D. Choi, in his seminal work on completely positive maps [10], describes the distinction between positive and completely positive maps on C^*-algebras. Choi's definition of a completely positive map may be paraphrased as follows: Consider a linear map $\Phi : \mathcal{A} \to \mathcal{B}$ between two C^*-algebras $\mathcal{A}$ and $\mathcal{B}$. The map Φ is *positive* if $\Phi(A) \geq 0$ for all positive $A \in \mathcal{A}$. Let $\mathcal{M}_n$ be the collection of all $n \times n$ complex matrices and $\mathcal{M}_n(\mathcal{A}) = \mathcal{A} \otimes \mathcal{M}_n$ be the C^*-algebra of $n \times n$ matrices over $\mathcal{A}$; meaning all $n \times n$ (block) matrices with the elements of the matrices being elements of $\mathcal{A}$. Now define $\Phi \otimes \mathbf{1}_n : \mathcal{M}_n(\mathcal{A}) \to \mathcal{M}_n(\mathcal{B})$ by $\Phi \otimes \mathbf{1}_n((A_{jk})_{1 \leq j,k \leq n}) = (\Phi(A_{jk}))_{1 \leq j,k \leq n}$. Here $(A_{jk})_{jk}$ denotes a block matrix with $A_{jk} \in \mathcal{A}$ occupying the jk-th block. In other words, it is the Kronecker product of the $n \times n$ matrix $M \in \mathcal{M}_n$ with the elements of $\mathcal{A}$. We say that Φ

is n-positive if $\Phi \otimes \mathbf{1}_n$ is positive. The set of all n-positive linear maps on $\mathcal{A}$ is denoted by $\mathbb{P}_n[\mathcal{A}\,,\,\mathcal{B}]$.

$$\Phi \text{ is said to be } \textit{completely positive} \text{ if } \Phi \in \mathbb{P}_\infty[\mathcal{A}\,,\,\mathcal{B}].$$

Choi goes on to prove several theorems on positivity and complete positivity including the useful result that if a map $\Phi : \mathcal{A} \to \mathcal{M}_n$ is n-positive then it is completely positive, where n is the dimensionality of the Hilbert space on which the C^*-algebra $\mathcal{A}$ is defined.

2.3.1 The witness

Let us leave Choi's definition of complete positivity aside for a moment and look at the "physical arguments" given for accepting only completely positive maps as reasonable choices for describing the evolution of open quantum systems. The following passage [18] is representative of similar arguments seen widely in the literature[2].

> A completely positive map is not only a reasonable map from density operators to density operators for S, but it is extensible in a trivial way to a reasonable map from density operators to density operators on any larger system $S + W$. Since we cannot exclude a priori that our system S is in fact initially entangled with some distant isolated system W, any acceptable Φ had better satisfy this condition.

[2]We have taken the liberty of making the mathematical notation uniform in the passages that are quoted

The reduced dynamics of the system S described by the map Φ is a result of the influence of some environment R on it. At this point there is no restriction of complete positivity on the map. The trick by which complete positivity is imposed on Φ is to introduce an auxiliary system called the *witness* W that is separate from R. The witness is assumed to be 'blind' in the sense that it does not interact with S and 'dead' in that it has no free evolution of its own. The motivation for introducing the witness is clear. Since the witness does not take part in the dynamics in any form we expect that its time evolution be given by the unit operator $\mathbf{1}_W$. From Choi's result it appears that to keep the action of $\Phi \otimes \mathbf{1}_W$ positive on *all* the states of $S + W$, Φ must be completely positive. Expecting $\Phi \otimes \mathbf{1}_W$ to be positive is perfectly reasonable because just the mere presence of W cannot suddenly make the dynamics of $S + W$ unphysical.

The subtle point that is often overlooked in the argument given above is the requirement that the system and the witness must be entangled or correlated in some other form with each other. If S and W are in a tensor product state of the form $\rho \otimes \rho_W$ with no correlations between their states then any positive but not necessarily completely positive map Φ extended to $\Phi \otimes \mathbf{1}_W$ will be positive on $S + W$ also. Entanglement or correlations between the system and anything outside of it introduces new elements into the dynamics and into the interpretation of Choi's result as we will see in the coming chapters. In the end, the argument using the witness turns out to be insufficient to exclude not completely positive maps as valid forms of

open quantum evolution precisely because of the entanglement needed to make it work. The rest of this dissertation is devoted to justifying the use of not completely positive maps in the study of open quantum systems and providing a consistent interpretation for the action of such maps.

The operational definition for complete positivity, $B \geq 0$ where B is the matrix representation of the map Φ, is better suited for computations. Choi's approach is useful for understanding and interpreting the action of the dynamical maps and for establishing the relationships between positivity and complete positivity.

2.4 Completely positive reduced dynamics

Since we shuffled around the elements of A to get the dynamical matrix B, the action of B on ρ is obviously going to look much different from the way A acts on ρ. The action of A on ρ is by simple matrix multiplication once ρ has been rearranged into a column vector. An advantage of recasting the linear transformation A into the dynamical matrix B which is hermitian in the pairs of indices rr' and $s's$ is that we can now represent the map in terms of the eigenvalues and eigenvectors of B in a convenient form; i.e,

$$\rho_{rs} = \sum_n \lambda_n \zeta_{rr'}^{(n)} \rho_{r's'} \zeta_{s's}^{(n)\dagger}, \tag{2.20}$$

If ρ is an $N \times N$ density matrix corresponding to an N-dimensional quantum system then B is an $N^2 \times N^2$ hermitian super-matrix and the index n can run over at most N^2 distinct values. In the case where B is completely positive

then all its eigenvalues, λ_n, are positive and they can be absorbed into the matrices $\zeta^{(n)}$ by defining $C^{(n)} \equiv \sqrt{\lambda_n}\zeta^{(n)}$. The dynamical map now takes the form

$$\rho_{rs} = \sum_n C^{(n)}_{rr'}\, \rho_{r's'}\, C^{(n)\dagger}_{s's} \tag{2.21}$$

with

$$\sum_n C^{(n)\dagger} C^{(n)} = 1 \tag{2.22}$$

following from the trace preservation condition. The form of the dynamical map in Eq. (2.21) is sometimes called the *operator sum representation* or the *Stinespring form* [19]. Note that unitary evolution is a special case of the dynamical map with a single non-zero eigenvalue:

$$\rho \longrightarrow U\rho U^\dagger \qquad ; \qquad U \equiv C^{(1)}.$$

The density matrices on which the dynamical maps act form a convex compact set. Since positive maps transform such a set into itself, they themselves form a convex compact set [14] (the set of completely positive maps also form a convex set lying inside the convex set of positive maps[3]). The convexity property means that any linear combination of positive maps with nonnegative coefficients which sum to unity is also another valid map. For instance the positive map B defined by

$$B = \sum_m k(m) B_m \quad ; \quad k(m) \geq 0 \quad ; \quad \sum_m k(m) = 1$$

[3]Positive maps form a convex cone but the condition that their action be trace preserving restricts the dynamical maps to a convex set. Completely positive trace preserving maps form a convex subset of this set.

is also a positive map if B_m are positive maps. It can also be shown that [10, 20] $1 \leq m \leq N^2$ where N is the dimensionality of the density matrices that the map acts on. Out of the convex set of positive maps we can pick out those maps which cannot be written as a sum of other maps. Such maps are called extremal. If a completely positive map is not extremal, its action can be written as

$$\rho \longrightarrow \sum_{m,n} k(m) C_m^{(n)} \rho C_m^{(n)\dagger}. \tag{2.23}$$

2.5 Completely positive maps as contractions

The dynamical matrix B has been introduced in the previous section as a mathematical construct that describes a general transformation that a density matrix can undergo. Now we look at the physical origins of the dynamical map. It is reasonable to expect that a given open quantum system interacts with only a limited number of systems in its environment. If we now consider the system and all the parts of the environment to which it is coupled to as one quantum system then that extended system can be treated as closed. The extended system therefore has to evolve unitarily. The dynamical map can be viewed as the dynamics that is induced on the system due to the unitary evolution of the extended system that includes the environment. To obtain the map we average over the effect of the environment starting from the state of the extended system using a partial trace operation.

Let S be the system of of interest and let R represent a 'reservoir' with

which S is interacting. Let the dimensionality of S be N and that of R be M. Since, at this point, we are interested in obtaining *completely positive* reduced dynamics for S, we have to choose a *direct product density matrix* (a *simply separable state*) as the initial state of the system and the reservoir. The dynamics of the coupled system is given by

$$\mathcal{R} = \rho_S \times \eta_R \longrightarrow U\rho_S \times \eta_R U^\dagger$$

where U is a unitary matrix in the direct product space $\mathcal{H}_\mathcal{S} \times \mathcal{H}_\mathcal{R}$ Using the index notation:

$$\rho_{rs} \times \eta_{ab} \longrightarrow U_{ra;r'a'}\rho_{r's'}\eta_{a'b'}U^*_{sb;s'b'}. \tag{2.24}$$

The evolution of the system S is extracted using the partial trace operation which is a contraction.

$$\rho_{rs} \longrightarrow \mathrm{tr}_R\left(U_{ra;r'a'}\rho_{r's'}\eta_{a'b'}U^*_{sb;s'b'}\right) = U_{rn;r'a'}\rho_{r's'}\eta_{a'b'}U^*_{sn;s'b'}.$$

For simplicity we assume that η can be made diagonal by a suitable unitary transformation in $\mathcal{H}_R$ with eigenvalues $\eta(1), \eta(2) \ldots \eta(n)$. Then the map on S is

$$\rho_{rs} \longrightarrow \sum_{\nu,n,r',s'} \eta(\nu)\, U_{rr'}(n,\nu)\rho_{r's'}U^*_{s's}(n,\nu). \tag{2.25}$$

Here the operator U has been rewritten in a manner suggestive of the form of a completely positive map that is not extremal, given in equation (2.23).

To get the form of the map in (2.23) it is sufficient that the dimensionality N of the reservoir to be the same as that of the system. i.e. $M = N$. With this restriction $\eta(\nu)$ could correspond to a mixed state. If we further

restrict η to correspond to a pure state so that it has only one eigenvalue then the map is extremal and reduces to the standard form (2.21)

$$\rho_{rs} = \sum_n U^{(n)}_{rr} \rho_{r's'} U^{(n)*}_{ss'} \simeq \sum_n C^{(n)} \rho C^{(n)\dagger}$$

in which n runs over $1 \leq n \leq N$. In other words extremal completely positive maps are contractions of unitary evolution in a space in which the system is coupled to a reservoir, of the same number of dimensions of the system, whose initial state is a pure projection. To obtain completely positive maps that are not extremal we should either let the reservoir state be mixed while keeping its dimensionality same as that of the system or else increase the dimensionality of the reservoir to N^2 while keeping the states of the reservoir pure.

We can also carry out the inverse construction where we start with a completely positive map and view it as a unitary transformation on a larger system. Given an extremal completely positive map of the form (2.21), we can construct a unitary matrix U in (at most) N^3 dimensions with:

$$U_{rn;r'1} = C^{(n)}_{rr'}.$$

The conditions on $C^{(n)}$ are transcribed into

$$\sum_{n,j} U^*_{rn;j1} U_{sn;j1} = \delta_{rs}$$

which is necessary for U to be a unitary matrix. The ambiguity in constructing the other elements of U, where the last index is not equal to 1, does not affect the map. In short, U can be constructed in such a fashion that it corresponds

to any given dynamical map on the system along with a particular choice of the states η of the reservoir.

It is significant to note here that we obtained a completely positive map out of the coupled unitary evolution of S and R because we chose the initial state of the two to be of the form $\rho \otimes \eta$. In Chapter 3 we will show that for generic choices of the initial states of $S + R$ the reduced dynamics is no longer completely positive. In situations where we have complete control over the initial state of the system of interest it is reasonable to claim that S and R starts off in a simple product state but otherwise we have no reason to expect that it be so.

2.6 Dynamical semi-group: the Kossakowski equation

In this section we take a brief detour and explore in detail some of the problems mentioned in the introduction in writing down differential equations describing open quantum evolution. We look at the special cases in which a dynamical map may be thought of as being generated by a sequence of infinitesimal transformations.

The dynamical maps $\rho \rightarrow B(t)\rho$ are labeled by the continuous time parameter with composition of two maps yielding another map of the same kind:

$$B(t_1) \cdot B(t_2) = B. \tag{2.26}$$

The maps do not, in general, form a one parameter group;

$$B(t_1) \cdot B(t_2) \neq B(t_1 + t_2). \tag{2.27}$$

Since the action of the maps are contractive in nature for arbitrary open quantum evolution one would not, in fact, expect a group structure in any case. On the other hand it is reasonable to ask whether it is possible to identify a semi-group structure for the composition of completely positive dynamical maps at least under certain restrictive, but broad, conditions.

Viewing the completely positive maps as contractions of the unitary evolution of an extended system provide clues as to how this may be accomplished. The system has an influence on the environment that must be regarded as non-trivial because we assume that the environment is also a quantum system with finite state space. If the influence that the system has on the environment affects the system back again then the net effect would be a map induced on the system that does not possess the semi-group property. If, on the other hand, we consider the map induced by the coupled evolution for *short* times so that the back-reaction has no significant effect then such maps can form a semi-group. So we consider the system and the environment evolving together for a short time t_0 and then we recouple the system S to *another copy* of the reservoir R and contract. This would lead to an iteration of $B(t_0)$ such that after nt_0 units of time, the dynamical matrix acting on S is

$$[B(t_0)]^n = \mathcal{B}(n)$$

$$\mathcal{B}(0) = 1 \quad ; \quad \mathcal{B}(n_1)\mathcal{B}(n_2) = \mathcal{B}(n_1 + n_2),$$

thus yielding a *discrete semi-group*. Such an evolution corresponds to the system encountering one reservoir R_1, decoupling from it, re-coupling to another similar reservoir R_2, and so on. For example, a system undergoing successive interactions with a stream of particles from its environment would have such a stochastic evolution for times large compared with t_0. We could interpolate this discrete semi-group with an analytic continuous semi-group. When the dynamical maps do form a semi-group we can construct the generator of the semi-group and use them to write down a differential equation for ρ_S of the form

$$\dot{\rho} = \mathcal{L}\rho. \tag{2.28}$$

This construction *ab initio* was carried out by Kossakowski [21, 22] (see also Lindbald [23]). A simplified derivation of the Kossakowski equation follows:

2.6.1 Deriving the Kossakowski master equation

We start from the representation of the completely positive map in terms of its eigenvector decomposition

$$\rho \to \sum_n C^{(n)} \rho C^{(n)\dagger}$$

in the vicinity of the identity. Then we could have

$$C^{(1)} = 1 + L^{(1)}\sqrt{\Delta t} \quad ; \quad C^{(n)} = L^{(n)}\sqrt{\Delta t} \quad n \geq 2. \tag{2.29}$$

Collecting terms up to linear order in Δt, we obtain

$$\begin{aligned}\rho_{\Delta t} &= (1+L^{(1)}\sqrt{\Delta t})\rho(1+L^{(1)}\sqrt{\Delta t})^{\dagger}+\Delta t\sum_{n\geq 2}L^{(n)}\rho L^{(n)\dagger}\\ &= \rho+\sqrt{\Delta t}L^{(1)}\rho+\sqrt{\Delta t}\rho L^{(1)\dagger}+\Delta t\sum_{n}L^{(n)}\rho L^{(n)\dagger}. \qquad (2.30)\end{aligned}$$

Now let

$$\begin{aligned}L^{(1)} &\equiv K^{(1)}-iH\sqrt{\Delta t},\\ L^{(1)\dagger} &\equiv K^{(1)}+iH\sqrt{\Delta t}\end{aligned}$$

so that

$$\rho_{\Delta t}-\rho=-i\Delta t[H,\rho]+\sqrt{\Delta t}\Big(K^{(1)}\rho+\rho K^{(1)}\Big)+\Delta t\sum_{n}L^{(n)}\rho L^{(n)\dagger}. \qquad (2.31)$$

Using the definitions in equation (2.29) we now rewrite the trace preservation condition on the map as

$$\big(1+L^{(1)}\sqrt{\Delta t}\big)^{\dagger}\big(1+L^{(1)}\sqrt{\Delta t}\big)+\Delta t\sum_{n\geq 2}L^{(n)\dagger}L^{(n)}=1.$$

It follows that

$$K^{(1)}=-\frac{1}{2}\sqrt{\Delta t}\sum_{n}L^{(n)\dagger}L^{(n)}. \qquad (2.32)$$

Using (2.32) in (2.31) we can write the change in ρ in the limit $\Delta t\to 0$ as

$$\frac{d\rho}{dt}=\mathfrak{L}\rho=-i[H,\rho]+\frac{1}{2}\sum_{n}\Big([L^{(n)}\rho,L^{(n)\dagger}]+[L^{(n)},\rho L^{(n)\dagger}]\Big). \qquad (2.33)$$

This is the Kossakowski-Lindblad master equation. The Kossakowski-Lindblad equation is *the most general allowed form* for quantum master equations if we assume complete positivity for the open dynamics. The first term on the right

hand side in (2.33) is like the familiar one from the von Neumann equation for isolated quantum systems. The last term containing $L^{(n)}$ represent the non-unitary part of the open evolution. We may call H the "Hamiltonian" part of the generator and $\pounds + i[H\,,\,\cdot]$ the dissipative part. It must be noted that in general H is not the same as the Hamiltonian H_0 of the free quantum system. Identifying the operators $L^{(n)}$ and constructing the generator $\pounds$ of the dynamical semi-group is possible in many cases of interest (for instance, see [4, 7, 24]). The open quantum evolution can then be treated as a Markov process governed by a differential equation. The dynamical evolution of the system can be traced continuously rather than in discrete steps when the maps are such that they allow a semi-group structure. Appropriate choices of $L^{(n)}$ can describe relaxation and decoherence that the system may undergo.

From the previous discussion we know that the Kossakowski-Lindblad equation gives the correct description of the irreversible evolution of an open quantum system in contact with a reservoir provided the decay time t_r or the correlations of the reservoir is much shorter than the typical relaxation times t_s of the system. If this condition is not met the dynamics of ρ will be given by a much more complicated integro-differential equation (a generalized master equation). The description of finite time translations of the system by the dynamical maps will still hold but as we noted in the beginning of this section, the maps will not have a semi-group structure. The generalized master equation can be shown to reduce to the Kossakowski-Lindblad form under suitable assumptions [7, 25].

Chapter 3

Two qubit example with initial entanglement

Entanglement is an enigmatic and uniquely fascinating quantum resource that has many uses and implications in quantum information theory. For instance entanglement opens the possibility of teleporting a quantum state (For a discussion on entanglement see Appendix A.2). The protocol for doing this is already well known [26] and the proof of principle has been established experimentally for several types of quantum systems including photons [27] and atoms [28, 29]. Quantum logical operations that use the entanglement that may exist between qubits can be combined into quantum algorithms that can be used to perform computations that transcend the capacity of any conceivable classical algorithm. The ever increasing ability to control and measure individual quantum systems with precision prompts us to ask how entanglement with an external system can modify the reduced dynamics of a quantum system that is being observed.

In the previous Chapter, when we constructed completely positive maps as contraction of the unitary evolution of an extended system, we made it a point to emphasize that the initial state of the extended system has to be a simply separable tensor product of the state of the system of interest

and the state of the environment. In this Chapter we construct a simple example in which this is not the case and study the new features that initial entanglement and other correlations introduces into the reduced dynamics induced by unitary evolution of the extended system.

3.1 Two qubit examples

Consider two qubits described by two sets of Pauli matrices σ_1, σ_2, σ_3 and τ_1, τ_2 and τ_3. We call one of the qubits "the system" and the other one "the environment". The initial states of the qubits expressed in terms of the Pauli matrices are respectively

$$\rho_0 = \frac{1}{2}(1 + a_i\sigma_i) = \frac{1}{2}\begin{pmatrix} 1+a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1-a_3 \end{pmatrix} \tag{3.1}$$

for the system and

$$\eta_0 = \frac{1}{2}(1 + b_j\tau_j) = \frac{1}{2}\begin{pmatrix} 1+b_3 & b_1 - ib_2 \\ b_1 + ib_2 & 1-b_3 \end{pmatrix} \tag{3.2}$$

for the environment with $i, j = 1, 2, 3$. The two qubit system is initially in an entangled state

$$\mathcal{R}_0 = \frac{1}{4}(1 + a_i\sigma_i + b_j\tau_j + c_{ij}\sigma_i\tau_j). \tag{3.3}$$

Note that $\mathrm{tr}_\eta[\mathcal{R}_0] = \rho_0$ and $\mathrm{tr}_\rho[\mathcal{R}_0] = \eta_0$ where $\mathrm{tr}_{\sigma,\rho}$ denote partial traces with respect to the system and the environment qubit states. The overall initial state $\mathcal{R}$ is an *entangled state* of the two qubits for generic values of c_{ij} (except for $c_{ij} = a_i b_j$, $c_{ij} = 0$ etc).

The interaction between the two qubits is specified by the Hamiltonian

$$H = \frac{1}{2}\omega\sigma_3\tau_3. \tag{3.4}$$

There is no special significance for this choice of H but later on we will see that it does not miss any of the interesting features that can arise in the reduced dynamics of the system qubit. A long, but straightforward, calculation (see Appendix D for details) shows that after time t the state of the two qubit system is[1]

$$\begin{aligned}
\mathcal{R}_t \;= e^{-iHt}\mathcal{R}_0 e^{iHt} \;= \frac{1}{4}\big[&(a_1\cos\omega t - c_{23}\sin\omega t)\sigma_1 \\
&+ (a_2\cos\omega t + c_{13}\sin\omega t)\sigma_2 \\
&+ a_3\sigma_3 \\
&+ (b_1\cos\omega t - c_{32}\sin\omega t)\tau_1 \\
&+ (b_2\cos\omega t + c_{31}\sin\omega t)\tau_2 \\
&+ b_3\tau_3 \\
&+ c_{11}\sigma_1\tau_1 \;+\; c_{12}\sigma_1\tau_2 \\
&+ (c_{13}\cos\omega t + a_2\sin\omega t)\sigma_1\tau_3 \\
&+ c_{21}\sigma_2\tau_1 \;+\; c_{22}\sigma_2\tau_2 \\
&+ (c_{23}\cos\omega t - a_1\sin\omega t)\sigma_2\tau_3 \\
&+ (c_{31}\cos\omega t + b_2\sin\omega t)\sigma_3\tau_1 \\
&+ (c_{32}\cos\omega t - b_1\sin\omega t)\sigma_3\tau_2 \\
&+ c_{33}\sigma_3\tau_3\big].
\end{aligned} \tag{3.5}$$

[1] We use units in which $\hbar = 1$ throughout this dissertation

When the overall state undergoes unitary evolution from $\mathcal{R}_0$ to $\mathcal{R}_t$ the evolution of the σ qubit is given by the changes in the parameters a_1, a_2 and a_3 which are respectively the expectation values of the operators σ_1, σ_2 and σ_3. These transformations are

$$\begin{aligned} a_1 \rightarrow a_1' &= a_1 \cos\omega t - c_{23} \sin\omega t \\ a_2 \rightarrow a_2' &= a_2 \cos\omega t + c_{13} \sin\omega t \\ a_3 \rightarrow a_3' &= a_3 \end{aligned} \tag{3.6}$$

The three mean values a_1', a_2' and a_3' describe the state of the σ qubit at time t. Equation (3.6) is the dynamics of the system qubit in the Heisenberg picture. Strictly speaking this is all we are interested in since we are looking at the reduced dynamics induced on the system by the unitary coupled evolution of the two qubits. So it is really not necessary that we compute all the terms in Eq. (3.5) but we can get away with just computing the expectation values of the operators $e^{iHt}\sigma_i e^{-iHt}$ in the initial state $\mathcal{R}_0$. We choose to compute the time evolution of the two qubit state in its entirety for illustrative purposes showing the changes that happen to the second qubit as well as to the entanglement shared between the two. If we are to remain true to the spirit of investigating open quantum dynamics we must be content in just knowing the dynamics of the system given by the changes in time of a_1, a_2 and a_3. The changes to a_1, a_2 and a_3 come from the coupled evolution to only one other qubit in this example. In general, to obtain the most general transformation, we must have the system qubit coupled to at least two other qubits. The one

qubit environment is sufficient for our investigations because it can lead to all possible *extremal maps* on the system.

The appearance of the parameters c_{13} and c_{23} in the reduced dynamics of the σ qubit leads to the reduced dynamics being not completely positive when c_{13} and c_{23} are such that the initial two qubit state is entangled. We look at the transformation (3.6) in detail in the next two sections and contrast it with completely positive dynamics that appear when the initial two qubit state is simply separable.

3.2 The induced map at one time

Look at (3.6) when ωt is $\pi/2$. Then the mean values are changed to

$$a_1' = -c_{23} \ , \qquad a_2' = c_{13} \ , \qquad a_3' = a_3 \tag{3.7}$$

We consider the c_{23}, c_{13} to be parameters that describe the effect of the dynamics of the two qubits that drives the evolution of the σ qubit, not quantities that are part of the description of the initial state of the σ qubit. What we do will apply to different initial states of the σ qubit for the same fixed c_{23}, c_{13}.

The density matrix in equation (3.1) that describes the state of the σ qubit at time zero is changed to the density matrix

$$\rho' = \frac{1}{2}(1 + a_i'\sigma_i) = \frac{1}{2}(1 - c_{23}\sigma_1 + c_{13}\sigma_2 + a_3\sigma_3) \tag{3.8}$$

that describes the state of the σ qubit when ωt is $\pi/2$. This is the same for *all* the different $\vec{a} \equiv \langle\vec{\sigma}\rangle$ that are compatible with the same fixed c_{23} and c_{13} in

describing a possible initial state for the two qubits. We will refer to these as the *compatible* $\vec{a}$. This is a new feature of the reduced dynamics when there is initial entanglement. Not all states are allowed as possible initial states ρ_0 of the system qubit. For instance, even if the two qubits are in an entangled two qubit pure state then it is easy to see that neither one of the two can be in a pure state by themselves. The partial trace used to compute the single qubit density matrices from the two qubit state means that the individual qubits must be in mixed states. Since certain states are not allowed as initial states of the σ qubit we consider the domain of only those states that are compatible with the specification of the parameters c_{23} and c_{13} that appear explicitly in the reduced dynamics in the example. We call this the *compatibility domain*. We discuss the compatibility domain in detail in chapter 4.

To be meaningful, a map has to act on a *substantial set* of states. To insure that we have something substantial to consider here, we will assume that the set of compatible $\vec{a}$ is substantial. We will exclude those values of c_{23} and c_{13} that do not at least allow three-dimensional variation in the directions of the compatible $\vec{a}$. For example, we will not let c_{13} be 1, because that would imply a_2 and a_3 are zero. The set of compatible $\vec{a}$ will be described more completely in the next chapter.

3.2.1 Properties of the dynamical map at $\omega t = \pi/2$

To treat the transformations in (3.6) induced on the σ qubit as a dynamical map we have to extend it to a linear map $\Phi_{\frac{\pi}{2}}$ of *all* 2×2 matrices to

2×2 matrices defined by

$$1' = 1 - c_{23}\sigma_1 + c_{13}\sigma_2 \ , \qquad \sigma_1' = 0 \ , \qquad \sigma_2' = 0 \ , \qquad \sigma_3' = \sigma_3 \ . \tag{3.9}$$

By viewing the dynamical map as a map of the basis matrices we are now moving away from looking at it as the reduced dynamics induced by the unitary evolution of an extended system. We now treat it as a mathematical object in its own right that describes open evolution without reference to the nature and influence of the environment around the system of interest. When applied to states of the system, Eq. (3.9) takes each density matrix ρ described by equation (3.1), for each compatible $\vec{a}$ in each different direction, to the density matrix

$$\rho' = \frac{1}{2}(1' + \vec{a} \cdot \vec{\sigma}') = \frac{1}{2} \begin{pmatrix} 1 + a_3 & -c_{23} - ic_{13} \\ -c_{23} + ic_{13} & 1 - a_3 \end{pmatrix} . \tag{3.10}$$

that is the same as that described by equation (3.8). The map $\Phi_{\frac{\pi}{2}}$ takes every Hermitian matrix to a Hermitian matrix. It does not map every positive matrix to a positive matrix. The map takes

$$P = \frac{1}{2}(1 + \sigma_3) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{3.11}$$

which is positive, to

$$P' = \Phi_{\frac{\pi}{2}} P = \frac{1}{2}(1 - c_{23}\sigma_1 + c_{13}\sigma_2 + \sigma_3) = \frac{1}{2} \begin{pmatrix} 2 & -c_{23} - ic_{13} \\ -c_{23} + ic_{13} & 0 \end{pmatrix} .$$

The eigenvalues of P' are

$$\lambda_{+,-} = \frac{1}{2} \left(1 \pm \sqrt{1 + c_{23}^2 + c_{13}^2} \right) .$$

Clearly λ_- is not positive for all non-zero values of $c_{23}$and c_{13}.

Of course if ρ is a density matrix that gives a compatible mean value $\vec{a}$, the map takes ρ, described by equation (3.1), to the density matrix $\rho' = \Phi_{\frac{\pi}{2}}\rho$ described by equation (3.8), which is positive. To see explicitly that ρ' is positive, we compute its eigenvalues,

$$\lambda^{\rho}_{+,-} = \frac{1}{2}\left(1 \pm \sqrt{a_3^2 + c_{23}^2 + c_{13}^2}\right). \tag{3.12}$$

If a_3 is compatible with c_{12} and c_{13} in describing a possible state for the two qubits, then

$$c_{23}^2 + c_{13}^2 + a_3^2 \leq 1 \tag{3.13}$$

so that λ^{ρ}_{+} and λ^{ρ}_{-} are both positive.

The important difference between the density matrix ρ and the positive matrix P described by equation (3.11) is the factor a_3 multiplying σ_3 in the density matrix. If a_3 is changed to 1, the inequality (3.13) can fail. The map can fail to take positive matrices to positive matrices when it extends beyond density matrices for *compatible* $\vec{a}$.

We can now apply Choi's definition to check if the map is completely positive. We extend the map $\Phi_{\frac{\pi}{2}}$ to 4×4 matrices by taking its tensor product, $\Phi^{(2)}_{\frac{\pi}{2}} \equiv \Phi_{\frac{\pi}{2}} \otimes \mathbf{1}_2$, with the identity map of 2×2 matrices. We now consider the action of $\Phi^{(2)}_{\frac{\pi}{2}}$ on a *positive* 4×4 matrix of the form

$$\Pi = \rho \otimes \xi = \frac{1}{4}(1 + a_i\sigma_i) \otimes (1 + z_j\tau_j). \tag{3.14}$$

Note that to use Choi's result, ξ can be any complex 2×2 matrix and not necessarily a density matrix. On the other hand ξ has to be positive in order

to make Π positive. All that we have to do to make ξ a density matrix is to normalize it so that it has unit trace. This can be done without loss of generality and so here we choose ξ to be a density matrix. Now we can legitimately interpret the action of the extended map as the dynamics of a system made up of one qubit undergoing open evolution along with another qubit with trivial dynamics. The physical requirement is that valid two qubit states be mapped to other valid positive two qubit states. The action of $\Phi^{(2)}_{\frac{\pi}{2}}$ on Π is given by the extension of (3.9):

$$\begin{aligned}
(\sigma_1\tau_k)' &= \sigma_1'\tau_k' &&= 0,\\
(\sigma_2\tau_k)' &= \sigma_2'\tau_k' &&= 0,\\
(\sigma_3\tau_k)' &= \sigma_3'\tau_k' &&= \sigma_3\tau_k,\\
\tau_k' = (1\cdot\tau_k)' &= 1'\tau_k' &&= (1 + a_1\sigma_1 + a_2\sigma_2)\tau_k,
\end{aligned}$$

for $k = 1, 2, 3$. This and the reinterpreted equations (3.9) define a linear map of 4×4 matrices to 4×4 matrices. If $\Phi_{\frac{\pi}{2}}$ is completely positive, then $\Phi^{(2)}_{\frac{\pi}{2}}$ should take every positive matrix Π to a positive matrix. The action of $\Phi^{(2)}_{\frac{\pi}{2}}$ on Π is to map it to

$$\Pi' = \Phi^{(2)}_{\frac{\pi}{2}}\Pi = \frac{1}{4}\left[1' + a_i\sigma_i' + b_j\tau_j' + a_ib_j(\sigma_i\tau_j)'\right]. \tag{3.15}$$

The eigenvalues of Π' are

$$\begin{aligned}
\pi_{1\,,\,2} &= \frac{1}{4}(1 \pm Z)(1 - A)\\
\pi_{3\,,\,4} &= \frac{1}{4}(1 \pm Z)(1 + A)
\end{aligned}$$

where

$$Z = \sqrt{z_1^2 + z_2^2 + z_3^2} \quad \text{and} \quad A = \sqrt{a_3^2 + c_{23}^2 + c_{13}^2}.$$

Since we already know that $Z \leq 1$ the only way that some of the eigenvalues of Π' can be negative is if $A \geq 1$. From (3.13) we know that $A \geq 1$ only if the ρ in $\Pi = \rho \otimes \xi$ is a density matrix that lies outside the compatibility domain of $\Phi_{\frac{\pi}{2}}$. Of course, according to Choi's theorem the map is not completely positive because we can easily find valid density matrices ρ such that the positive matrix Π is taken into Π' which is not positive by $\Phi_{\frac{\pi}{2}}^{(2)}$. The fact that all such ρ lie outside the compatibility domain of $\Phi_{\frac{\pi}{2}}$ is a factor that has to be taken into account when we interpret the not completely positive nature of the maps that represent the reduced dynamics when there is initial entanglement. We will take up the issue of interpretation in detail in Chapter 7.

We can see that the compatibility domain is enough to give the linearity of the map physical meaning. Applied to density matrices, the linearity of the map says that if density matrices ρ_1 and ρ_2 are mapped to ρ_1' and ρ_2' then each density matrix

$$\nu = q\rho_1 + (1-q)\rho_2 \tag{3.16}$$

with $0 < q < 1$ is mapped to

$$\nu' = q\rho_1' + (1-q)\rho_2'. \tag{3.17}$$

Suppose ρ_1 and ρ_2 are density matrices for the σ qubit that give mean values $\vec{a}_{\rho_1}$ and $\vec{a}_{\rho_2}$. If both $\vec{a}_{\rho_1}$ and $\vec{a}_{\rho_2}$ are compatible with the same c_{23} and c_{13} in

describing an initial state of the two qubits, then so is

$$\vec{a}_\tau = q\vec{a}_{\rho_1} + (1-q)\vec{a}_{\rho_2}. \tag{3.18}$$

The compatibility domain is convex. Explicitly, if Π_{ρ_1} and Π_{ρ_2} are density matrices for the two qubits written in the form of equation (3.3) with $\vec{a}_{\rho_1}$ and $\vec{a}_{\rho_2}$ for $\vec{a}$ and the same c_{23} and c_{13}, then

$$\Pi_\nu = q\Pi_{\rho_1} + (1-q)\Pi_{\rho_2} \tag{3.19}$$

is a density matrix for the two qubits written in the same form with $\vec{a}_\nu$ for $\vec{a}$ and the same c_{23} and c_{13}. If ρ_1 and ρ_2 are in the compatibility domain, then so are all the ν defined by equation (3.16). For these, the linearity described by equations (3.16) and (3.17) has a meaningful physical interpretation.

3.2.2 A special case: The initial state is simply separable

A different map is an option if the initial state of the two qubits is a product state or if at least

$$c_{23} = a_2 b_3\,, \qquad c_{13} = a_1 b_3. \tag{3.20}$$

Then the density matrix ρ' described by equation (3.8) is

$$\rho' = \frac{1}{2}(1 - a_2 b_3 \sigma_1 + a_1 b_3 \sigma_2 + a_3 \sigma_3).$$

This is obtained from equation (3.1) with the linear map of 2×2 matrices defined either by equations (3.9) or by

$$1' = 1\,, \qquad \sigma_1' = b_3\sigma_2\,, \qquad \sigma_2' = -b_3\sigma_1\,, \qquad \sigma_3' = \sigma_3. \tag{3.21}$$

With the latter, every positive matrix maps to a positive matrix. In fact the map is completely positive.

This completely positive map is defined by equations (3.21) for a given fixed value of b_3. That puts no restrictions on $\vec{a}$, no limits on the initial state of the σ qubit. Every $\vec{a}$ is compatible with any b_3 in describing an initial state of the two qubits for which equations (3.20) hold; every state of the σ qubit can be combined with any state of the τ qubit in a product state for the two qubits. However we will see that the $\vec{a}$ compatible with given nonzero c_{23} and c_{13} in product states for the two qubits fill only a two-dimensional set embedded in the three-dimensional compatibility domain.

The completely positive map defined by equations (3.21) is an option only when equations (3.20) hold. Then both maps, from equations (3.9) and (3.21), reproduce the evolution of the σ qubit. There is a map defined by equations (3.9) for almost every initial state of the two qubits, with c_{23} and c_{13} changing continuously from state to state. Switching to the completely positive map when equations (3.20) hold would be a discontinuous change.

3.3 Time dependence

From the transformations to a_1, a_2 and a_3 in equation (3.6) for any t, we see that the reduced dynamics for the σ qubit is given by the map Φ_t

defined as follows:

$$1' = 1 + (-c_{23}\sigma_1 + c_{13}\sigma_2)\sin\omega t$$
$$\sigma_1' = \sigma_1\cos\omega t\,, \qquad \sigma_2' = \sigma_2\cos\omega t\,, \qquad \sigma_3' = \sigma_3. \tag{3.22}$$

Φ_t is a linear map $Q \to Q'$ of all 2×2 matrices to 2×2 matrices described by

$$Q^t_{rs} = \sum_{r's'} B_{rr';ss'}Q_{r's'} \tag{3.23}$$

where B is the matrix representation of the map Φ^t. The matrix B is given by (see Appendix B)

$$B = \begin{pmatrix} 1 & 0 & \frac{1}{2}c^*\sin\omega t & \cos\omega t \\ 0 & 0 & 0 & \frac{1}{2}c^*\sin\omega t \\ \frac{1}{2}c\sin\omega t & 0 & 0 & 0 \\ \cos\omega t & \frac{1}{2}c\sin\omega t & 0 & 1 \end{pmatrix} \tag{3.24}$$

where $c = -c_{23} + ic_{13}$ and the rows and columns of B are in the order 11, 12, 21, 22.

A vector

$$\psi_{1 \text{ or } 3} = \begin{pmatrix} \lambda \\ \frac{1}{2}c^*\sin\omega t \\ \frac{1}{2}c\sin\omega t \\ \lambda \end{pmatrix} \tag{3.25}$$

is an eigenvector of B with eigenvalue λ if

$$\lambda^2 - \lambda(1+\cos\omega t) - \frac{1}{4}|c|^2\sin^2\omega t = 0.$$

This yields two eigenvalues

$$\begin{aligned} \lambda_1 &= \frac{1}{2}\left(1+\cos\omega t + \sqrt{(1+\cos\omega t)^2 + |c|^2\sin^2\omega t}\right) \\ \lambda_3 &= \frac{1}{2}\left(1+\cos\omega t - \sqrt{(1+\cos\omega t)^2 + |c|^2\sin^2\omega t}\right) \end{aligned} \tag{3.26}$$

and eigenvectors

$$\begin{aligned} \psi_{1 \text{ or } 3} &= \psi_1 \quad \text{for} \quad \lambda = \lambda_1 \\ &= \psi_3 \quad \text{for} \quad \lambda = \lambda_3. \end{aligned} \tag{3.27}$$

Note that ψ_1 and ψ_3 are orthogonal because

$$\lambda_1 \lambda_3 = -\frac{1}{4}|c|^2 \sin^2 \omega t.$$

The squares of the lengths of the eigenvectors are

$$\begin{aligned} ||\psi_n||^2 &= 2\left(\lambda_n^2 + \frac{1}{4}|c|^2 \sin^2 \omega t\right) \\ &= 2\lambda_n(1 + \cos \omega t) + |c|^2 \sin^2 \omega t \end{aligned} \tag{3.28}$$

for $n = 1, 3$. A vector

$$\psi_{2 \text{ or } 4} = \begin{pmatrix} \lambda \\ -\frac{1}{2}c^* \sin \omega t \\ \frac{1}{2}c \sin \omega t \\ -\lambda \end{pmatrix} \tag{3.29}$$

is an eigenvector of B with eigenvalue λ if

$$\lambda^2 - \lambda(1 - \cos \omega t) - \frac{1}{4}|c|^2 \sin^2 \omega t = 0.$$

This yields two eigenvalues

$$\begin{aligned} \lambda_2 &= \frac{1}{2}\left(1 - \cos \omega t + \sqrt{(1 - \cos \omega t)^2 + |c|^2 \sin^2 \omega t}\right) \\ \lambda_4 &= \frac{1}{2}\left(1 - \cos \omega t - \sqrt{(1 - \cos \omega t)^2 + |c|^2 \sin^2 \omega t}\right) \end{aligned} \tag{3.30}$$

and eigenvectors

$$\begin{aligned} \psi_{2 \text{ or } 4} &= \psi_2 \quad \text{for} \quad \lambda = \lambda_2 \\ &= \psi_4 \quad \text{for} \quad \lambda = \lambda_4. \end{aligned} \tag{3.31}$$

Note that ψ_2 and ψ_4 are orthogonal because

$$\lambda_2 \lambda_4 = -\frac{1}{4}|c|^2 \sin^2 \omega t.$$

The squares of the lengths of the eigenvectors are

$$\begin{aligned} ||\psi_n||^2 &= 2\left(\lambda_n^2 + \frac{1}{4}|c|^2 \sin^2 \omega t\right) \\ &= 2\lambda_n(1 - \cos \omega t) + |c|^2 \sin^2 \omega t \end{aligned} \tag{3.32}$$

for $n = 2, 4$.

We see that, in all but a few exceptional cases, B has two positive eigenvalues λ_1 and λ_2 and two negative eigenvalues λ_3 and λ_4. That means the map is not completely positive; for a completely positive map, B is a positive matrix and its eigenvalues are all non-negative. A plot of the eigenvalues of B as a function of ωt when $|c|^2$ is $1/2$ is shown in Figure 3.1. The two negative eigenvalues λ_3 and λ_4 go to zero when ωt is $n\pi$; the map is the identity map for even n and rotation by π around the z axis for odd n. In Figure 3.2 the four eigenvalues are plotted as a function of $|c|^2$ at $\omega t = \pi/4$. For all values of c_{23} and c_{13} for which $|c|^2 \neq 0$, at least one of the eigenvalues of B is negative.

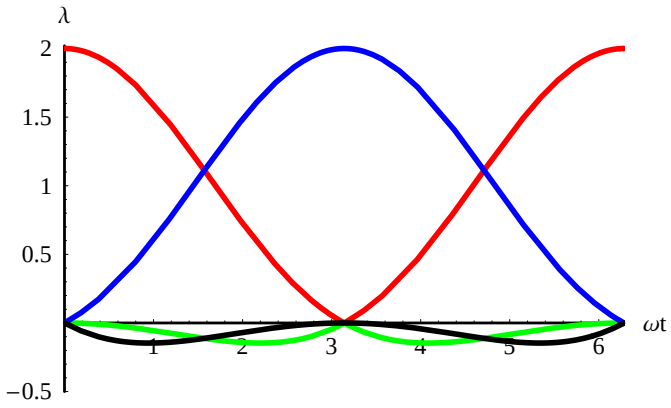

Figure 3.1: The eigenvalues of B as a function of ωt when $|c|^2$ is $\frac{1}{2}$. The red line is λ_1, the blue line is λ_2, the green line is λ_3, and black line is λ_4.

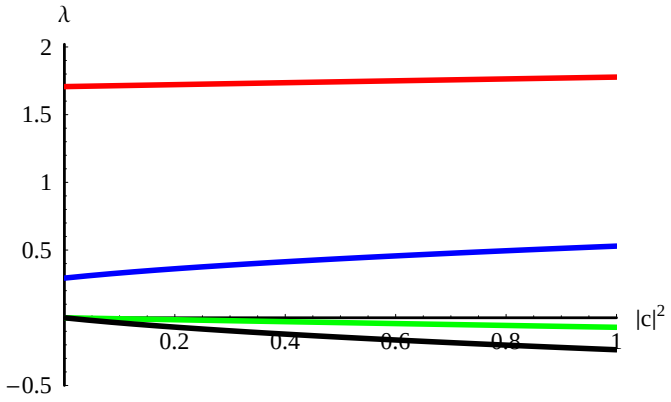

Figure 3.2: The eigenvalues of B as a function of $|c|^2$ when ωt is $\frac{\pi}{4}$. The red line is λ_1, the green line is λ_2, the blue line is λ_3, and black line is λ_4.

The spectral decomposition

$$B = \sum_{n=1}^{4} \lambda_n |n\rangle\langle n| \tag{3.33}$$

with

$$|n\rangle = \frac{1}{||\psi_n||}|\psi_n\rangle$$

yields

$$B_{rr';ss'} = \sum_{n=1}^{4} \lambda_n \langle r\, r'|n\rangle\langle s\, s'|n\rangle^* = \sum_{n=1}^{4} \mathrm{sign}(\lambda_n) C^{(n)}_{rr'} C^{(n)\dagger}_{s's} \tag{3.34}$$

with

$$C^{(n)}_{rr'} = \sqrt{|\lambda_n|}\langle r\, r'|n\rangle = \frac{\sqrt{|\lambda_n|}}{||\psi_n||}\langle r\, r'|\psi_n\rangle \tag{3.35}$$

so equation (3.23) is

$$Q'_{rs} = \sum_{n=1}^{4} \mathrm{sign}(\lambda_n) \sum_{r's'} C^{(n)}_{rr'} Q_{r's'} C^{(n)\dagger}_{s's}$$

or

$$Q' = \sum_{n=1}^{4} \mathrm{sign}(\lambda_n) C^{(n)} Q C^{(n)\dagger}.$$

Since $\mathrm{Tr}Q' = \mathrm{Tr}Q$ for all Q for our map,

$$\sum_{n=1}^{4} \mathrm{sign}(\lambda_n) C^{(n)\dagger} C^{(n)} = 1. \tag{3.36}$$

Except for the minus signs, these equations are the same as for completely positive maps. Explicitly we have

$$C^{(n)} = \sqrt{\frac{|\lambda_n|}{2\lambda_n(1+\cos\omega t) + |c|^2 \sin^2 \omega t}} \left[\lambda_n + \frac{1}{2}(-c_{23}\sigma_1 + c_{13}\sigma_2)\sin\omega t\right] \tag{3.37}$$

for $n = 1, 3$, and

$$C^{(n)} = \sqrt{\frac{|\lambda_n|}{2\lambda_n(1-\cos\omega t) + |c|^2 \sin^2 \omega t}} \left[\lambda_n \sigma_3 + \frac{i}{2}(c_{13}\sigma_1 - c_{23}\sigma_2)\sin\omega t\right] \tag{3.38}$$

for $n = 2, 4$.

3.3.1 Case 1: ωt is small

For small ωt and nonzero $|c|$

$$\begin{aligned}
\lambda_1 &= 2 - \frac{1}{2}(\omega t)^2 + \frac{1}{8}|c|^2(\omega t)^2 \\
\lambda_2 &= \frac{1}{2}|a|\omega t + \frac{1}{4}(\omega t)^2 + \frac{1}{16|c|}(\omega t)^3 \\
\lambda_3 &= -\frac{1}{8}|c|^2(\omega t)^2 \\
\lambda_4 &= -\frac{1}{2}|a|\omega t + \frac{1}{4}(\omega t)^2 - \frac{1}{16|c|}(\omega t)^3
\end{aligned} \tag{3.39}$$

and

$$\begin{aligned}
C^{(1)} &= 1 + \frac{\omega t}{4}(-c_{23}\sigma_1 + c_{13}\sigma_2) - \frac{(\omega t)^2}{8} \\
C^{(2)} &= \sqrt{\frac{|c|}{8}}\left[\sqrt{\omega t} + \frac{(\omega t)^{\frac{3}{2}}}{2|c|}\right]\sigma_3 + i\sqrt{\frac{1}{8|c|}}\sqrt{\omega t}(c_{13}\sigma_1 + c_{23}\sigma_2) \\
C^{(3)} &= \frac{\omega t}{4}(-c_{23}\sigma_1 + c_{13}\sigma_2) - \frac{|c|^2}{16}(\omega t)^2 \\
C^{(4)} &= \sqrt{\frac{|c|}{8}}\left[-\sqrt{\omega t} + \frac{(\omega t)^{\frac{3}{2}}}{2|c|}\right]\sigma_3 + i\sqrt{\frac{1}{8|c|}}\sqrt{\omega t}(c_{13}\sigma_1 + c_{23}\sigma_2).
\end{aligned} \tag{3.40}$$

3.3.2 Case 2: c_{13} and c_{23} are zero

When the parameters c_{13} and c_{23} are zero all forms of initial entanglement that affects the dynamics of the system of interest vanishes. In this case

we expect to find that the map is completely positive. The four eigenvalues of the dynamical matrix B are now

$$\begin{aligned} \lambda_1 &= 1 + \cos\omega t \\ \lambda_2 &= 1 - \cos\omega t \\ \lambda_3 &= 0 \\ \lambda_4 &= 0 \end{aligned} \tag{3.41}$$

which means that the map is indeed completely positive. The eigenvectors of B are

$$\begin{aligned} C^{(1)} &= \frac{1}{\sqrt{2}}\sqrt{1+\cos\omega t} = \cos(\omega t/2) \\ C^{(2)} &= \frac{1}{\sqrt{2}}\sqrt{1-\cos\omega t}\sigma_3 = -i\sin(\omega t/2)\sigma_3 \\ C^{(3)} &= 0 \\ C^{(4)} &= 0. \end{aligned} \tag{3.42}$$

Setting c_{12} and c_{23} to zero is not the same as treating the system and the reservoir as initially separable. It is actually doing more than that. By setting these parameters to zero we are effectively assuming that the system is in a tensor product state with an environment that is fully mixed. We will return to this special case in chapter 6 in the context of looking at the dynamical maps as affine transformations. The case where the initial state of the system and the reservoir is separable with the reservoir being in any state is considered next. In this case also we expect to end up with a dynamical map that is completely positive.

3.3.3 Time dependence without initial entanglement

In the absence of initial entanglement between the two qubits the map in (3.22) is modified to

$$1' = 1 + b_3(-a_2\sigma_1 + a_1\sigma_2)\sin\omega t$$
$$\sigma_1' = \sigma_1\cos\omega t\,, \qquad \sigma_2' = \sigma_2\cos\omega t\,, \qquad \sigma_3' = \sigma_3. \tag{3.43}$$

The map is completely positive and in matrix form it is given by

$$B = \begin{pmatrix} 1 & 0 & 0 & \cos\omega t - ib_3\sin\omega t \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \cos\omega t + ib_3\sin\omega t & 0 & 0 & 1 \end{pmatrix}. \tag{3.44}$$

Two of the eigenvalues of B, $\lambda_{3\,,4} = 0$ while the other two are also positive semi-definite and are given by

$$\lambda_{1\,,2} = 1 \pm \sqrt{\cos^2\omega t + b_3^2\sin^2\omega t}.$$

The corresponding eigenvectors are

$$\psi_1 = \begin{pmatrix} \frac{\cos\omega t - ib_3\sin\omega t}{\sqrt{\cos^2\omega t + b_3^2\sin^2\omega t}} \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad , \quad \psi_2 = \begin{pmatrix} -\frac{\cos\omega t - ib_3\sin\omega t}{\sqrt{\cos^2\omega t + b_3^2\sin^2\omega t}} \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

and

$$\psi_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad \psi_4 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Using

$$||\psi_1||^2 = ||\psi_2||^2 = 2 \quad \text{and} \quad ||\psi_3||^2 = ||\psi_4||^2 = 1$$

we obtain

$$C^{(1)} = \sqrt{\frac{\lambda_1}{2}} \begin{pmatrix} \frac{\cos\omega t - i b_3 \sin\omega t}{\sqrt{\cos^2\omega t + b_3^2 \sin^2\omega t}} & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.45}$$

$$C^{(2)} = \sqrt{\frac{\lambda_2}{2}} \begin{pmatrix} -\frac{\cos\omega t - i b_3 \sin\omega t}{\sqrt{\cos^2\omega t + b_3^2 \sin^2\omega t}} & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.46}$$

and

$$C^{(3)} = C^{(4)} = 0. \tag{3.47}$$

For small values of ωt we have

$$\begin{aligned} C^{(1)} &\simeq 1 - \frac{(1-b_3)^2(\omega t)^2}{8} \\ C^{(2)} &\simeq -\frac{1}{2}(1-b_3)\omega t\ \hat{\sigma}_3 \end{aligned} \tag{3.48}$$

3.3.4 The initial state is separable but not simply separable

The discussion so far has focused on the initial state of the two qubits being either entangled or simply separable. An intermediate possibility that we have to consider is when the initial state is separable but not a simple product state: Let us now assume that $\mathcal{R}$ is of the form

$$\mathcal{R} = \sum_{n=1}^{N} p_n \rho^n \otimes \eta^n \quad ; \quad N \geq 2 \tag{3.49}$$

with the system density matrix given by

$$\rho = \sum_{n=1}^{N} p_n \rho^n = \frac{1}{2}\left(1 + \sum_{i=1}^{3} a_i \sigma_i\right) \tag{3.50}$$

where

$$\rho^n = \frac{1}{2}\left(1 + \sum_{i=1}^{3} a_i^n \sigma_i\right) \quad \text{and} \quad a_i \equiv \sum_{n=1}^{N} p_n a_i^n. \tag{3.51}$$

Contraction of the unitary evolution of $\mathcal{R}$ yields a map on ρ of the form

$$\rho \rightarrow = \sum_{n=1}^{N} p_n B^n \rho^n = \widetilde{B} \sum_{n=1}^{N} p_n \rho^n = \widetilde{B}\rho, \tag{3.52}$$

where all B^n are completely positive maps. The transformations given in equation (3.6) now becomes

$$\begin{aligned} a_1(t) &= a_1 \cos\omega t - \sum_{n=1}^{N} p_n a_2^n b_3^n \sin\omega t \\ a_2(t) &= a_2 \cos\omega t + \sum_{n=1}^{N} p_n a_1^n b_3^n \sin\omega t \\ a_3(t) &= a_3 \end{aligned} \tag{3.53}$$

If all b_3^n are identical then the state is simply separable and the dynamical map is completely positive. On the other hand, if we treat the last terms of the first two equations in (3.53) as inhomogeneous shifts in a_1 and a_2 then the map looks very much like the case where $\mathcal{R}$ was entangled and we expect to get a not completely positive map describing the reduced dynamics of the system.

3.3.4.1 Example: the $n = 2$ case

Let us now consider the special case where $n = 1, 2$ with $p_1 = p$ and $p_2 = 1 - p$. Using Eq. (3.53) we can compute

$$\begin{aligned} 1 \pm a_3(t) &= 1 \pm a_3 \\ a_1(t) - i a_2(t) &= (a_1 - i a_2)\cos\omega t + \kappa^* \sin\omega t \\ a_1(t) + i a_2(t) &= (a_1 + i a_2)\cos\omega t + \kappa \sin\omega t \end{aligned} \tag{3.54}$$

where

$$\kappa = i[p(a_1^1 + ia_2^1)b_3^1 + (1-p)(a_1^2 + ia_2^2)b_3^2].$$

The effects of the (classical) correlations in the initial mixed state on the induced map is bundled together into the inhomogeneous term d. The A matrix corresponding to the map is easily written down:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2}\kappa^* \sin\omega t & \cos\omega t & 0 & \frac{1}{2}\kappa^* \sin\omega t \\ \frac{1}{2}\kappa \sin\omega t & 0 & \cos\omega t & \frac{1}{2}\kappa \sin\omega t \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.55}$$

The corresponding dynamical matrix B is

$$B = \begin{pmatrix} 1 & 0 & \frac{1}{2}\kappa^* \sin\omega t & \cos\omega t \\ 0 & 0 & 0 & \frac{1}{2}\kappa^* \sin\omega t \\ \frac{1}{2}\kappa \sin\omega t & 0 & 0 & 0 \\ \cos\omega t & \frac{1}{2}\kappa \sin\omega t & 0 & 1 \end{pmatrix}, \tag{3.56}$$

with eigenvalues

$$\begin{aligned} \lambda_{1\,,3} &= \frac{1}{2}\left(1 + \cos\omega t \pm \sqrt{(1+\cos\omega t)^2 + |\kappa|^2 \sin^2\omega t}\right) \\ \lambda_{2\,,4} &= \frac{1}{2}\left(1 - \cos\omega t \pm \sqrt{(1-\cos\omega t)^2 + |\kappa|^2 \sin^2\omega t}\right). \end{aligned} \tag{3.57}$$

It is easy to see that for generic values of the parameters a_i^n, b_i^n and p the eigenvalues of B are not positive semi-definite at all times signifying that an initial mixed (not simply separable) state also induces not completely positive dynamics on the system of interest.

Chapter 4

The compatibility and positivity domains

The compatibility domain has an important role to play in interpreting the action of not completely positive reduced dynamics. In this chapter we construct the compatibility domain for the example in chapter 3 and investigate it in detail. We also look at the *the positivity domain* which is the set of all states ρ of the σ qubit that are transformed to positive matrices by the action of the map defined at any fixed time t. The intersection of the positivity domains at all times is also studied and it is shown to be identical to the compatibility domain.

4.1 The compatibility domain

Once the parameters c_{23} and c_{13} that appear explicitly in the reduced dynamics of the system qubit are fixed, the compatibility domain is the set of all possible values of the vector (a_1, a_2, a_3) for which

$$\mathcal{R}_0 = \frac{1}{4}(1 + a_i\sigma_i + b_j\tau_j + c_{ij}\sigma_i\tau_j) \tag{4.1}$$

is a valid two qubit density matrix. In other words, for any (a_1, a_2, a_3) and fixed c_{23} and c_{13}, if there exists at least one choice of b_j, c_{11}, c_{12}, c_{21}, c_{22}, c_{31},

c_{32} and c_{33} for which $\mathcal{R}$ is a positive matrix of unit trace then that particular $(a_1,\, a_2,\, a_3)$ lies in the compatibility domain.

Suppose c_{23} and c_{13} are given. To write equations for the compatibility domain, we do a change of coordinates:

$$\begin{aligned} \sigma_+ &= \frac{c_{13}\sigma_1 + c_{23}\sigma_2}{\sqrt{c_{13}^2 + c_{23}^2}} \\ \sigma_- &= \frac{c_{23}\sigma_1 - c_{13}\sigma_2}{\sqrt{c_{13}^2 + c_{23}^2}}. \end{aligned} \tag{4.2}$$

We can use σ_+ and σ_- to rewrite the two qubit density matrix $\mathcal{R}$ in (4.1) with $a_1,\, a_2,\, a_3$ replaced by $a_+,\, a_-,\, a_3$ and c_{ij} replaced by $c_{kj},\ k = +,\, -,\, 3$. Using (4.2) we get c_{-3} is zero and

$$c_{+3} = \langle \sigma_+ \tau_1 \rangle = \sqrt{c_{13}^2 + c_{23}^2}. \tag{4.3}$$

An advantage of using this coordinate system is that the dynamical map is specified by the single fixed value of c_{+3} with $c_{-3} = 0$. The compatibility domain is the set of $\vec{a}$, or $a_+,\, a_-,\, a_3$, that are compatible with the given c_{+3} and zero c_{-3} in describing a possible initial state for the two qubits.

4.1.1 Sections of the compatibility domain

Basic outlines of the compatibility domain are easy to see. When a_+ is zero, the compatibility domain includes the $a_-,\, a_3$ such that

$$a_-^2 + a_3^2 + c_{+3}^2 \leq 1 \tag{4.4}$$

because for these

$$\Pi = \frac{1}{4}(1 + a_-\sigma_- + a_3\sigma_3 + c_{+3}\sigma_+\tau_3) \tag{4.5}$$

is a density matrix for the two qubits. Larger a_- and a_3 are not included. If

$$(x_-)^2 + (x_3)^2 + (c_{+3})^2 = 1$$

and $r > 1$, then

$$\begin{aligned}\Pi &= \frac{1}{4}\Big(1 + rx_-\sigma_- + rx_3\sigma_3 + c_{+3}\sigma_+\tau_3 \\ &\qquad + b_j\tau_j + z_{33}\sigma_3\tau_3 + \sum_{j=1}^{3}\sum_{k=1}^{2} z_{jk}\sigma_j\tau_k\Big)\end{aligned}$$

is not a density matrix for any b_j and z_{jk} because

$$W = \frac{1}{4}(1 - x_-\sigma_- - x_3\sigma_3 - c_{+3}\sigma_+\tau_3)$$

is a density matrix and

$$\mathrm{T}r[\Pi W] = \frac{1}{4}(1 - r(x_-)^2 - r(x_3)^2 - (c_{+3})^2) < 0.$$

When a_+ is zero, the compatibility domain is just the circular area described by (4.4); it cannot be extended in any direction in the a_-, a_3 plane (described by any ratio of a_- and a_3). This projection of the compatibility domain on the a_-, a_3 plane is shown in Figure 4.1 for the case where c_{+3} is $1/\sqrt{2}$.

When a_3 is zero, the compatibility domain is the elliptical area of a_-, a_+ such that

$$\frac{a_-^2}{1 - c_{+3}^2} + a_+^2 \leq 1. \tag{4.6}$$

To see this, we find the conditions for which the eigenvalues of

$$\Pi = \frac{1}{4}(1 + b_3\tau_3 + a_+\sigma_+ + a_-\sigma_- + a_3\sigma_3 + c_{+3}\sigma_+\tau_3 + c_{33}\sigma_3\tau_3) \tag{4.7}$$

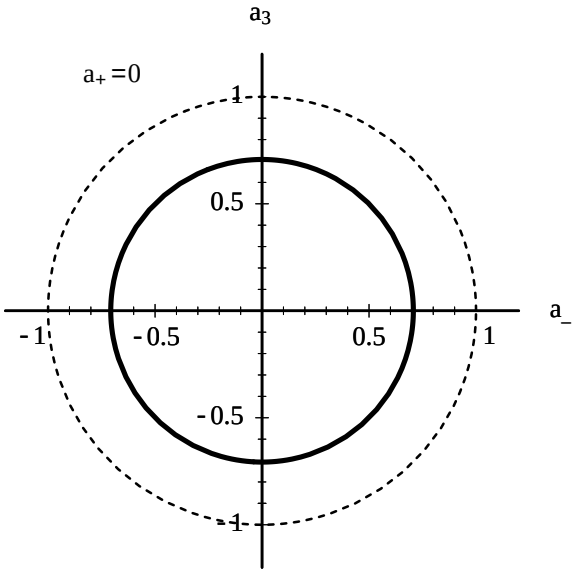

Figure 4.1: Section of the compatibility domain when $c_{+3} = \frac{1}{\sqrt{2}}$ and $a_+ = 0$. The area enclosed by the thick solid line is the compatibility domain. The dotted line shows the unit circle.

are all nonnegative so that Π is a density matrix for the two qubits. This particular choice of Π comes about in the following manner. We want to keep c_{+3} at a fixed value. But c_{+3} denotes the correlation between σ_+ polarization of the system qubit and the τ_3 polarization of the environment qubit. For as many possible values of a_+, we want to keep this correlation constant while at the same time keeping the two qubit density matrix positive. We expect that the allowed values of a_+ for which this can be done will depend on the coefficients of all the terms in the two qubit density matrix that contain τ_3. All such terms are included in Π except for c_{-3} which we want to be zero. Let

$$\Pi = \frac{1}{4}(1 + b_3\tau_3 + M).$$

Then

$$M^2 = a_+^2 + a_-^2 + a_3^2 + c_{+3}^2 + c_{33}^2 + 2a_3c_{33}\tau_3 + 2a_+c_{+3}\tau_3.$$

The eigenvalues of M are the square roots of the eigenvalues of M^2. When τ_3 has eigenvalue $+1$, the eigenvalues of Π are

$$\frac{1}{4}(1 + b_3 \pm \sqrt{m_+^2})$$

where m_+^2 is M^2 with τ_3 replaced by its eigenvalue $+1$. When τ_3 has eigenvalue -1, the eigenvalues of Π are

$$\frac{1}{4}(1 - b_3 \pm \sqrt{m_-^2})$$

where m_-^2 is M^2 with τ_3 replaced by its eigenvalue -1. The eigenvalues of Π are all nonnegative if

$$m_+^2 \leq (1 + b_3)^2 \tag{4.8}$$

$$m_-^2 \leq (1 - b_3)^2 \tag{4.9}$$

and $b_3^2 \leq 1$. When a_3 is zero, the areas of a_+, a_- allowed by the inequalities (4.8) and (4.9) are largest when c_{33} is zero. Then as b_3 varies from -1 to 1 the inequalities (4.8) and (4.9) describe the area of an ellipse with foci at $\pm c_{+3}$ on the a_+ axis; they say that the distance from a point with coordinates (a_+, a_-) to the focus at $-c_{+3}$ is bounded by $1 + b_3$ and the distance to the focus at c_{+3} is bounded by $1 - b_3$, so the sum of the distances is bounded by 2. That gives the elliptical area described by (4.6). We conclude that it is the compatibility domain when a_3 is zero. This conclusion is not changed if Π is given additional terms involving τ_1, τ_2, $\sigma_j\tau_1$, $\sigma_j\tau_2$. Each eigenvalue of M that

we considered to find the projection of the compatibility domain in the a_+, a_- plane is a diagonal matrix element $(\psi, \Pi\psi)$ with ψ being an eigenvector of τ_3 as well as being an eigenvector of the Π we considered, so $(\psi, \tau_1\psi)$, $(\psi, \tau_2\psi)$, $(\psi, \sigma_j\tau_1\psi)$, $(\psi, \sigma_j\tau_2\psi)$ are zero. Additional terms will change the eigenvalues and eigenvectors of Π but will not change the diagonal matrix elements we considered. They have to be nonnegative if Π is a density matrix. That is all we need to show that the inequality (4.6) describes the compatibility domain when a_3 is zero. The projection of the compatibility domain on the a_+, a_- plane is shown in Figure 4.2 for the case where c_{+3} is $1/\sqrt{2}$.

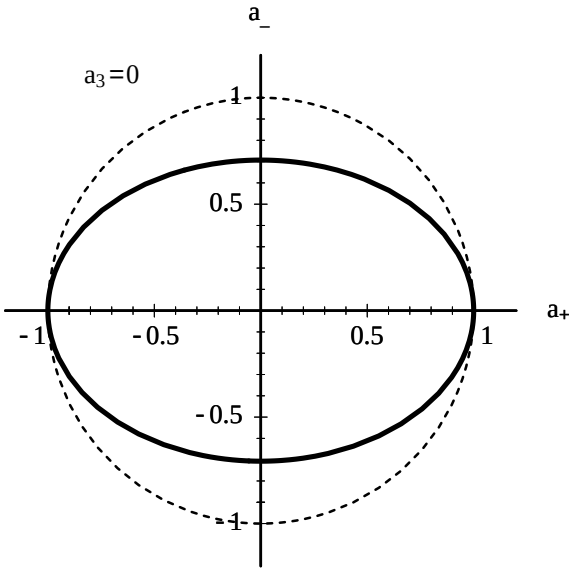

Figure 4.2: Section of the compatibility domain when $c_{+3} = \frac{1}{\sqrt{2}}$ and $a_3 = 0$.

When c_{23} and c_{13} are not both zero, all the product states (simply separable states) for the two qubits that are compatible with the given c_{+3}

and zero c_{-3} are for $\vec{a}$ in the projection of the compatibility domain in the a_+, a_3 plane. If

$$\begin{aligned} a_- b_3 &= c_{-3} = 0 \\ a_+ b_3 &= c_{+3} \neq 0 \end{aligned}$$

then $a_- = 0$ and

$$a_+^2 \geq c_{+3}^2. \tag{4.10}$$

There is a compatible product state for each such a_+ and each a_3 such that

$$a_3^2 \leq 1 - a_+^2, \tag{4.11}$$

with $a_- = 0$. The $\vec{a}$ for compatible product states fill the two areas in the a_+, a_3 plane bounded by sections of the unit circle from (4.11) and straight lines from (4.10). These areas are shown in Figure 4.3 for the case where c_{+3} is $1/\sqrt{2}$.

Since $\vec{a}$ cannot be outside the unit circle for any state, these sections of the unit circle are on the boundary of the compatibility domain. We can conclude that the boundary of the projection of the compatibility domain in the a_+, a_3 plane is completed by straight lines with constant values of a_3 between the sections of the unit circle, because we proved the compatibility domain is convex and from (4.4), (4.11) and (4.10) we see that a_3^2 cannot be larger when a_+ is zero than it is at the termini of the sections of the unit circle. The complete boundary in shown in Figure 4.3 for the case where c_{+3} is $1/\sqrt{2}$.

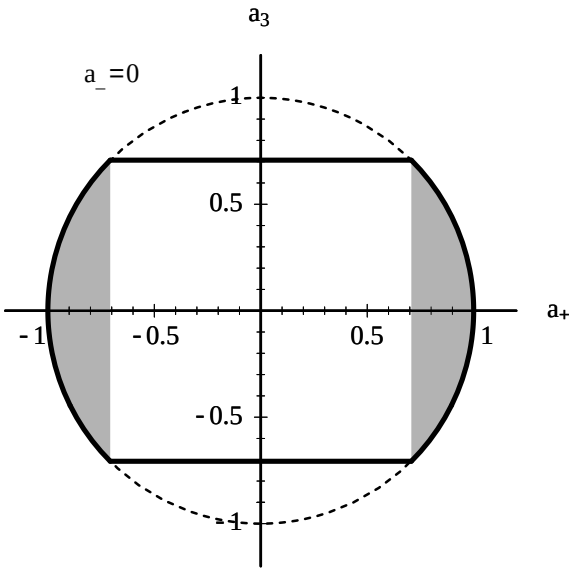

Figure 4.3: Section of the compatibility domain when $c_{+3} = \frac{1}{\sqrt{2}}$ and $a_- = 0$. The shaded area shows the $\langle \vec{\sigma} \rangle$ for product states compatible with the given c_{+3} and zero c_{-3}.

4.1.2 The whole compatibility domain

From the three orthogonal sections of the compatibility domain we now construct the whole domain in a_1, a_2, a_3 space. We will show that the compatibility domain is the set of $\vec{a}$ where

$$\sqrt{(a_+^2 + a_-^2 + c_{+3}^2)^2 - 4a_+^2 c_{+3}^2} \leq 2 - 2a_3^2 - a_+^2 - a_-^2 - c_{+3}^2. \tag{4.12}$$

First let us see what this says. Squaring both sides of (4.12) gives

$$a_+^2 + a_-^2 + a_3^2 + c_{+3}^2 - \frac{a_+^2 c_{+3}^2}{1 - a_3^2} \leq 1. \tag{4.13}$$

When a_+ is zero, (4.13) gives

$$a_-^2 + a_3^2 + c_{+3}^2 \leq 1$$

which is the inequality (4.4) that describes the circular projection of the compatibility domain in the a_-, a_3 plane. When a_3 is zero, from (4.13) we obtain,

$$a_+^2(1-c_{+3}^2)+a_-^2 \leq 1-c_{+3}^2$$

which is the inequality (4.6) that describes the elliptical projection of the compatibility domain in the a_+, a_- plane. Using (4.13) we can write down equations for sections of the compatibility domain in planes parallel to the a_+, a_- plane. If a_3^2 is between zero and $1-c_{+3}^2$, then

$$\frac{a_-^2}{1-c_{+3}^2-a_3^2}+\frac{a_+^2}{1-a_3^2} \leq 1. \tag{4.14}$$

A contour of the compatibility domain at constant a_3 is an ellipse. As a_3^2 approaches $1-c_{+3}^2$ the semi-minor axis shrinks to zero and the semi-major axis goes to c_{+3}, so the ellipse reduces to a line from $-c_{+3}$ to c_{+3} along the a_+ axis.

When a_- is zero, it is easier to start from the inequality (4.12) rather than (4.13) and we obtain

$$a_3^2 \leq 1-\frac{a_+^2+c_{+3}^2}{2}-\frac{|a_+^2-c_{+3}^2|}{2}, \tag{4.15}$$

which is (4.11) when $a_+^2 \geq c_{+3}^2$ and is

$$a_3^2 \leq 1-c_{+3}^2 \tag{4.16}$$

when $a_+^2 \leq c_{+3}^2$. That describes the area bounded by sections of the unit circle and straight lines that is the projection of the compatibility domain in the a_+, a_3 plane.

When c_{+3} is zero, (4.12) just says that $\vec{a}$ is on or inside the unit sphere; then there is no restriction on $\vec{a}$ from compatibility. A three-dimensional view of the compatibility domain is shown in Figure 4.4 for the case where c_{+3} is $1/\sqrt{2}$.

The inequality (4.12) puts a bound on a_3^2 for each a_+ and a_-. In particular, it says a_3^2 can never be larger than the values it has when a_- is zero; the bound (4.16) holds for the entire compatibility domain. For a_3^2 within this bound, the left side of (4.13) is an increasing function of a_+^2. The inequality (4.13) puts a bound on a_-^2 for each a_+ and a_3 and a bound on a_+^2 for each a_- and a_3.

To show that the set of $\vec{a}$ described by (4.12) is indeed in the compatibility domain, we show that for each $\vec{a}$ that satisfies (4.12) there is a Π of the form

$$\Pi = \frac{1}{4}(1 + b_1\tau_3 + a_+\sigma_+ + a_-\sigma_- + a_3\sigma_3 + c_{+3}\sigma_+\tau_3 + c_{33}\sigma_3\tau_3),$$

which is the same as in (4.7), that is a density matrix for the two qubits. We let

$$b_3 = \frac{a_+c_{+3}}{1 - a_3^2} \tag{4.17}$$

and

$$c_{33} = a_3b_3. \tag{4.18}$$

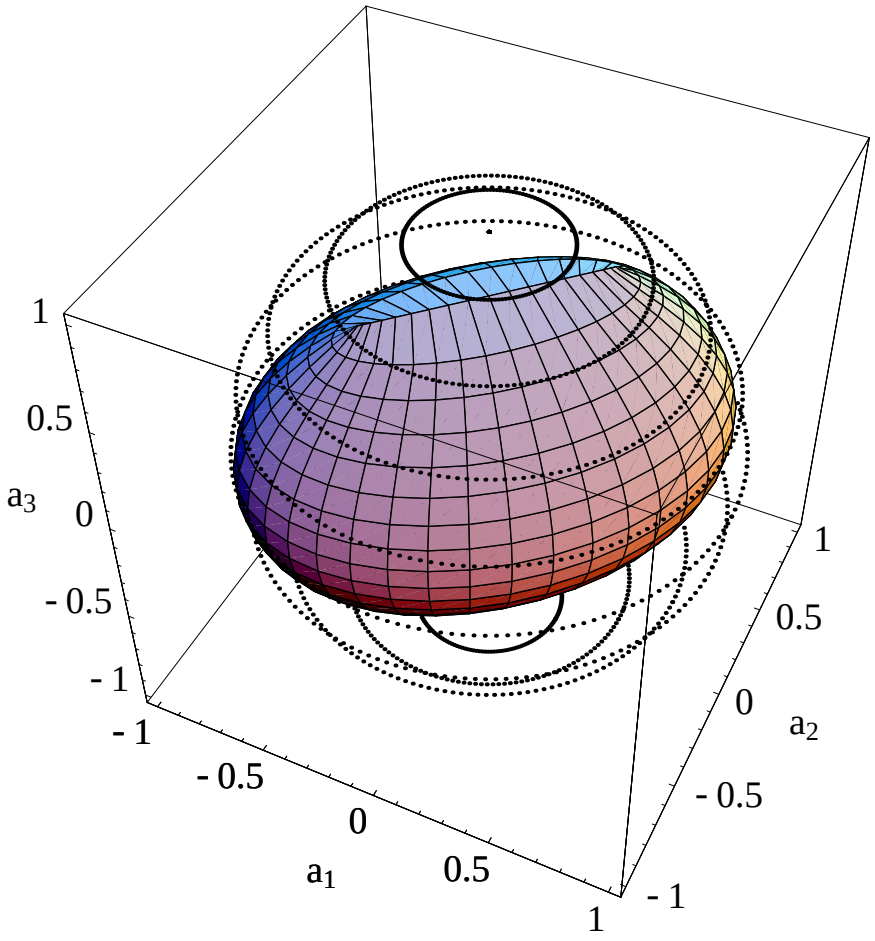

Figure 4.4: The compatibility domain generated using *Mathematica* for the case where c_{23} and c_{13} are both $\frac{1}{2}$. The dotted sphere is the unit sphere (the Bloch sphere) that represents all possible states of the qubit.

Then the inequalities (4.8) and (4.9) tell us that for Π to be a positive matrix,

$$m_{\pm}^2 \leq (1 \pm b_3)^2$$

where

$$m_{\pm}^2 = a_+^2 + a_-^2 + a_3^2 + c_{+3}^2 + c_{33}^2 \pm 2a_3c_{33} \pm 2a_+c_{+3}.$$

It is easy to verify that for the choice of b_1 and c_{33} in equation (4.17) and (4.18), $m_{\pm}^2$ is less than $(1 \pm b_1)^2$. For Π to be a valid two qubit density matrix we have to verify that $-1 \leq b_1 \leq 1$ for the choice made in (4.17). From (4.12) we see that,

$$|b_3| \leq \frac{|a_+|}{c_{+3}} \leq 1 \tag{4.19}$$

for $a_+^2 \leq c_{+3}^2$, and from (4.11), which holds for any $\vec{a}$,

$$|b_3| \leq \frac{c_{+3}}{|a_+|} \leq 1 \tag{4.20}$$

for $a_+^2 \geq c_{+3}^2$. Thus we see that $-1 \leq b_1 \leq 1$ as it should be for Π to be a density matrix.

The inequality (4.13) by itself does not imply that $\vec{a}$ is in the compatibility domain. The equality limit of (4.13) is a quadratic equation for a_3^2. The equality limit of (4.12) is one solution. In the other solution, the sign of the square root in (4.12) is changed. That changes the sign of the term with the absolute value in (4.15), which extends the boundary to include the entire area of the unit circle in the a_+, a_3 plane. The bounds (4.16) on a_3^2 and (4.19) on $|b_3|$ do not hold for the other solution. They are not implied by (4.12).

4.2 A different approach for obtaining the compatibility domain

A necessary and sufficient condition for any matrix to be positive semi-definite is that all its minors along the principal diagonal are all positive semi-definite. If we apply this condition to the six 2×2 minors along the diagonal of the two qubit density matrix $\mathcal{R}$ we obtain the following equations:

$$\begin{aligned} (1+a_3)^2 - (b_3+c_{33})^2 &\geq (b_1+c_{31})^2 + (b_2+c_{32})^2 \\ (1-a_3)^2 - (b_3-c_{33})^2 &\geq (b_1-c_{31})^2 + (b_2-c_{32})^2 \end{aligned} \tag{4.21}$$

$$\begin{aligned} (1+c_{33})^2 - (a_3+b_3)^2 &\geq (c_{11}+c_{22})^2 + (c_{12}+c_{21})^2 \\ (1-c_{33})^2 - (a_3-b_3)^2 &\geq (c_{11}-c_{22})^2 + (c_{12}-c_{21})^2 \end{aligned} \tag{4.22}$$

$$\begin{aligned} (1+b_3)^2 - (a_3+c_{33})^2 &\geq (a_1+c_{13})^2 + (a_2+c_{23})^2 = (a_+ + c_{+3})^2 + a_-^2 \\ (1-b_3)^2 - (a_3-c_{33})^2 &\geq (a_1-c_{13})^2 - (a_2-c_{23})^2 = (a_+ - c_{+3})^2 + a_-^2 \end{aligned} \tag{4.23}$$

From equations (4.21) and (4.22) it is clear that to find the largest domain of values of $\{a_1, a_2, a_3\}$ that are compatible with two qubit density matrices keeping c_{13} and c_{23} fixed, we should choose b_1, b_2, c_{11}, c_{12}, c_{21}, c_{22}, c_{31} and c_{32} to be zero. Equation (4.23) may be re-written as

$$\begin{aligned} a_+^2 + a_-^2 + a_3^2 + c_{+3}^2 + c_{33}^2 + 2a_+c_{+3} + 2a_3c_{33} &\leq (1+b_3)^2 \\ a_+^2 + a_-^2 + a_3^2 + c_{+3}^2 + c_{33}^2 - 2a_+c_{+3} - 2a_3c_{33} &\leq (1-b_3)^2. \end{aligned} \tag{4.24}$$

Equation (4.24) is the same as equations (4.8) and (4.9) from which we obtained the section of the compatibility domain when a_3 is zero. For fixed

non-zero values of a_3 we obtain from (4.24) the ellipses with decreasing semi-major and semi-minor axes that form sections for the solid in Fig. 4.4.

4.3 The positivity domain

In the previous section we have shown that the set of $\vec{a}$ described by the inequality (4.12) is in the compatibility domain of the map defined by the contraction of unitary evolution of an initially entangled two qubit system. The compatibility domain is the same for all times. In a larger domain, which we call the *positivity domain*, every positive matrix is mapped to a positive matrix. The positivity domain depends on the time t. We will show that the set of $\vec{a}$ described by the inequality (4.12) is also the intersection of all the positivity domains for different t. This means that the intersection of the positivity domains for all times is the same as the compatibility domain; the compatibility domain cannot be larger, because it must be in every positivity domain for every t.

The positivity domain for each t is easily found from the map of the expectation values

$$\begin{aligned} a_1' &= a_1 \cos\omega t - c_{23} \sin\omega t \\ a_2' &= a_2 \cos\omega t + c_{13} \sin\omega t \\ a_3' &= a_3. \end{aligned} \tag{4.25}$$

Regardless of whether $\vec{a}$ is compatible, the density matrix of the system corresponding to $\vec{a}$, described by $\rho = 1/2(1 + a_i\sigma_1)$, is mapped to a positive matrix,

which is the density matrix for $\vec{a}\,'$, given by $\rho' = 1/2(1 + a'_i\sigma_i)$, if

$$a_1'^2 + a_2'^2 + a_3'^2 \leq 1 \tag{4.26}$$

which means $\vec{a}\,'$ is on or inside the unit sphere described by

$$a'_1 = \sin\theta\cos\varphi\,, \quad a'_2 = \sin\theta\sin\varphi\,, \quad a'_3 = \cos\theta \tag{4.27}$$

with θ, φ varying over all directions. Then $\vec{a}$ is on or inside the surface described by

$$\begin{aligned} a_1 &= c_{23}\tan\omega t + \frac{\sin\theta\cos\varphi}{\cos\omega t} \\ a_2 &= -c_{13}\tan\omega t + \frac{\sin\theta\sin\varphi}{\cos\omega t} \\ a_3 &= \cos\theta \quad ; \quad 0 \leq \theta \leq \pi\ ;\ 0 \leq \varphi \leq 2\pi \end{aligned} \tag{4.28}$$

which is obtained from the unit sphere by moving the center of the sphere through distances $(c_{23}\tan\omega t)$ and $(-c_{13}\tan\omega t)$ in the x and y directions and stretching the x and the y dimensions by a factor of $1/\cos\omega t$. The positivity domain is the intersection of this surface and its interior with the unit sphere and its interior, since $\vec{a}$ must also be on or inside the unit sphere. The positivity domain for different values of ωt is shown in Figure 4.5.

When ωt is $\pi/2$, the restriction (4.26) is just that

$$a_3^2 \leq 1 - c_{23}^2 - c_{13}^2. \tag{4.29}$$

Then the positivity domain is the part of the unit sphere where a_3^2 is within this bound. If c_{23} and c_{13} are not both zero, and t is not zero, the positivity

domain does not include the north pole point that corresponds to the matrix P of equation (3.11).

If c_{23} and c_{13} are both zero, the positivity domain is the entire interior and surface of the unit sphere. Then the map takes every density matrix to a density matrix and every positive matrix to a positive matrix. In fact the map is completely positive for all t. The two eigenvalues of the dynamical matrix B that are generally negative, λ_3 and λ_4, are in this case zero, so $C(3)$ and $C(4)$ are also zero. That leaves two positive eigenvalues

$$\lambda_1 = 1 + \cos\omega t\,, \qquad \lambda_2 = 1 - \cos\omega t \tag{4.30}$$

and just

$$C(1) = \sqrt{\frac{1+\cos\omega t}{2}}\,, \qquad C(2) = \sqrt{\frac{1-\cos\omega t}{2}}\sigma_3. \tag{4.31}$$

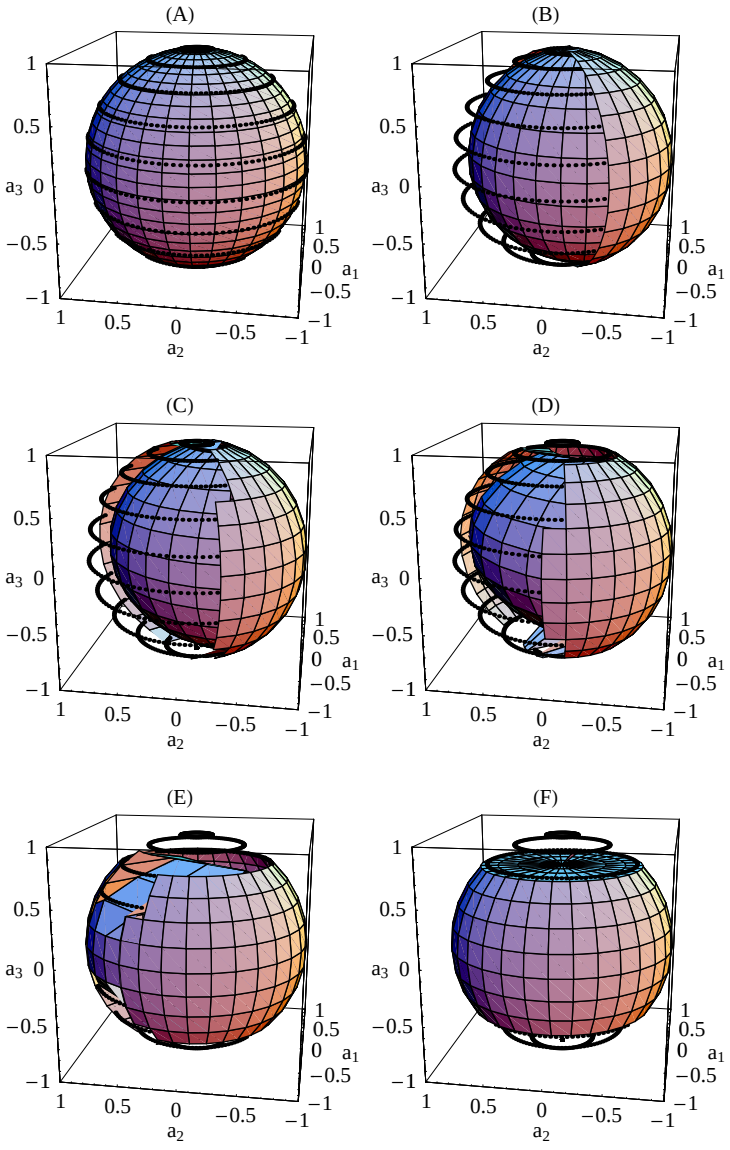

Figure 4.5: The positivity domains for (left to right) $\omega t = 0, \frac{\pi}{10}, \frac{2\pi}{10}, \frac{3\pi}{10}, \frac{4\pi}{10}$ and $\frac{\pi}{2}$ when $-c_{23} = c_{13} = \frac{1}{2}$. The surface of the unit sphere is shown with dotted lines where it is not the surface of the positivity domain.

4.4 The intersection of positivity domains

Consider three sets: the intersection of all the positivity domains for different t, the compatibility domain, and the set of $\vec{a}$ described by the inequality (4.12). We know these sets are nested; the intersection of the positivity domains contains the compatibility domain because every positivity domain contains the compatibility domain, and we showed that the compatibility domain contains the set of $\langle\vec{\sigma}\rangle$ described by (4.12). Now we will show that these three sets are the same; we will show that every point on the boundary of the set of $\langle\vec{\sigma}\rangle$ described by (4.12) is also on the boundary of a positivity domain for some t.

In terms of the a_+, a_- used to describe the compatibility domain, the equations (4.28) for $\vec{a}$ on the boundary of the positivity domain for time t are

$$\begin{aligned} a_+ &= -\frac{\sin\theta}{\cos\omega t}\sin(\varphi-\alpha) \\ a_- &= c_{+3}\tan\omega t - \frac{\sin\theta}{\cos\omega t}\cos(\varphi-\alpha) \\ a_3 &= \cos\theta \end{aligned} \tag{4.32}$$

with

$$-c_{23} = c_{+3}\cos\alpha \quad , \quad c_{13} = c_{+3}\sin\alpha. \tag{4.33}$$

If

$$\sin\omega t = \frac{c_{+3}\cos(\varphi-\alpha)}{\sin\theta} = \frac{c_{+3}\cos(\varphi-\alpha)}{\sqrt{1-a_3^2}} \tag{4.34}$$

then

$$\begin{aligned} a_+ &= -\sin\theta\sin\beta = -\sqrt{1-a_3^2}\,\sin\beta \\ a_- &= -\sqrt{\sin^2\theta - c_{+3}^2}\,\cos\beta = -\sqrt{1-a_3^2-c_{+3}^2}\,\cos\beta \end{aligned} \tag{4.35}$$

where

$$\begin{aligned} \sin\beta &= \frac{\sin(\varphi-\alpha)}{\cos\omega t} \\ \cos\beta &= \frac{\sqrt{\sin^2\theta - c_{+3}^2}\,\cos(\varphi-\alpha)}{\sin\theta\cos\omega t} \\ \tan\beta &= \frac{\sin\theta}{\sqrt{\sin^2\theta - c_{+3}^2}}\,\tan(\varphi-\alpha). \end{aligned} \tag{4.36}$$

It is easy to check that the sum of the squares of the formulas for $\sin\beta$ and $\cos\beta$ is 1, so the designations $\sin\beta$ and $\cos\beta$ are allowed. Each $\vec{a}$ described by these equations is on the boundary of a positivity domain. Equations (4.35) also describe the ellipses of (4.14) that are the contours of the boundary of the set of $\vec{a}$ described by the inequality (4.12). From equations (4.36) we see that all values of β from 0 to 2π are included as $\varphi-\alpha$ varies from 0 to 2π, so the whole of each ellipse is included. The bound (4.16) on a_3^2 ensures that (4.34) does not ask $|\sin\omega t|$ to be larger than 1 for any $\vec{a}$ that satisfies (4.12), so all the ellipses of (4.14) are included. Every point on the boundary of the set of $\vec{a}$ described by (4.12) is on the boundary of a positivity domain. This completes our proof that the compatibility domain and the intersection of the positivity domains both are the set of $\vec{a}$ described by the inequality (4.12).

There is no reason to expect that the intersection of all the positivity domains coincides with the compatibility domain. All we really require is that

the compatibility domain be inside the positivity domain for all times. The fact that the intersection of the positivity domains is identical to the compatibility domain is a rather surprising result in the example that we considered. There are some indications that in the generic case the compatibility domain is not identical but lies within the intersection of the positivity domains.

4.5 Discussion

The definition of the compatibility domain stands quite independent of the dynamical map that we wish to study. Even if we were not interested in any dynamical map we can still ask the following question: given an entangled state of a bipartite system with certain correlations having fixed values, what are the states of the subsystems that are allowed? The question is directly connected to Schrödinger's view on entanglement [30] (see Appendix A.1). The statement is that when there is entanglement, a complete knowledge of the whole system precludes us from knowing the states of the subsystems precisely. In our case complete knowledge of the extended system includes knowing the (fixed) values of the correlations $\langle \sigma_i \tau_j \rangle = c_{ij}$. The consequence of keeping these values fixed is that not all states of the system of interest are allowed. The most obvious example of a state that is not allowed is a pure state with $a_3 = 1$. Pure states correspond to complete knowledge of the subsystem which, as Schrödinger says, is something that is not always allowed if there is entanglement.

Finding the set of all allowed states of the subsystems given that the

expectation values of certain correlations in the global state are fixed is a well defined problem. Something that can be solved independent of what the reason for fixing these correlations at certain values are. In our case the reason for fixing them is the dynamical map at hand. The map may have been obtained by observations made *only* on the subsystem of interest without any knowledge about the other subsystem. We then seek to understand the origin of the map as following from the correlations between the two subsystems and the interaction between them.

The positivity domain, on the other hand, is well defined without even talking about an extended system or correlations in that extended system. Given a map we can blindly apply it to all possible states of the subsystem and figure out a subset of states on which the map is positive preserving.

When we put the notion of the compatibility domain and the positivity domain together we come across a consistent physical interpretation for the action of not completely positive maps. We observe that quantities that appear as parameters in the map can be understood as expectation values of correlations in the extended system; the dynamics of which led to the map on the system. All that we need now for the not completely positive map to acceptable as a possible description of open quantum evolution is that the compatibility arising from our construction of the extended state lie within the intersection of positivity domains at all times of the map. If this is so we can automatically restrict the action of the map on a set of states on which it is positive preserving.

Chapter 5

General forms for not completely positive reduced dynamics

The example we considered in the chapters 3 and 4 looked at two interacting qubits with initial entanglement between them. It is possible to generalize the results that we obtained in the case of the qubits to the case where we have two interacting quantum systems with larger state spaces. In this chapter we consider the reduced dynamics of an N-dimensional quantum system induced by the extended unitary evolution of a bipartite system with an arbitrarily large but finite dimensional Hilbert space.

5.1 N-dimensional system

Consider a quantum system described by $N \times N$ matrices. The $N \times N$ Hermitian matrices form a real linear space of N^2 dimensions with inner product

$$(A\,,\ B) = \mathrm{Tr}[A^\dagger B] = \sum_{j,k=1}^{N} A^*_{kj} B_{kj}. \tag{5.1}$$

Taking N^2 linearly independent Hermitian matrices that include the unit matrix 1, orthogonalizing them with a Gram-Schmidt process using the inner product (5.1), starting with the unit matrix, and multiplying by positive num-

bers for normalization, yields N^2 Hermitian matrices $F_{\mu 0}$ for $\mu = 0, 1, \ldots N^2-1$ such that F_{00} is 1 and

$$\mathrm{Tr}[F_{\mu 0} F_{\nu 0}] = N\delta_{\mu\nu}. \tag{5.2}$$

Every $N \times N$ matrix is a linear combination of the N^2 matrices $F_{\mu 0}$.

A state of this quantum system is described by a density matrix

$$\rho = \frac{1}{N}\left(1 + \sum_{\nu=1}^{N^2-1} f_\nu F_{\nu 0}\right). \tag{5.3}$$

Equations (5.2) imply that

$$\langle F_{\mu 0}\rangle = \mathrm{Tr}[F_{\mu 0}\rho] = f_\mu \tag{5.4}$$

for $\mu = 1, 2, \ldots N^2 - 1$ and $\langle F_{00}\rangle = 1$, so

$$\rho = \frac{1}{N}\left(1 + \sum_{\alpha=1}^{N^2-1} \langle F_{\alpha 0}\rangle F_{\alpha 0}\right). \tag{5.5}$$

Knowing ρ is equivalent to knowing the $N^2 - 1$ mean values $\langle F_{\mu 0}\rangle$ for $\mu = 1, 2, \ldots N^2 - 1$. The state is described either by the density matrix or by these mean values. We can see how the state changes in time by learning how these mean values change in time.

5.2 Reduced dynamics

Suppose this first system is entangled with and interacting with a second system described by $M \times M$ matrices. Let $F_{0\mu}$ for $\mu = 0, 1, \ldots M^2 - 1$ be Hermitian $M \times M$ matrices such that F_{00} is 1 and

$$\mathrm{Tr}[F_{0\mu} F_{0\nu}] = M\delta_{\mu\nu}. \tag{5.6}$$

The combined system is described by $NM \times NM$ matrices. Every $NM \times NM$ matrix is a linear combination of the matrices $F_{\mu 0} \otimes F_{0\nu}$ which are Hermitian and linearly independent. We use notation that identifies $F_{\mu 0}$ with $F_{\mu 0} \otimes 1$ and $F_{0\nu}$ with $1 \otimes F_{0\nu}$ and let

$$F_{\mu\nu} = F_{\mu 0} \otimes F_{0\nu}. \tag{5.7}$$

For these $NM \times NM$ matrices

$$\mathrm{Tr}[F_{\mu\nu} F_{\alpha\beta}] = NM\ \delta_{\mu\alpha}\delta_{\nu\beta}. \tag{5.8}$$

In the Heisenberg picture, evolution produced by a Hamiltonian H for the combined system changes each matrix $F_{\mu\nu}$ to a matrix

$$e^{iHt} F_{\mu\nu} e^{-iHt} = \sum_{\alpha=0}^{N^2-1} \sum_{\beta=0}^{M^2-1} t_{\mu\nu;\alpha\beta} F_{\alpha\beta} \tag{5.9}$$

with real $t_{\mu\nu;\alpha\beta}$. Since

$$\mathrm{Tr}\left[e^{iHt} F_{\mu\nu} e^{-iHt} e^{iHt} F_{\alpha\beta} e^{-iHt}\right] = \mathrm{Tr}[F_{\mu\nu} F_{\alpha\beta}], \tag{5.10}$$

the $t_{\mu\nu;\alpha\beta}$ form an orthogonal matrix, so $t^{-1}_{\alpha\beta;\mu\nu}$ is $t_{\mu\nu;\alpha\beta}$ and

$$e^{-iHt} F_{\alpha\beta} e^{iHt} = \sum_{\mu=0}^{N^2-1} \sum_{\nu=0}^{M^2-1} t_{\mu\nu;\alpha\beta} F_{\mu\nu}. \tag{5.11}$$

Since F_{00} is 1,

$$t_{00;\alpha\beta} = \delta_{0\alpha}\delta_{0\beta}\,, \qquad t_{\mu\nu;00} = \delta_{\mu 0}\delta_{\nu 0}. \tag{5.12}$$

Forming an orthogonal matrix is not the only property the $t_{\mu\nu;\alpha\beta}$ need to have. They must also yield

$$e^{iHt} F_{\mu\nu} e^{-iHt} = e^{iHt} F_{\mu 0} e^{-iHt} e^{iHt} F_{0\nu} e^{-iHt} \tag{5.13}$$

and the same with the time parameter t changed to $-t$.

The mean values $\langle F_{\mu 0}\rangle$ for $\mu = 1, 2, \ldots N^2 - 1$ that describe the state of the first system at time zero are changed to the mean values

$$\langle F_{\mu 0}\rangle' = \langle e^{iHt} F_{\mu 0} e^{-iHt}\rangle = d_\mu + \sum_{\alpha=1}^{N^2-1} t_{\mu 0;\alpha 0}\langle F_{\alpha 0}\rangle \tag{5.14}$$

that describe the state of the first system at time t, with

$$d_\mu = \sum_{\alpha=0}^{N^2-1}\sum_{\beta=1}^{M^2-1} t_{\mu 0;\alpha\beta}\langle F_{\alpha\beta}\rangle. \tag{5.15}$$

Mean values $\langle F_{\alpha 0}\rangle$ that describe the state of the first system at time t are in equation (5.14) but not in (5.15). We consider the d_μ, as well as the $t_{\mu 0;\alpha 0}$ to be parameters that describe the effect on the first system of the dynamics of the combined system that drives the evolution of the first system, not part of the description of the initial state of the first system.

The density matrix ρ of equation (5.5) that describes the state of the first system at time zero is changed to the density matrix

$$\rho' = \frac{1}{N}\left(1 + \sum_{\mu=1}^{N^2-1}\langle F_{\mu 0}\rangle' F_{\mu 0}\right) \tag{5.16}$$

that describes the state at time t. Equations (5.14) imply that this state is

$$\rho' = \frac{1}{N}\left(1 + \sum_{\mu=1}^{N^2-1} d_\mu F_{\mu 0} + \sum_{\alpha=1}^{N^2-1}\langle F_{\alpha 0}\rangle \sum_{\mu=1}^{N^2-1} t_{\mu 0;\alpha 0} F_{\mu 0}\right). \tag{5.17}$$

Equation (5.17) for ρ' can be obtained another way. In the Schrödinger picture the density matrix

$$\Pi = \frac{1}{NM}\left(1 + \sum_{\alpha=1}^{N^2-1}\langle F_{\alpha 0}\rangle F_{\alpha 0} + \sum_{\alpha=0}^{N^2-1}\sum_{\beta=1}^{M^2-1}\langle F_{\alpha\beta}\rangle F_{\alpha\beta}\right) \tag{5.18}$$

that represents the state of the combined system at time zero is changed at time t to

$$\begin{aligned} e^{-iHt}\Pi e^{iHt} &= \frac{1}{NM}\left(1+\sum_{\alpha=1}^{N^2-1}\langle F_{\alpha 0}\rangle\sum_{\mu=1}^{N^2-1}t_{\mu 0;\alpha 0}F_{\mu 0}\right. \\ &\quad +\sum_{\alpha=1}^{N^2-1}\langle F_{\alpha 0}\rangle\sum_{\mu=0}^{N^2-1}\sum_{\nu=1}^{M^2-1}t_{\mu\nu;\alpha 0}F_{\mu\nu} \\ &\quad +\sum_{\alpha=0}^{N^2-1}\sum_{\beta=1}^{M^2-1}\langle F_{\alpha\beta}\rangle\sum_{\mu=1}^{N^2-1}t_{\mu 0;\alpha\beta}F_{\mu 0} \\ &\quad \left.+\sum_{\alpha=0}^{N^2-1}\sum_{\beta=1}^{M^2-1}\langle F_{\alpha\beta}\rangle\sum_{\mu=0}^{N^2-1}\sum_{\nu=1}^{M^2-1}t_{\mu\nu;\alpha\beta}F_{\mu\nu}\right) \end{aligned} \tag{5.19}$$

according to equations (5.11). Taking the partial trace of this over the states of the second system eliminates the $F_{\mu\nu}$ for ν not zero and gives equation (5.17) for the density matrix of the first system at time t with equations (5.15) for the d_μ. Since this involves working with the larger system longer, it does not appear to be the easier way to actually carry out a calculation.

5.3 Properties of the dynamical map

The map from density matrices (5.5) at time zero to density matrices (5.17) at time t holds for all the varying mean values $\langle F_{\alpha 0}\rangle$ that are compatible with fixed mean values $\langle F_{\alpha\beta}\rangle$ in the d_μ in describing a possible initial state for the combined system. We will refer to them as compatible $\langle F_{\alpha 0}\rangle$. Almost all initial states of the combined system allow the compatible $\langle F_{\alpha 0}\rangle$ to vary as N^2-1 independent variables. We will consider only those initial states.

The map of density matrices extends to a linear map of all $N \times N$ matrices to $N \times N$ matrices defined by

$$1' = 1 + \sum_{\mu=1}^{N^2-1} d_\mu F_{\mu 0}\,, \qquad F'_{\alpha 0} = \sum_{\mu=1}^{N^2-1} t_{\mu 0;\alpha 0} F_{\mu 0}. \tag{5.20}$$

It takes the density matrix (5.5) to the density matrix (5.17) for each of the varying compatible $\langle F_{\alpha 0}\rangle$. It takes every Hermitian matrix to a Hermitian matrix.

The latter property alone is the foundation for basic forms of the map. This statement is independent of our other considerations.

Lemma 5.3.1. *If a linear map $Q \to Q'$ of $N \times N$ matrices to $N \times N$ matrices maps every Hermitian matrix to a Hermitian matrix, then in the description of the map by*

$$Q'_{rs} = \sum_{r',s'=1}^{N} B_{rr';ss'} Q_{r's'} \tag{5.21}$$

the $N^2 \times N^2$ matrix B is uniquely determined by the map and is Hermitian,

$$B^*_{rr';ss'} = B_{ss';rr'}, \tag{5.22}$$

and there are $N \times N$ matrices $C^{(n)}$ for $n = 1, \ldots N^2$ such that

$$Q' = \sum_{n=1}^{p} C^{(n)} Q C^{(n)\dagger} - \sum_{n=p+1}^{N^2} C^{(n)} Q C^{(n)\dagger} \tag{5.23}$$

for all Q, and

$$Tr[C^{(m)\dagger} C^{(n)}] = 0 \tag{5.24}$$

for $m \neq n$, for $m, n = 1, \ldots N^2$.

Proof: Let E_{jk} be the $N \times N$ matrices defined by

$$[E_{jk}]_{lm} = \delta_{lj}\delta_{mk}. \tag{5.25}$$

Clearly $E_{jk}^\dagger = E_{kj}$. If the map takes every Hermitian matrix to a Hermitian matrix, then $(\mathrm{Re}[E_{jk}])'$ and $(\mathrm{Im}[E_{jk}])'$ are Hermitian and

$$\{(E_{jk})'\}^\dagger = \{(\mathrm{Re}[E_{jk}])' + i(\mathrm{Im}[E_{jk}])'\}^\dagger = (\mathrm{Re}[E_{jk}])' - i(\mathrm{Im}[E_{jk}])' = (E_{jk}^\dagger)'. \tag{5.26}$$

Equations (5.21) and (5.25) give

$$[E'_{jk}]_{rs} = \sum_{r',s'} B_{rr';ss'}\delta_{r'l}\delta_{s'k} = B_{rl;sk} \tag{5.27}$$

which shows that the map determines a unique B, and with

$$(E'_{jk})^\dagger = (E_{jk}^\dagger)' = E'_{kj} \tag{5.28}$$

implies that $B^*_{sr';rs'} = B_{rs';sr'}$ which is the same as equation (5.22).

Since B is Hermitian, it has a spectral decomposition

$$B = \sum_{n=1}^{N^2} \lambda_n |n\rangle\langle n| \tag{5.29}$$

where the $|n\rangle$ are orthonormal eigenvectors of B and the λ_n are eigenvalues. The λ_n are real, but they are not necessarily all different, non-zero, or non-negative. We label them so that

$$\lambda_n \geq 0 \quad \text{for} \quad n = 1, \ldots p \qquad ; \qquad \lambda_n \leq 0 \quad \text{for} \quad n = p+1, \ldots N^2. \tag{5.30}$$

Then

$$B_{rr';ss'} = \sum_{n=1}^{p} \sqrt{|\lambda_n|}\langle r\, r'|n\rangle\langle n|s\, s'\rangle\sqrt{|\lambda_n|} - \sum_{n=p+1}^{N^2} \sqrt{|\lambda_n|}\langle r\, r'|n\rangle\langle n|s\, s'\rangle\sqrt{|\lambda_n|}. \tag{5.31}$$

Let

$$C^{(n)}_{rr'} = \sqrt{|\lambda_n|}\langle r\, r'|n\rangle. \tag{5.32}$$

Then equation (5.21) is

$$Q'_{rs} = \sum_{n=1}^{p}\sum_{r's'} C^{(n)}_{rr'} Q_{r's'} C^{(n)*}_{ss'} - \sum_{n=p+1}^{N^2}\sum_{r's'} C^{(n)}_{rr'} Q_{r's'} C^{(n)*}_{ss'} \tag{5.33}$$

so the map is described by equation (5.23), and

$$\begin{aligned} \mathrm{Tr}[C^{(m)\dagger}C^{(n)}] \quad &= \textstyle\sum_{rr'} C^{(m)*}_{rr'} C^{(n)}_{rr'} \\ &= \textstyle\sum_{rr'} \sqrt{|\lambda_m|}\langle m|r\, r'\rangle\langle r\, r'|n\rangle\sqrt{|\lambda_n|} = |\lambda_n|\langle m|n\rangle \end{aligned} \tag{5.34}$$

which is zero for $m \neq n$ in accord with equation (5.24).

This completes the proof of the Lemma.

The maps we are considering, those described by equations (5.20), have the additional property that

$$\mathrm{Tr}\ Q' = \mathrm{Tr}\ Q \tag{5.35}$$

for every Q. This implies that

$$\sum_{n=1}^{p} C^{(n)\dagger}C^{(n)} - \sum_{n=p+1}^{N^2} C^{(n)\dagger}C^{(n)} = 1 \tag{5.36}$$

because

$$\text{Tr } Q = \text{Tr } Q' = \text{Tr}\left[\left(\sum_{n=1}^{p} C^{(n)\dagger}C^{(n)} - \sum_{n=p+1}^{N^2} C^{(n)\dagger}C^{(n)}\right) Q\right] \tag{5.37}$$

implies that in the linear space of $N \times N$ matrices with the inner product defined by the trace as in (5.1), the difference between the two sides of equation (5.36) has zero inner product with every matrix Q and therefore must be zero. From equations (5.25) and (5.27) we see also that the trace-preserving property described by (5.35) implies that

$$\sum_{r} B_{rr';rs'} = \text{Tr}[E'_{r's'}] = \text{Tr}[E_{r's'}] = \delta_{r's'}. \tag{5.38}$$

Conversely, either equation (5.36) or (5.38) implies that Tr Q' equals Tr Q for every matrix Q. From equation (5.38) we see in particular that Tr B is N.

5.4 The Kossakowski equation for NCP maps

Extending the Kossakowski equation to not completely positive maps is straightforward. Let B be the dynamical matrix corresponding to such a map acting on an N dimensional open quantum system. Let $\{\lambda_\alpha\}$ and $\{\nu_\beta\}$ be the positive and negative eigenvalues of B with $\alpha = 1, \ldots m$, $\beta = 1, \ldots n$ and $m + n \leq N^2$. From equation (5.33) we see that the action of the map can be written in the form

$$\rho \to B\rho = \sum_{n=1}^{p} C^{(n)}\rho C^{(n)\dagger} - \sum_{n=p+1}^{N^2} C^{(n)}\rho C^{(n)\dagger} \tag{5.39}$$

where

$$\begin{aligned} C^{(n)} &\equiv \sqrt{\lambda_n}\xi(n) \quad ; \quad n = 1, \dots p \\ C^{(n)} &\equiv \sqrt{|\nu_n|}\zeta(n) \quad ; \quad n = p+1, \dots N^2, \end{aligned}$$

$\xi(n)$ and $\zeta(n)$ denoting the eigenvectors of B corresponding to the two sets of eigenvalues. Following equation (2.29) in the derivation of the Kossakowski equation in section 2.6 we define

$$\begin{aligned} C^{(1)} &= 1 + L^{(1)}\sqrt{\Delta t}, \\ C^{(n)} &= L^{(n)}\sqrt{\Delta t} \quad ; \quad n = 2, \dots p, \\ C^{(n)} &= \widetilde{L}^{(n)}\sqrt{\Delta t} \quad ; \quad n = p+1, \dots N^2. \end{aligned}$$

Carrying through the rest of the calculation just as in page 25 we obtain

$$\begin{aligned} \frac{d\rho}{dt} = \mathcal{L}\rho &= -i[H,\rho] + \frac{1}{2}\sum_{n=1}^{p}\Big([L^{(n)}\rho, L^{(n)\dagger}] + [L^{(n)}, \rho L^{(n)\dagger}]\Big) \\ &\quad -\frac{1}{2}\sum_{n=p+1}^{N^2}\Big([\widetilde{L}^{(n)}\rho, \widetilde{L}^{(n)\dagger}] + [\widetilde{L}^{(n)}, \rho\widetilde{L}^{(n)\dagger}]\Big), \quad (5.40) \end{aligned}$$

which is the extension of the Kossakowski equations to not completely positive maps when such maps form a continuous semi-group.

Chapter 6

More on dynamical maps of density matrices

The dynamical maps − whether they are completely positive or not − represent physical processes that a quantum system undergoes. Quite often there is the need to re-construct these dynamical processes from experimental data. In this Chapter we briefly describe how a dynamical map can be constructed from knowing the states of the system at two different times. This reconstruction is made possible by the knowledge of the mathematical properties of dynamical maps. We explore the structure of such maps which may or may not be completely positive and also present a way of parameterizing them. An alternate way of looking at the dynamical maps as affine transformations on the set of density matrices is also discussed.

6.1 Quantum process tomography

The method designed for experimentally determining complete information about a quantum process (dynamical map) is called *quantum process tomography* [16, 31, 32]. Knowledge of the dynamical maps acting on qubits due to the effects of its environment are needed if we are to correct for errors due to decoherence and other sources that inevitably creep into controlled

quantum processes like quantum gates.

Process tomography is a familiar procedure in classical physics and often appears in the form of "black box" problems. Given a black box with an input and output the aim is to reconstruct the process that happens within the box provided we have the ability to send any input we want into the box and measure the output that is produced. If the process that happens inside the box is linear and classical it is possible to find the response function of the box in many situations.

In our case we have a quantum black box. Inputs and outputs of the box are density matrices and we know that the process is linear. We assume here that we have some means of generating desired inputs at will and measuring the outputs accurately. We know that the process inside the box comes about due to the interaction of the input state with an unknown quantum or classical system inside the box. This process can always be described in terms of a dynamical map. The problem is to determine this unknown map.

From Eq. (5.33) in chapter 5 the general transformation on an input $N \times N$ density matrix is

$$\rho' = \sum_{n=1}^{p} C^{(n)} \rho C^{(n)\dagger} - \sum_{n=p+1}^{N^2} C^{(n)} \rho C^{(n)\dagger}. \tag{6.1}$$

Using the N^2 matrices $F_{\alpha 0}$ from the previous chapter we can write

$$C^{(n)} = \sum_{\alpha=0}^{N^2-1} c_{\alpha}^{(n)} F_{\alpha 0}. \tag{6.2}$$

In terms of the basis matrices $F_{\alpha 0}$ the map can be written in the form

$$\rho' = B\rho = \sum_{\alpha=0}^{N^2-1} \sum_{\beta=0}^{N^2-1} \chi_{\alpha\beta} F_{\alpha 0} \rho F_{\beta 0}^{\dagger} \tag{6.3}$$

where

$$\chi_{\alpha\beta} = \sum_{n} c_{\alpha}^{(n)} c_{\beta}^{(n)*}. \tag{6.4}$$

The map is now completely determined by the complex matrix $\chi_{\alpha\beta}$. The quantum process tomography we describe here is designed to find this matrix and from it the map.

Let ρ^j, $1 \leq j \leq N^2$ be a set of linearly independent *density matrices* that form a basis set for all $N \times N$ density matrices. We can always write

$$\rho^j = \frac{1}{N} \left(\mathbf{1} + \sum_{\alpha=1}^{N^2-1} a_{\alpha}^{j} F_{\alpha 0} \right)$$

even though $F_{\alpha 0}$ are themselves not density matrices.

We can now send each of the ρ^j into the quantum black box and measure the output $B\rho^j$ and we know express the output of the box as

$$B\rho^j = \bar{\rho}^j = \sum_{k} \theta_{jk} \rho^k. \tag{6.5}$$

Since $\bar{\rho}^j$ is known, θ_{jk} can be found provided $B\rho^j \neq B\rho^{j'}$ for $j \neq j'$. Since we have chosen the basis set ρ^j and the set of matrices $F_{\alpha 0}$ we can always compute theoretically the action of $F_{\alpha 0}$ on ρ^j:

$$F_{\alpha 0} \rho^j F_{\beta 0}^{\dagger} = \sum_{k} \Phi_{jk}^{\alpha\beta} \rho^k \tag{6.6}$$

where $\Phi_{jk}^{\alpha\beta}$ is a complex matrix that is completely determined. Using Eq. (6.5) and (6.6) we obtain

$$\sum_k \sum_{\alpha\beta} \chi_{\alpha\beta} \Phi_{jk}^{\alpha\beta} \rho^k = \sum_k \theta_{jk} \rho^k. \tag{6.7}$$

From the linear independence of ρ^k it follows that

$$\sum_{\alpha\beta} \chi_{\alpha\beta} \Phi_{jk}^{\alpha\beta} = \theta_{jk}. \tag{6.8}$$

Since we know θ_{jk} from the experimental results and $\Phi_{jk}^{\alpha\beta}$ from our computations we can find

$$\chi = \Phi^{-1}\theta \tag{6.9}$$

where Φ^{-1} must be thought of as a generalized inverse taken after flattening out θ and χ into column vectors just as we did earlier in the construction of the linear maps of matrices. Again, one must keep in mind that θ can be computed only if the inputs ρ^j into the black box can be chosen so that $B\rho^j \neq B\rho^{j'}$ for $j \neq j'$.

We see that it is indeed possible to find the nature of an unknown quantum processes by sending known inputs through the process and measuring the output. Experimentally this has been done in several simple systems (see for instance, [17] and references therein). In many of these experiments the quantum processes that are measured turn out to be not completely positive. What is interesting in the present context is that in many of these cases there has been attempts to explain the lack of complete positivity as a consequence of errors in the experiments. We hold the view that the measured

processes turn out to be not completely positive because of correlations that the input states have with its environment and to the black box because of imperfect control over initializing the inputs. This is a more natural way of explaining the observed lack of complete positivity rather than attributing it to experimental error.

Now that we know how to reconstruct a dynamical map by determining its action on known input states we turn our attention to ways of looking at the dynamical map that will give further insight into the nature of the physical process that leads to the map. As a first step we introduce a method of parameterizing not completely positive maps of density matrices in next section.

6.2 Parameterizing not completely positive maps

Consider action of an (extremal) map which is not completely positive on a density matrix, which we know can be expressed in the form

$$\rho \longrightarrow \sum_{n=1}^{p} C^{(n)} \rho C^{(n)\dagger} - \sum_{m=1}^{n} D^{(m)} \rho D^{(m)\dagger} \tag{6.10}$$

with

$$C^{(n)}_{rr'} = (\lambda_n)^{1/2} \zeta^{(n)}_{rr'}$$

and

$$D^{(m)}_{rr'} = (|\nu_m|)^{1/2} \eta^{(m)}_{rr'}$$

where λ_n and ν_m are the positive and negative eigenvalues of the map while $\zeta^{(n)}_{rr'}$ and $\eta^{(m)}_{rr'}$ are the corresponding eigenvectors. Here we have chosen to change

the notation a bit and use two different symbols C and D for the matrices coming from the positive and negative eigenvectors of the map for clarity in the following discussion.

The trace condition on the map can be written in the form

$$\sum_{n=1}^{p} C^{(n)\dagger} C^{(n)} - \sum_{m=1}^{q} D^{(m)\dagger} D^{(m)} = 1_{N\times N}. \tag{6.11}$$

The positivity condition yields the general result

$$\sum_{n=1}^{p} C^{(n)\dagger} u_n u_n^{\dagger} C^{(n)} - \sum_{m=1}^{q} D^{(m)\dagger} u_m u_m^{\dagger} D^{(m)} \geq 0 \tag{6.12}$$

Taking the trace on both sides of equation (6.11) we obtain:

$$\sum_{n=1}^{p} \mathrm{tr}\left[C^{(n)\dagger} C^{(n)}\right] - \sum_{m=1}^{q} \mathrm{tr}\left[D^{(m)\dagger} D^{(m)}\right] = N \tag{6.13}$$

Define

$$\sum_{n=1}^{p} C^{(n)\dagger} C^{(n)} = J \geq 0 \tag{6.14}$$

$$\sum_{m=1}^{n} D^{(m)\dagger} D^{(m)} = K \geq 0. \tag{6.15}$$

Since $C^{(n)\dagger}C^{(n)}$ is Hermitian so is J. We can therefore perform a unitary transformation U that diagonalizes J. By the trace condition the same unitary transformation automatically diagonalizes K. Then equation (6.11) becomes

$$\tilde{J} - \tilde{K} = 1$$

where $\tilde{J} = UJU^{\dagger}$ and $\tilde{K} = UKU^{\dagger}$

Let the eigenvalues of $\tilde{J}$ be j_i^2 and those of $\tilde{K}$ be k_i^2 $(0 \leq i \leq N)$. Since $\tilde{J} = \mathrm{diag}(j_1^2, j_2^2 \ldots j_N^2)$ and $\tilde{K} = \mathrm{diag}(k_1^2, k_2^2 \ldots k_N^2)$ we have the relation

$$j_i^2 = k_i^2 + 1$$

from the trace condition.

Define φ_i so that

$$j_i = \cosh\varphi_i \qquad , \qquad k_i = \sinh\varphi_i.$$

Now define

$$C^{(n)} = [\cosh\varphi]\ M^{(n)} \tag{6.16}$$

$$D^{(m)} = [\sinh\varphi]\ N^{(m)} \tag{6.17}$$

where we have extracted the matrices $[\cosh\varphi]$ and $[\sinh\varphi]$ from the matrices $C^{(n)}$ and $D^{(m)}$ respectively. It follows from equations (6.14) and (6.15) that

$$\sum_{n=1}^{p} M^{(n)\dagger} M^{(n)} = 1 \tag{6.18}$$

$$\sum_{m=1}^{q} N^{(m)\dagger} N^{(m)} = 1. \tag{6.19}$$

Parameterizing the matrices M and N are already known. In the cases where $\sinh\varphi = 0$, for all φ, we have only a smaller set of matrices to parameterize and this is identical to the case of having a completely positive map. Here we assume that $\sinh\varphi \neq 0$ and see how many parameters we need to write the map in the most general case (up to a unitary transformation).

Since the matrices $M^\dagger M$ are hermitian we first choose a unitary transformation W_1 that can diagonalize $M^{(1)\dagger}M^{(1)}$:

$$W_1^\dagger M^{(1)\dagger}M^{(1)}W_1 = \begin{pmatrix} \cos^2\theta_1^{(1)} & & & 0 \\ & \cos^2\theta_2^{(1)} & & \\ & & \ddots & \\ 0 & & & \cos^2\theta_N^{(1)} \end{pmatrix}$$

We can make further simplifications on $M^{(1)\dagger}M^{(1)}$ by noting the following: We can make an orthogonal coordinate transformation that transforms the density matrix $\rho(t)$ on which the map acts on i.e.

$$\rho(t) \longrightarrow \gamma(t)\rho(t)\gamma^\dagger(t),$$

or, equivalently,

$$\rho_{rs}(t) \longrightarrow \gamma_{rr'}(t)\gamma^*_{s's}\rho_{r's'}(t).$$

The transformation of the map B under the change of basis is given by

$$B \longrightarrow OBO^\dagger \quad ; \quad O_{rr';ss'} = \gamma_{rs}\delta_{r',s'}.$$

Since O is unitary matrix, the transformed map is equivalent to the original map. This freedom that we have to make orthogonal transformations on the coordinate system may be used to fix $\cos\theta_1^{(1)} = 1$. Thus we parameterize $M^{(1)}$ using $N-1$ angles $\theta_i^{(1)}$; $2 \le i \le N$.

Applying the transformation W_1 to both sides of equation (6.18) we obtain

$$\sum_{n=2}^{m} \tilde{M}_1^{(n)\dagger}\tilde{M}_1^{(n)} = \begin{pmatrix} 0 & & & 0 \\ & \sin^2\theta_2^{(1)} & & \\ & & \ddots & \\ 0 & & & \sin^2\theta_N^{(1)} \end{pmatrix} \tag{6.20}$$

Where $\tilde{M}_1^{(n)} = W_1^\dagger M^{(n)} V_1$ for $2 \leq n \leq p$. V_1 is another unitary matrix that reduces $\tilde{M}_1^n$ to the form that we want. We can now focus on the set of $(N-1) \times (N-1)$ matrices $M_1^{(n)}$ defined as

$$M_1^{(n)} \equiv \begin{pmatrix} \sin\theta_2^{(1)} & & & 0 \\ & \sin\theta_3^{(1)} & & \\ & & \ddots & \\ 0 & & & \sin\theta_N^{(1)} \end{pmatrix} \tilde{M}_1^{(n)} \quad ; \quad 2 \leq n \leq N$$

where we have dropped the first row and column of $\tilde{M}_1^{(n)}$ on the right hand side of the equation and also extracted the factor containing $\sin\theta_i^{(i)}$ from it. We assume that none of the $\sin\theta_i^{(i)}$ are zero since we are interested in computing the maximum number of parameters required for describing a generic extremal map that is not completely positive.

From equation (6.20) it follows that

$$\sum_{n=2}^{m} M_1^{(n)\dagger} M_1^{(n)} = 1_{(N-1)\times(N-1)}$$

the matrix $M_1^{(2)}$ in the first term of this sum can be parameterized using $N-2$ parameters using exactly the same procedure as before. Using a unitary transformation W_2 and a further orthogonal transformation (if needed) we can transform $M_1^{(2)}$ to the following form as before

$$M_1^{(2)} \longrightarrow \begin{pmatrix} 1 & & & 0 \\ & \cos\theta_2^{(2)} & & \\ & & \ddots & \\ 0 & & & \cos\theta_{N-1}^{(2)} \end{pmatrix}$$

Repeating this procedure m times, we parameterize all the matrices $C^{(n)}$. $D^{(m)}$ can also be parameterized in the same fashion. The total number of parameters

needed can be computed as follows. There are N angles φ_i. To parameterize the matrices $M^{(n)}$ we need $(N-1)+(N-2)+\ldots(N-p)$ parameters and for $N^{(m)}$ we need $(N-1)+(N-2)+\ldots(N-q)$ parameters. So in total we need

$$N^2 - \frac{p(p-1)+q(q-1)}{2} \tag{6.21}$$

parameters.

Note that the matrices $C^{(n)}$ and $D^{(m)}$ are determined only up to $p+q$ unitary matrices according to

$$C^{(n)} \longrightarrow C^{(n)}U^{(n)}$$

which leave equation (6.13) unchanged. We can see this also in the manner we defined $\tilde{M}_1^{(n)} = W_1^\dagger M^{(n)} V_1$ where we had to introduce the arbitrary unitary matrix V_1.

6.3 Dynamical maps as affine transformations

In fig. 2.1 and 4.5 we see the deformations of the unit sphere of all one qubit states when a few different types of dynamical maps act on it. The transformations that the unit sphere undergoes seem to arrange themselves into two classes:

- Homogeneous transformations that rotate and scale the unit sphere along various directions keeping its center fixed at the origin
- Inhomogeneous transformations that shift the entire sphere uniformly in some direction.

Motivated by this observation we can try to represent the dynamical maps; whether they be completely positive or not; in an affine form:

$$B\rho = \Xi\rho + K \tag{6.22}$$

where Ξ is the homogeneous part and K the inhomogeneous part that is independent of the density matrix ρ of the system.

It has been shown that it is always possible to write a dynamical map in this form [33–35]. Rewriting the map as an affine transformation is straightforward starting from the construction of the map as a contraction of the unitary evolution of an extended system. We have,

$$\rho^U = B\rho = \mathrm{tr}_R \left[U \mathcal{R}_{SR} U^\dagger \right] \tag{6.23}$$

where $\mathcal{R}_{SR}$ denotes the combined state of an $N-$dimensional system coupled to an $M-$dimensional reservoir and U is a unitary transformation on the combined state. Let ρ and ρ_R denote the reduced density matrices of the system and the reservoir respectively. We can re-write Eq. (6.23) as

$$\rho^U = \mathrm{tr}_R \left[U\rho \otimes \frac{1}{M}\mathbf{1}_R U^\dagger \right] + \mathrm{tr}_R \left[U \left(\mathcal{R}_{SR} - \rho \otimes \frac{1}{M}\mathbf{1}_R \right) U^\dagger \right] \tag{6.24}$$

where we have separated out the terms in the map based on their dependence on the starting state ρ. We now identify

$$\begin{aligned} \Xi\rho &= \mathrm{tr}_R \left[U\rho \otimes \frac{1}{M}\mathbf{1}_R U^\dagger \right] \\ K &= \mathrm{tr}_R \left[U \left(\mathcal{R}_{SR} - \rho \otimes \frac{1}{M}\mathbf{1}_R \right) U^\dagger \right]. \end{aligned} \tag{6.25}$$

We see from Eq. (6.25) that Ξ is a completely positive unital map.

6.3.1 General forms for Ξ and K

Using the basis matrices $F_{\alpha 0}$, $F_{0\beta}$ and $F_{\alpha\beta} = F_{\alpha 0} \otimes F_{0\beta}$ that we introduced in chapter 5 we can write down expressions for Ξ and K. The starting point is to notice that the unitary transformation U in Eq. (6.23) can always be written as

$$U = e^{-iHt} = \sum_{\mu=0}^{M^2-1} G^{(\mu)} \otimes F_{0\mu} \tag{6.26}$$

where G^{μ} are a set of operators on the system density matrix. In general $\{G^{(\mu)}\}$ does not form an orthonormal set but $F_{0\mu}$, as we know, do form such a set. The initial states of the system and the reservoir (reduced density matrices) are

$$\rho = \frac{1}{N}\left(\mathbf{1} + \sum_{\alpha=1}^{N^2-1} \langle F_{\alpha 0}\rangle F_{\alpha 0}\right), \tag{6.27}$$

$$\rho_R = \frac{1}{M}\left(\mathbf{1} + \sum_{\beta=1}^{M^2-1} \langle F_{0\beta}\rangle F_{0\beta}\right). \tag{6.28}$$

The initial state of the combined system is

$$\mathcal{R}_{SR} = \frac{1}{NM}\left(\mathbf{1} + \sum_{\alpha=1}^{N^2-1} \langle F_{\alpha 0}\rangle F_{\alpha 0} + \sum_{\beta=1}^{M^2-1} \langle F_{0\beta}\rangle F_{0\beta} + \sum_{\alpha=1}^{N^2-1}\sum_{\beta=1}^{M^2-1} \langle F_{\alpha\beta}\rangle F_{\alpha\beta}\right) \tag{6.29}$$

Using Eq. (6.26), (6.27) and (6.25) we obtain

$$\begin{aligned}
\Xi\rho &= \frac{1}{NM}\left(1 + \sum_{\alpha=1}^{N^2-1} \langle F_{\alpha 0}\rangle \sum_{\mu=0}^{M^2-1}\sum_{\nu=0}^{M^2-1} G^{(\mu)} F_{\alpha 0} G^{(\nu)\dagger} \mathrm{tr}_R\left[F_{0\mu} F_{0\nu}\right]\right) \\
&= \frac{1}{N}\left(1 + \sum_{\alpha=1}^{N^2-1}\sum_{\mu=0}^{M^2-1} \langle F_{\alpha 0}\rangle G^{(\mu)} F_{\alpha 0} G^{(\mu)\dagger}\right)
\end{aligned} \tag{6.30}$$

where we have used

$$\mathrm{tr}_R\left[F_{0\mu}F_{0\nu}\right] = M\delta_{\mu\nu}.$$

In a similar fashion we obtain the inhomogeneous part of B as

$$K = \frac{1}{N}\sum_{\alpha=0}^{N^2-1}\sum_{\beta=1}^{M^2-1}\langle F_{\alpha\beta}\rangle \sum_{\mu=0}^{M^2-1}\sum_{\nu=0}^{M^2-1} G^{(\mu)}F_{\alpha 0}G^{(\nu)\dagger}\frac{1}{M}\mathrm{tr}_R\left[F_{0\mu}F_{0\beta}F_{0\nu}\right]. \qquad (6.31)$$

Note that the inhomogeneous part K does not contain any terms with $\langle F_{\alpha 0}\rangle$ in it which means that it does not depend explicitly on ρ and it is a common shift for *all* ρ when the map B acts on them. The homogeneous part in Eq. (6.30) appears as the contraction of the unitary evolution of the systems coupled to the reservoir in the *maximally mixed state*. In other words Ξ is sensitive only to the state of the system and the interaction Hamiltonian connecting the system to the reservoir while it is not sensistive to the particular state of that the reservoir is in.

6.3.2 The map in the two qubit example in affine form

Let us now turn to re-writing the dynamical map obtained in chapter 3 for the two qubit example we considered. Since both the system and the reservoir are qubits we have

$$F_{00} = \mathbf{1}_{2\times 2} \quad ; \quad F_{\alpha 0} = \sigma_\alpha \quad ; \quad F_{0\beta} = \tau_\beta \quad , \quad \alpha,\, \beta = 1,2,3 \qquad (6.32)$$

where σ_α and τ_β are two sets of Pauli matrices. The unitary time evolution operator for the two qubit system corresponding to the Hamiltonian in Eq. (3.4) is

$$U(t) = \exp\left[-i\frac{1}{2}\omega t\sigma_3\tau_3\right] = \cos\left(\omega t/\,2\right) - i\sigma_3\tau_3\sin(\omega t/2). \qquad (6.33)$$

Using Eq. (6.26) and (6.32) we immediately obtain

$$G^{(0)} = \cos(\omega t/2) = \begin{pmatrix} \cos(\omega t/2) & 0 \\ 0 & \cos(\omega t/2) \end{pmatrix}, \tag{6.34}$$

$$G^{(3)} = -i\sigma_3 \sin(\omega t/2) = \begin{pmatrix} -i\sin(\omega t/2) & 0 \\ 0 & i\sin(\omega t/2) \end{pmatrix} \tag{6.35}$$

and $G^{(1)} = G^{(2)} = 0$. Comparison with Eq. (3.42) shown us that the $G-$matrices are the same as the eigenvectors for the dynamical matrix in the example when the parameters c_{13} and c_{23} are set to zero.

It is through the inhomogeneous shift K that the state of entanglement of the subsystems S and R affects the reduced dynamics of S. Using Eq. (6.31) we find that for our example

$$K = \frac{1}{2}(-c_{23}\sigma_1 + c_{12}\sigma_2)\sin\omega t \tag{6.36}$$

which is consistent with Eq. (3.22).

Chapter 7

Discussion and conclusion

Choi's approach to defining completely positive maps[1] has led to much discussion about the physical interpretation of completely positive and not completely positive dynamical maps. In the light of the understanding gained here, it is easy to see the problems with the arguments that a map describing the most general evolution of an open quantum system *has to be completely positive*. In this chapter we discuss how such arguments may be addressed and how a consistent picture of open quantum dynamics that may not be completely positive can be constructed.

7.1 The questions raised by Pechukas

In a paper entitled *Reduced dynamics need not be completely positive* [36], Pechukas directly questions the validity of assuming that the most general open quantum dynamics is described in terms of only completely positive maps. He, like us, concludes that completely positive dynamical maps cannot provide an accurate description of the dynamics in several situations that are physically quite reasonable. Pechukas' motivation for considering more general

[1] See page 15

possibilities like not completely positive maps is simple. In Chapter 2 we have already seen that a whole lot of dynamical possibilities are forbidden if only completely positive transformations are allowed. Pechukas considers relaxation behavior of quantum systems that under certain circumstances may proceed in a manner that is forbidden by complete positivity. Consider, for example, a qubit relaxing to equilibrium, ρ_{eq}: suppose that the process, in the basis of the eigenvectors of ρ_{eq}, is

$$\rho = \begin{pmatrix} p^{eq} + \epsilon & \delta \\ \delta & 1 - p^{eq} - \epsilon \end{pmatrix} \rightarrow \begin{pmatrix} p^{eq} + \zeta\epsilon & \beta\delta \\ \beta\delta & 1 - p^{eq} - \zeta\epsilon \end{pmatrix} \tag{7.1}$$

with ζ and β positive and both less than or equal to one. Let this relaxation process be described by a completely positive map of the form

$$\rho \rightarrow \Phi\rho = \sum_{\alpha} C(\alpha)\rho C(\alpha)^{\dagger} \quad ; \quad C(\alpha) = \begin{pmatrix} a_\alpha & c_\alpha \\ d_\alpha & b_\alpha \end{pmatrix}.$$

If we regard $\{a_\alpha\}$, $\{b_\alpha\}\ldots$ as vectors $\mathbf{a}$, $\mathbf{b}\ldots$ then it turns out that

$$\beta = (\mathbf{a}\,,\,\mathbf{b}) \qquad \text{and} \qquad \zeta = (\mathbf{a}\,,\,\mathbf{a}) + (\mathbf{b}\,,\,\mathbf{b})$$

and therefore using the Schwarz inequality

$$\beta \leq \frac{\zeta + 1}{2}. \tag{7.2}$$

Wince we are dealing with a relaxing system, we could write ζ and β as exponentials;

$$\zeta = e^{-t/T_1} \qquad \text{and} \qquad \beta = e^{-t/T_2},$$

and then we have $T_2 \leq 2T_1$. The relaxation rates of the diagonal elements cannot be faster than the off diagonal elements just from the restriction that

we have completely positive dynamics. Pechukas' main point is that such restrictions on the relaxation rates are artificial because it arises out of the very general assertion that the reduced dynamics be completely positive which is made without any reference to the specifics of the system. Moreover, the condition $T_2 \leq 2T_1$ does not even correspond to observations and numerical investigations in cases where the system under observation is strongly coupled to others around it [37–39]. The restriction $T_2 \leq 2T_1$coming from complete positivity can be generalized [40, 41]. If there are three principal directions for relaxation in a system and if γ_1, γ_2, γ_3 are the relaxation rates along these directions then γ_1, γ_2, γ_3 have to satisfy the following triangle inequality if complete positivity is to hold,

$$\gamma_1 + \gamma_2 > \gamma_3 \ , \quad \gamma_2 + \gamma_3 > \gamma_1 \ , \quad \gamma_3 + \gamma_1 > \gamma_2. \tag{7.3}$$

If one were to start from the point of view that the most general transformations on a quantum state must exactly be that - the most general - without any further restrictions, then one is tempted to reconsider the reasons why reduced dynamics is assumed to be exclusively completely positive.

7.2 The witness test and complete positivity

We have seen in chapter 2 that starting from Choi's result, the usual strategy for imposing complete positivity on the reduced dynamics of open systems is to introduce an auxiliary system called the *witness* into the problem. Let ρ be state of the system S that interacts with a reservoir R and let ρ_W

the state of the witness W. The witness is decoupled from the system and it does not evolve in time. In other words, it is blind ($H_{SW}^{(int)} = 0$) and dead ($H_W = 0$). If the state of the system evolves according to the dynamical map Φ then Choi's theorem tells us that $\Phi \otimes \mathbf{1}_W$ will always preserve the positivity of states of the combined system $S + W$ if Φ is completely positive. Since we expect the dynamics of the system and the witness to be described by $\Phi \otimes \mathbf{1}_W$ because of the way the witness is defined, the usual conclusion is that Φ has to be completely positive in order to preserve the positivity of the state $\mathcal{R}_{SW}$ of the system and the witness at all times. In Pechukas' own words:

> One may reasonably doubt this argument. It is very powerful magic. W sits apart from $S + R$ and does nothing; by doing so, it forces the motion of S to be completely positive, with dramatic physical consequences such as $T_2 \leq 2T_1$ for exponential two state relaxation. Ones doubts are strengthened by calculations of Skinner and co-workers [37–39] on strong coupling models for two-state relaxation; in some cases the relaxation looks almost exponential, but with $T_2 \geq 2T_1$.

From our discussion of open quantum dynamics with initial entanglement, we have already seen some of the problems in arguing that reduced dynamics must be completely positive based on Choi's results. Asserting that we require all $\mathcal{R}_{SW}$ to be mapped to other positive matrices is not really one that we can always make because all possible choices of ρ are not allowed in $\mathcal{R}_{SW}$ if we simultaneously state that the system is interacting with and possi-

bly entangled to a reservoir R. The reservoir R being distinct from the witness W. So, even if some choices of $\mathcal{R}_{SW}$ gets mapped to negative matrices by the map $\Phi \otimes \mathbf{1}_W$, we cannot claim that Φ is not an allowed dynamical transformation as long as ρ is not *compatible* with an entangled state of $S + R$. The action of extensions of Φ to formally valid states of $S + W$ should not be used to deduce a physical interpretation of the action of Φ. We should consider the action of Φ only on physically valid states of $S + W$ and in the example in page 37 we have seen that such action presents no problems of consistency.

There are further subtleties with the witness test. Even if S and W are not interacting, they need to share entanglement for the test to work. This means that the allowed states of the system are not only restricted by its correlations with the environment, they will be further restricted by the entanglement with the witness itself.

7.2.1 The role of entanglement in the witness test

An important point that was mentioned in chapter 2 is that the system and the witness has to share entanglement for $\Phi \otimes \mathbf{1}$ to be not positive on $\mathcal{R}_{SW}$. Let us look more closely at the role of entanglement between S and W in making the case for complete positivity. Let S be a *qubit* with density matrix ρ. Since the the map Φ acts on a two dimensional Hilbert space, it is sufficient to show that Φ is 2-positive in order to show that it is completely positive [10]. With this in mind we choose the witness to be a qubit also with density matrix ρ_W. Let us keep the initial states of the system and witness

completely general and let

$$\begin{aligned} \rho &= \tfrac{1}{2}(1 + a_j\sigma_j) &= \frac{1}{2}\begin{pmatrix} 1+a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1-a_3 \end{pmatrix} \\ \rho_W &= \tfrac{1}{2}(1 + w_k\tau_k) &= \frac{1}{2}\begin{pmatrix} 1+w_3 & w_1 - iw_2 \\ w_1 + iw_2 & 1-w_3 \end{pmatrix}. \end{aligned} \tag{7.4}$$

Define

$$\alpha \equiv \sqrt{a_1^2 + a_2^2 + a_3^2} \quad \text{and} \quad \omega \equiv \sqrt{w_1^2 + w_2^2 + w_3^2}.$$

For ρ and ρ_W to be states, we require $-1 \leq a, w \leq 1$. If we assume that there is no entanglement between S and W then from the way the witness is defined, we know that the initial state of $S + W$ is a simple product state

$$\mathcal{R}_{SW}^{(sep)} = \frac{1}{4}(1 + a_j\sigma_j) \otimes (1 + w_k\tau_k).$$

The eigenvalues of $\mathcal{R}_{SW}^{(sep)}$ are

$$\begin{aligned} \lambda_1 &= \frac{1}{4}(1-\alpha)(1-\omega), \qquad \lambda_2 = \tfrac{1}{4}(1-\alpha)(1+\omega), \\ \lambda_3 &= \frac{1}{4}(1+\alpha)(1-\omega), \qquad \lambda_4 = \tfrac{1}{4}(1+\alpha)(1+\omega) \end{aligned} \tag{7.5}$$

which are all positive semi-definite. So we know that the initial state of $S+W$ is a positive density matrix. Starting from this valid two qubit state, let us apply a map on ρ which we know to be positive but not completely positive. An easy choice is the transposition map $\mathbf{T}$. The action of $\mathbf{T}$ on ρ is to change a_2 to $-a_2$ and leave a_1 and a_3 unchanged. This transformation does not change α and hence does not change λ_i. In other words, we find that $\mathcal{R}_{SW}^{(sep)'} = (\mathbf{T} \otimes \mathbf{1}_W)\mathcal{R}_{SW}^{(sep)}$ is also a positive matrix.

Another example is a map that Choi introduces in [10] as one that is $(n-1)$ positive but not n positive:

$$\Phi^C(A) = \{(n-1)(\mathrm{tr}\, A)\}\mathbf{1}_n - A.$$

The action of Φ^C (with $n = 2$) on ρ is

$$\rho' = \Phi^C(\rho) = \frac{1}{2}\begin{pmatrix} 1-a_3 & -a_1+ia_2 \\ -a_1-ia_2 & 1+a_3 \end{pmatrix}. \tag{7.6}$$

In other words, $a_j \to -a_j$, $j = 1, 2, 3$. Again, this transformation does not change α and therefore $\mathcal{R}_{SW}^{(sep)C} = (\Phi^C \otimes \mathbf{1}_W)\mathcal{R}_{SW}^{(sep)}$ is a positive matrix for all possible choices of ρ and ρ_W.

We see that two not completely positive maps $\mathbf{T}$ and Φ^C pass the "witness test" and appear to be valid descriptions of the evolution of S if we assume that there is no entanglement between S and W. For the transpose map in the two qubit case this, of course, makes a lot of sense because $\mathbf{T} \otimes \mathbf{1}_W$ is just the Peres' partial transpose criterion [42] for detecting entanglement. The partial transpose is indeed positive preserving on all separable states and ceases to be so only on entangled $\mathcal{R}$. Similarly Choi shows that Φ^C is 1-positive and not 2-positive by considering action of $\Phi^C \otimes \mathbf{1}_2$ on the matrix

$$(E_{jk})_{1\le j,k,n} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

which, up to a normalization factor, is the fully entangled two qubit state. It also is a (block) matrix $M \in \mathcal{M}_2$ with each of its elements in turn being 2×2

matrices belonging to the C^*-algebra of single qubit operators. Specifically

$$\begin{aligned} M_{11} &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(1+\sigma_3) \\ M_{12} &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_1 + i\sigma_2) \\ M_{21} &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_1 - i\sigma_2) \\ M_{22} &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(1-\sigma_3). \end{aligned}$$

We see that the device of introducing the witness W that does not interact with S is inadequate to restrict the dynamics of S to completely positive transformations if there is no entanglement between S and W. This fact is not always emphasized when the witness is introduced even if it is pretty well known. The action of a given map Φ, when extended to $\Phi \otimes \mathbf{1}_n$ can fail to be positive on generic elements of $\mathcal{M}_n(\mathcal{A})$ while at the same time being positive on all $\rho \otimes \rho_W$.

The problem at hand might well be the evolution of an open quantum system. Still, one has to assume that system along with its environment can be considered in isolation with no residual interaction or entanglement with anything outside. If S and W are entangled $-$ a fact that seems crucial for the witness test to work $-$ then there must have been some sort of direct or indirect interaction between the two at some point and hence W should really be part of the definition of the environment of S.

When we have the witness which is entangled to S but not interacting with it (without changing the entanglement between S and R), all that

happens is that the domain of allowed states of S is further restricted. How precisely the compatibility domain is restricted depends now of the nature of the tripartite entanglement between S, R and W. But what we do know about the new compatibility domain in the presence of the witness is that it must be a *subset of the compatibility domain without the witness*. So $\Phi \otimes \mathbf{1}_W$ on all the states $\mathcal{R}_{SW} = \mathrm{tr}_R[\mathcal{R}_{SRW}]$ such that $\rho = \mathrm{tr}_{RW}[\mathcal{R}_{SRW}]$ is positive even for not positive Φ. In short, the presence of the witness does not really create any new issues with respect to the physical interpretation of not positive reduced dynamics of S. So it appears that there is no reason to restrict the reduced dynamics of an open system to being exclusively completely positive in nature. *Not completely positive maps are just as good.*

7.3 The assignment map

An alternate approach that leads to only completely positive maps as admissible forms of reduced dynamics was pointed out by Alicki [43, 44] in response to Pechukas. When viewed as the contraction of unitary evolution of an extended system, the action of a dynamical map on a density matrix looks like a combination of three separate maps. The first one, called an *assignment map* Δ, assigns a bipartite state $\mathcal{R}_{SR}$ of the system and the environment to each state ρ of the system, i.e. $\Delta : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_{S+R})$ where $\mathcal{B}(\mathcal{H})$ denote the C^*-algebra of positive trace class operators on a Hilbert space $\mathcal{H}$. The second and third pieces of the dynamical map are the unitary map that moves $\mathcal{R}_{SR}$ forward in time and the partial trace operation which gives us, in the end,

$\rho(t)$. The unitary map and the partial trace are both completely positive. So the nature of the dynamical map now depends on the what the assignment map Δ is.

Pechukas, in [36] proves that the only *linear* assignment that works for every $\rho \in \mathcal{B}(\mathcal{H}_S)$ is the product assignment

$$\Delta\rho = \mathcal{R}_{RS} = \rho \otimes \eta \tag{7.7}$$

where η is a *fixed* reservoir density matrix. A generalization of the proof due to T. F. Jordan [5] is given in Appendix C. We have seen in Chapter 2 that if the initial state is a simple product state the corresponding reduced dynamics is completely positive. It is certainly possible to consider other kinds of assignment maps. Alicki [43], in his reply to Pechukas, lists the following three "natural" conditions on Δ that restricts it to being product assignment:

1. Linearity: Δ preserves mixtures in the sense that

$$\Delta \sum_i p_i \rho^i = \sum_i p_i \mathcal{R}^i_{SR} \qquad ; \qquad \sum_i p_i = 1.$$

2. Consistency: Δ is consistent in the sense that

$$\mathrm{tr}_R[\mathcal{R}_{SR}] = \rho.$$

3. Positivity: $\Delta\rho$ is positive *for all* ρ.

We see from previous discussion that the positivity condition on Δ is quite unnecessary and unjustifiable. Strangely enough, the positivity condition is considered essential by several authors on the grounds that even if it

possible to restrict ourselves to those ρ for which $\Delta\rho$ is positive there is no operational prescription of specifying such a subset of all available system states. A lot of effort has been put into putting the assignment map in a rigorous mathematical footing; see for instance [45]. From the example in Chapter 3 we see immediately that there indeed is such a well motivated and physically meaningful prescription for choosing a subset of ρ on which the action of Δ is to give a positive density matrix for the $S + R$ system. If we restrict ρ to the compatibility domain fixed by the parameters of the dynamical map then we can find an assignment map consistent with the map that returns a valid bipartite density matrix for any ρ.

If we remove the positivity condition, the assignment map need not be the product assignment which leads to completely positive reduced dynamics. The product assignment has other serious drawbacks. If we require that the the assignment map be consistent with the dynamical evolution in that $\mathcal{R}_{SR}$ be of the form $\rho\otimes\eta$ at all times, we are forced into several approximations like weak coupling between S and R or a fast relaxation time for R compared to S. This is because any generic interaction between S and R will entangle the two in a short time unless the reservoir decoheres rapidly. An entangled $\mathcal{R}_{SR}$ is definitely not of the form $\rho\otimes\eta$. One hopes that under some approximation, the bipartite state stays on or close to the set of simply separable states. This is an unusually restrictive assumption which does not hold up in many experimental situations. For the description of open quantum dynamics to be truly general, we must abandon the simple product assignment and the completely positive

maps that come along with it. With a more general assignment defined on a subset of compatible system states, the open quantum dynamics can be not completely positive. In fact, as we have seen, the map need not even be positivity preserving when applied to states outside the compatibility domain.

If the dynamical map is meant to apply to a set of ρ that all evolve in time as a result of the same cause, the $\mathcal{R}_{SR}$ assigned to these ρ should not differ in ways that would change the cause of evolution of the ρ. This is the reason why we treat the correlations $\langle\sigma_1\tau_3\rangle = c_{13}$ and $\langle\sigma_2\tau_3\rangle = c_{23}$ that appear in the example in Chapter 3 as parameters with *fixed* values. Since the assignment map corresponding to not completely positive evolution is not a simple product assignment, each ρ in the compatibility domain has to be paired up with a different state ρ_R of the reservoir to be consistent with the observed dynamics of S and the entanglement in $\mathcal{R}_{SR}$ In other words, corresponding to each different state of S there is a state $\rho_R = \mathrm{tr}_S[\mathcal{R}_{SR}]$ that is coupled to it. Does this mean it is handled differently? If a map is meant to describe evolution that has a definite physical cause, does an assignment that is not a simple product do the job?

In the compatibility domain that we describe, the evolution of all the states is clearly the result of the same cause. It can be described by a single map that has physical meaning. Working with mean values helps make this clear. We do not need a complete description of the state of $S + R$ at time zero. It does not need to stand alone, independent of the unitary evolution, and accommodate any unitary evolution. The compatibility domain depends

on the unitary evolution. In our example, the compatibility domain depends on the mean values that are the parameters c_{23} and c_{13}. That these mean values are the relevant parameters depends on our choice of Hamiltonian. The compatibility domain is unlimited when c_{23} and c_{13} are zero. Then the map is completely positive, but that does not require an initial state described by a density matrix that is a product. It must be noted that even if the compatibility domain of a given map is well defined, it is not clear whether there is a general method of identifying it easily. The algorithm for finding the compatibility domain for a given system and its observed dynamics is easily written down but computing the domain is a hard problem because it involves searching for a set of points in many dimensional parameter space[2].

Talking about dynamical maps in terms of the assignment map and its properties is to a certain extent like putting the cart before the horse! The system S is the only one that we are able to directly observe. The combined state of the system and the reservoir is not accessible to us. After all, that is the whole point of studying *open* quantum systems. By knowing the time evolution of S in a particular experiment we are able to reconstruct the dynamical map. Quantum process tomography will give us the values of the parameters (like c_{23} and c_{13} in the example) that are relevant for the dynamics of the system. From the knowledge of these parameters it is possible to decide whether the observed dynamics is completely positive map. According to the kind of dynamics that is observed, we can then reconstruct an assignment map that associates with

[2]Ten parameter space for the example in chapter 3

each observed system density matrix a state of the $S+R$ system. This extended state might be entangled or not as the case may be. Once this assignment map, which is not necessarily a product assignment, is fixed it would then shed light on the influence of the environment on the system of interest and on its dynamics in the context of the external influences on it. At this point one can reasonably ask useful questions like how the influence of the environment may be limited to prevent decoherence or, at the other extreme, how this influence may lead to a projective measurement on the system.

7.4 Who's afraid of not completely positive maps?

In a recent paper entitled "Quantum process tomography of a single solid state qubit" [17], Howard et al look the relaxation of the state of a qubit. The qubit is a nitrogen impurity atom next to a vacancy in a diamond lattice. Two atomic levels of the Nitrogen atom are isolated and used as a qubit. The qubit can be manipulated using electron spin resonance and can be initialized to any desired state and quantum process tomography used to reconstruct the map representing its relaxation. The following is a passage from the paper:

> The process obtained directly from experimental data is often unphysical i.e. non-trace-preserving or not completely positive. In such cases it is necessary to search for a physical process which is closest in some sense to the experimental results. In this case we used a least squares fit between the experimentally determined Φ and a Hermitian parameterization of a physical $\bar{\Phi}$ while enforcing

complete positivity and trace preservation.

We expect the carbon atoms in the diamond lattice around the qubit to play at least some part in the relaxation of the qubit. The qubit in turn is in a *lattice* with these other atoms and it is difficult to imagine that the qubit has no correlations or entanglement with the surrounding atoms. Putting the two observations together there is reason to believe that the lack of complete positivity of the measured maps might be due to the entanglement that the qubit shares with its surroundings. The experimental results could therefore have a more direct explanation in terms of not completely positive maps. Instead, in [17], the lack of complete positivity of the measured process is interpreted as a consequence of errors in the experiment. A similar point of view is taken in [46] as well.

The accepted wisdom with respect to open quantum dynamics is that complete positivity for reduced dynamics is unavoidable. In spite of Pechukas' work the question of the limitations of completely positive dynamics have remained relatively unexplored until recently [47, 48]. For dynamical maps the effort seems to be concentrated on finding acceptable ways to avoid introducing not completely positive ones [15, 43, 49, 50]. For instance, an alternate approach that is sometimes utilized to force complete positivity on the reduced dynamics is to re-define the system and the environment in a suitable manner so that new "dressed" system and environment are weakly coupled. In such cases complete positivity for the dynamics of the new 'system' becomes a good approximation. On the other hand, the direct approach of using

not completely positive maps to describe the open quantum evolution of the original system may provide a clearer understanding of its dynamics at least in systems with small dimensional Hilbert spaces. We have shown that there is no reason to shy away from such a direct approach based on claims that not completely positive evolution has no consistent physical interpretation and meaning.

Quantum information processors are often conceived in such a manner that the each qubit can be initialized to specific un-entangled initial states [1] before unitary transformations are performed on them to build up a computation. It is argued that the ability to decohere the qubits and initialize them is a valid reason for considering only completely positive dynamics for describing quantum information processors and communication channels. Even in this case where we expect a lot of control over the dynamics of the system it is not always reasonable to assume complete positivity. This is because any rudimentary quantum algorithm will involve several operations or gates involving interactions between more than one qubit. Even if the effect of the first quantum gate on a qubit that we are tracking is described by a completely positive map, the action of the next gate need not be so because the first multi-qubit gate will introduce entanglement into the system of qubits. Subsequent operations will, in general, induce not completely positive reduced dynamics on each one of the qubits.

Using not completely positive maps to describe open quantum dynamics is evidently well motivated by experimental considerations as well as by the

potential insights such maps may provide into the nature of entanglement. We have shown in the preceding Chapters how such maps may be constructed and how their action interpreted. There seems to be no reason at all to shy away from considering such maps.

7.5 Conclusion

The question we looked at is what is the best description of the most general physical evolution of an open quantum system? What kind of map is needed to describe evolution of states of a system S caused by dynamics of $S + R$? Our analysis suggests that the dynamics is in general not described by a completely positive map. Such maps can take some positive matrices to negative ones unless the domain of action of the map is restricted. This then raises the question of justifying the choice of a subset of states of S on which the map can act while preserving physical meaning. Introduction of the idea of compatibility domain shows that the choice of the domain of action of a not completely positive map comes naturally from the initial entanglement between S and R.

We conclude that not completely positive maps are just as good as completely positive maps in describing open quantum evolution. When using not completely positive maps one has to be careful in defining the domain of action of the map. The not completely positive nature of the map must be understood as a consequence of the correlations or entanglement that the system may have with its surroundings. These correlations define a compatibility

domain which in turn gives meaning to the restricted domain in which the maps make physical sense. Preliminary experimental evidence also suggests that not completely positive maps are needed to describe observed quantum processes.

7.5.1 Future directions

The example we studied in Chapter 3 is a particularly simple one because we took both the system and the reservoir to be single qubits. The interaction between S and R was also chosen to be a simple one. An arbitrary dynamical matrix B acting on the state of a qubit can always be constructed as the contraction of the unitary evolution of the system qubit and two other qubits. So extending the example to three qubits with one of them treated as the system and the other two as the reservoir is required if we are to study all possible open dynamics of a qubit. More general Hamiltonians for the qubits including terms with free evolution of the individual qubits, in addition to interaction terms between them, needs to be considered too. The compatibility domains and the positivity domains for these cases is expected to be much more complicated. In our example we had the intersection of all the positivity domains being exactly equal to the compatibility domain. This need not be so in all cases. Still, it has to be verified that the compatibility domain lies inside the intersection of all positivity domains.

Finding the generators of the not completely positive maps is an avenue of research where more needs to be done. The conditions (if any) under which

not completely positive open dynamics can be treated as a Markov process needs to be explored. We have outlined the form of the Kossakowski-Lindblad type quantum master equation corresponding to not completely positive open dynamics in Chapter 5. Finding the generators $L^{(n)}$ and $\widetilde{L}^{(n)}$ that appear in Eq. (5.40) for specific examples is a challenging problem.

The mathematical properties of not completely positive maps of C^*-algebras are rather well understood [14, 51–54]. Once the conceptual difficulties in accepting not completely positive maps as a description of open quantum dynamics is removed the physical implications of the mathematical results can be fully explored. We expect that this would contribute significantly to our understanding of the nature of entanglement and the details of the quantum measurement process.

Appendices

Appendix A

Qubits and Entanglement

The two state quantum system is a central player in all our discussions. This is in part because of the simplicity afforded by such systems and in part because we want to explore the relevance of our results to quantum information theory. In the language of quantum information theory, any quantum system with a two dimensional Hilbert space is a *qubit* which is short for a *QUantum BInary digiT*.

A.1 Qubits

One of the basic ideas in information theory - classical or quantum - is that information can be encoded in a wide varieties of equivalent forms. Whether it is a sentence, a number, a mathematical formula, a picture, a movie or a complete symphony, inside the ubiquitous computer, they are all stored as a sequence of ones and zeros; a string of classical *bits*. The qubit has an analogous role in the paradigm of quantum information theory. Any $2n$ dimensional Hilbert space $\mathcal{H}$ has an equivalent representation in terms of $n-$qubits of the form $\otimes_{i=1}^{n}\mathcal{H}^2$. So an arbitrary quantum system and the processes that it undergoes can be simulated in a *quantum computer* with an

appropriate number of qubits. This is in line with Feynman's original conception of a quantum computer [55] as a device dedicated to simulating quantum processes that by their very nature are extremely inefficiently simulated by a classical computer.

In reality a qubit is an idealization since physical systems with exactly two dimensional Hilbert spaces are difficult to come by. Still, in many cases very good approximations to an ideal qubit can be constructed. Internal states of atoms trapped in optical lattices, States of superconducting structures with Josephson junctions, Molecules containing atoms with prescribed nuclear spins probed using nuclear magnetic resonance techniques are just a few of the tried and tested ways of constructing physical representations of qubits. For the purposes of the discussion that follows, it is sufficient that we view a qubit as an abstract two state quantum system. The two spin states of a spin 1/2 particle is a nice clean choice for visualizing a qubit when such visualizations are called for.

Since we will be concentrating on the features of the open evolution of quantum systems with finite dimensional Hilbert spaces, a good starting point is to look at such dynamics involving a few qubits. Both the system of interest and the its environment can be considered to be a one or more qubits without loss of generality[1]. The simplest case is when the system is just one qubit and so is the environment which will be discussed in detail in Chapter

[1]The case where the system or the environment have infinite dimensional Hilbert spaces is beyond the scope of the present work

3. In a sense, systems and environments of modest sizes present a greater scope for finding novel behavior because we already know much about large systems and environments using the well established statistical techniques to understand the dynamics. The middle ground between the microscopic and the macroscopic is the place where a lot is still unknown as far as open system evolution goes.

A.2 Entanglement

With more than one quantum system (qubit) in the picture we encounter the possibility of there being *entanglement* between them. The consequences of such entanglement will be important in our investigations of open system dynamics. It is therefore worthwhile to briefly go over what it means for two quantum systems to be entangled. Erwin Schrödinger gave the name *"Verschränkung" to correlations that can exist between quantum systems that has no classical analogue [56].* The original name means something like "holding of hands" but it got translated to "entanglement". The term entanglement seems to have taken on several different flavors since its introduction. While Dirac [57] considered the defining character of quantum mechanics to be *superposition*, Schrödinger emphasized that superposition was relevant for classical wave phenomena. He identified *entanglement* as the definitive character of quantum systems. To capture these aspects of entanglement we take a page out of an article by Bruss [58] and collect together the points of view about entanglement of various important people in the fields of quantum physics and

quantum information theory.

Einstein, Podolsky and Rosen initiated the long debates on the meaning of quantum theory by expressing the opinion that an entangled wave function does not describe physical reality in a complete way [59]. Schrödinger pointed out that for an entangled state the best possible knowledge of the whole state ends up precluding the best possible knowledge of the parts [56]. For John Bell, entanglement signified a correlation that is stronger than any classical correlation. Asher Peres playfully describes entanglement as a trick that quantum magicians use to produce phenomena that cannot be used by classical magicians. Charles Bennett showed that entanglement is a "quantum resource" that can be used to perform the teleportation of quantum states [26]. For Peter Shor, the inventor of the first substantial algorithm designed for a quantum computer [60], entanglement is a global structure of the wave function that makes quantum algorithms more efficient in some tasks that any conceivable classical counterpart. Finally for the Horodeckis' [61] entanglement presented a reason to consider positive maps in physics; a theme that will be central to our discussion also.

Interactions of any sort between two quantum systems leaves a mark on both of them that persists even if the two systems are prevented from having any further contact with each other. This, of course, is not something unique to quantum systems. Two classical systems that interact with each other; say, through a collision can end up bearing signatures of the interaction for quite a long time. A fender-bender collision between two cars bears the signs of the

accident until one spends a bit of money at the mechanics'!

The persistent effects of the interaction between two (or more) quantum systems that show up in measurements made on each system even after they are isolated from each other is entanglement. The quantum nature of the persistent effect is in that it does not reside in each subsystem separately. The prototypical system that illustrates the various, often counter-intuitive, aspects of the phenomenon of quantum entanglement is the following:

Imagine that a quantum particle of total angular momentum zero decays into two pieces, each carrying spin 1/2. Conservation of angular momentum requires that the state of the system after the original particle has dissociated must be of the form

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right).$$

Here the up and the down arrows represent the components of the spin of the first and the second particle measured along a particular direction (we choose the z-direction).

Even if we assume that the two particles have no further interaction with each other after they are created the two still seem to be inseparably connected by just being in the combined quantum state $|\psi\rangle$. The state $|\psi\rangle$ is a coherent superposition of the two particle states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. Consequently, if a measurement on the first particle yields the result that it is in the $|\uparrow\rangle$ state then that means that we have picked up the $|\uparrow\downarrow\rangle$ component of the superposition and therefore the second particle must be in the state $|\downarrow\rangle$. Yet,

one could argue that given the original state $|\psi\rangle$ the second particle by itself is a mixture of $|\uparrow\rangle$ and $|\downarrow\rangle$ states. It is then as if the measurement on the first particle transforms the second particle automatically from a mixed state to a definite spin state. This apparent 'transformation' seems inevitable even if we assume that the second particle is totally isolated from the first particle at all times except at the instant of their creation from the original particle.

Viewed as a single two particle state, the effects of the quantum entanglement in $|\psi\rangle$ presents no particular conceptual difficulties. Observing the first particle in the $|\uparrow\rangle$ state simply means that we have observed the $|\uparrow\downarrow\rangle$ component of the original superposition. The difficulties come in when we stipulate that a consequence of the fact that the two particles do not interact with each other once they are created is that the result of a measurement on each of then should be understandable in terms of their individual quantum states rather than in terms of the combined state $|\psi\rangle$. Deliberately avoiding such treacherous discussions on the connection between entanglement, causality and the nature of physical reality we merely state that there is sufficient experimental evidence to substantiate the reality of the phenomena of quantum entanglement [62].

Appendix B

Constructing the dynamical matrix B

The transformation brought about on the system qubit by the coupled evolution of the system and the environment qubit in the example when there is initial entanglement is from

$$\rho_0 = \frac{1}{2}(1 + a_i\sigma_i) = \frac{1}{2}\begin{pmatrix} 1+a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1-a_3 \end{pmatrix} \tag{B.1}$$

to

$$\rho_t = \frac{1}{2}\begin{pmatrix} 1+a_3 & (a_1 - ia_2)\cos\omega t + c^*\sin\omega t \\ (a_1 + ia_2)\cos\omega t + c\sin\omega t & 1-a_3 \end{pmatrix} \tag{B.2}$$

where

$$c = -c_{23} + ic_{13}.$$

If we now cast both ρ_0 and ρ_t into column vectors of the form

$$\rho = \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ \rho_{22} \end{pmatrix},$$

then by inspection it is easy to determine that the linear transformation that connects ρ_t to ρ_0 is given by the matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2}c^*\sin\omega t & \cos\omega t & 0 & \frac{1}{2}c^*\sin\omega t \\ \frac{1}{2}c\sin\omega t & 0 & \cos\omega t & \frac{1}{2}c\sin\omega t \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{B.3}$$

From equation (2.9) we have

$$A_{rs;r's'} = B_{rr';ss'}$$

and rearranging the elements of the A matrix accordingly gives us

$$B = \begin{pmatrix} 1 & 0 & \frac{1}{2}c^* \sin\omega t & \cos\omega t \\ 0 & 0 & 0 & \frac{1}{2}c^* \sin\omega t \\ \frac{1}{2}c \sin\omega t & 0 & 0 & 0 \\ \cos\omega t & \frac{1}{2}c \sin\omega t & 0 & 1 \end{pmatrix}. \tag{B.4}$$

The transformation rules from the A to B matrix are given below in explicit detail

$$[A]_{11} = A_{11;11} = B_{11;11} = [B]_{11}$$
$$[A]_{12} = A_{11;12} = B_{11;12} = [B]_{12}$$
$$[A]_{13} = A_{11;21} = B_{12;11} = [B]_{21}$$
$$[A]_{14} = A_{11;22} = B_{12;12} = [B]_{22}$$
$$[A]_{21} = A_{12;11} = B_{11;21} = [B]_{13}$$
$$[A]_{22} = A_{12;12} = B_{11;22} = [B]_{14}$$
$$[A]_{23} = A_{12;21} = B_{12;21} = [B]_{23}$$
$$[A]_{24} = A_{12;22} = B_{12;22} = [B]_{24}$$
$$[A]_{31} = A_{21;11} = B_{21;11} = [B]_{31}$$
$$[A]_{32} = A_{21;12} = B_{21;12} = [B]_{32}$$
$$[A]_{33} = A_{21;21} = B_{22;11} = [B]_{41}$$
$$[A]_{34} = A_{21;22} = B_{22;12} = [B]_{42}$$
$$[A]_{41} = A_{22;11} = B_{21;21} = [B]_{33}$$
$$[A]_{42} = A_{22;12} = B_{21;22} = [B]_{34}$$

$$[A]_{43} = A_{22;21} = B_{22;21} = [B]_{43}$$
$$[A]_{44} = A_{22;22} = B_{22;22} = [B]_{44}$$

The easy way to do the transformation from A to B is the following: Take each row of A and fold them into 2×2 matrices: First row:

$$(1, 0, 0, 0) \to \mathcal{B}_{11} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Second row:

$$\left(\frac{1}{2}c^* \sin\omega t,\ \cos\omega t,\ 0,\ \frac{1}{2}c^* \sin\omega t\right) \to \mathcal{B}_{12} = \begin{pmatrix} \frac{1}{2}c^* \sin\omega t & \cos\omega t \\ 0 & \frac{1}{2}c^* \sin\omega t \end{pmatrix}$$

Third row:

$$\left(\frac{1}{2}c \sin\omega t,\ 0,\ \cos\omega t,\ \frac{1}{2}c \sin\omega t\right) \to \mathcal{B}_{21} = \begin{pmatrix} \frac{1}{2}c \sin\omega t & 0 \\ \cos\omega t & \frac{1}{2}c \sin\omega t \end{pmatrix}$$

Fourth row:

$$(0,\ 0,\ 0,\ 1) \to \mathcal{B}_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Now rearrage it back into a block matrix

$$B = \begin{pmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} \\ \mathcal{B}_{21} & \mathcal{B}_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \frac{1}{2}c^* \sin\omega t & \cos\omega t \\ 0 & 0 & 0 & \frac{1}{2}c^* \sin\omega t \\ \frac{1}{2}c \sin\omega t & 0 & 0 & 0 \\ \cos\omega t & \frac{1}{2}c \sin\omega t & 0 & 1 \end{pmatrix}.$$

Appendix C

Generalization of Pechukas' result

We present here a generalization of a result by Pechukas [36] due to T. F. Jordan on the connection between the nature of the assignment map and the types of reduced dynamics.

Theorem C.0.1. *If a linear map applies to all density matrices ρ_A for a subsystem A and assigns each ρ_A a density matrix ρ_{AB}^A for the combined system AB so that*

$$Tr_B[\rho_{AB}^A] = \rho_A, \tag{C.1}$$

then, for every ρ_A,

$$\rho_{AB}^A = \rho_A \otimes \rho_B \tag{C.2}$$

with ρ_B a density matrix for the subsystem B that is the same *for all ρ_A.*

Proof. The first step, which Pechukas [36] did, is to show that every pure-state density matrix ρ_A is assigned a product density matrix, as in (C.2), with ρ_B possibly different for different ρ_A. For completeness we include a slightly different presentation of this step. If ρ_A represents a pure state, there is an orthonormal basis of state vectors $|\psi_j\rangle$ for A, with $j = 1, 2, \ldots$, such that ρ_A is $|\psi_1\rangle\langle\psi_1|$. We combine these with orthonormal state vectors $|\phi_k\rangle$ for B to make

an orthonormal basis of product vectors $|\psi_j\phi_k\rangle$ for AB. Since ρ_{AB}^A is positive, each $\langle\psi_j\phi_k|\rho_{AB}^A|\psi_j\phi_k\rangle$ is non-negative and, from (C.1), if j is not 1,

$$\langle\psi_j\phi_k|\rho_{AB}^A|\psi_j\phi_k\rangle \leq \langle\psi_j|\mathrm{Tr}_B[\rho_{AB}^A]|\psi_j\rangle = \langle\psi_j|\psi_1\rangle\langle\psi_1|\psi_j\rangle = 0. \tag{C.3}$$

Since ρ_{AB}^A is positive, it is the square of a Hermitian operator. Thus we see that $\rho_{AB}^A|\psi_j\phi_k\rangle$ is zero if j is not 1 and

$$\langle\psi_j\phi_r|\rho_{AB}^A|\psi_k\phi_s\rangle = \delta_{j1}\delta_{k1}\langle\psi_1\phi_r|\rho_{AB}^A|\psi_1\phi_s\rangle. \tag{C.4}$$

Let

$$\rho_B^A = \mathrm{T}r_A[\rho_{AB}^A]. \tag{C.5}$$

Then

$$\rho_B^A = \langle\psi_1|\rho_{AB}^A|\psi_1\rangle. \tag{C.6}$$

and

$$\rho_{AB}^A = |\psi_1\rangle\langle\psi_1| \otimes \rho_B^A. \tag{C.7}$$

That completes the first step of the proof.

The second step, which completes the proof of the theorem, is to show that ρ_B is the same for all pure-state density matrices ρ_A. Pechukas [36] did this for the case where A is a qubit. We show that the proof an be easily extended to any quantum system [63]. Suppose $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthonormal

state vectors for A. Let

$$\begin{aligned} |\psi_3\rangle &= \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{i}{\sqrt{2}}e^{i\beta}|\psi_2\rangle \\ |\psi_4\rangle &= \frac{1}{\sqrt{2}}|\psi_1\rangle - \frac{i}{\sqrt{2}}e^{i\beta}|\psi_2\rangle \\ |\psi_5\rangle &= \cos\alpha\,|\psi_1\rangle + \sin\alpha\,e^{i\beta}|\psi_2\rangle \\ |\psi_6\rangle &= \sin\alpha\,|\psi_1\rangle - \cos\alpha\,e^{i\beta}|\psi_2\rangle. \end{aligned} \tag{C.8}$$

Then $|\psi_3\rangle$ and $|\psi_4\rangle$ are orthogonal, $|\psi_5\rangle$ and $|\psi_6\rangle$ are orthogonal, and $|\langle\psi_1|\psi_3\rangle|^2$, $|\langle\psi_1|\psi_4\rangle|^2$, $|\langle\psi_2|\psi_3\rangle|^2$, $|\langle\psi_2|\psi_4\rangle|^2$, $|\langle\psi_3|\psi_5\rangle|^2$, $|\langle\psi_3|\psi_6\rangle|^2$, $|\langle\psi_4|\psi_5\rangle|^2$, $|\langle\psi_4|\psi_6\rangle|^2$ are all $1/2$. The length of each vector $|\psi_k\rangle$ is 1, so $|\psi_k\rangle\langle\psi_k|$ is a pure-state density matrix for A. The map assigns it a product density matrix

$$\rho_{AB}(|\psi_k\rangle\langle\psi_k|) = |\psi_k\rangle\langle\psi_k| \otimes \rho_B(k) \tag{C.9}$$

as in (C.7) with $\rho_B(k)$ short notation for $\rho_B(|\psi_k\rangle\langle\psi_k|)$.

Since the map is linear, it follows from

$$\frac{1}{2}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|) = \frac{1}{2}(|\psi_3\rangle\langle\psi_3| + |\psi_4\rangle\langle\psi_4|) \tag{C.10}$$

that

$$\frac{1}{2}(|\psi_1\rangle\langle\psi_1|\,\rho_B^1 + |\psi_2\rangle\langle\psi_2|\,\rho_B^2) = \frac{1}{2}(|\psi_3\rangle\langle\psi_3|\,\rho_B^3 + |\psi_4\rangle\langle\psi_4|\,\rho_B^4). \tag{C.11}$$

Taking partial mean values $\langle\psi_1|\ldots|\psi_1\rangle$, $\langle\psi_2|\ldots|\psi_2\rangle$, $\langle\psi_3|\ldots|\psi_3\rangle$ of this last equation (C.11) yields three equations that imply ρ_B^1, ρ_B^2, ρ_B^3 and ρ_B^4 all are the same. Doing everything starting from (C.10) again with $1, 2, 3, 4$ changed to $3, 4, 5, 6$ shows that ρ_B^3, ρ_B^4, ρ_B^5 and ρ_B^6 all are the same. Any state vector

for A is in a subspace spanned by $|\psi_1\rangle$ and a vector $|\psi_2\rangle$ orthogonal to $|\psi_1\rangle$, so $|\psi_5\rangle$ with fixed $|\psi_1\rangle$ and varying α, β and $|\psi_2\rangle$ can represent any pure state for A. If ρ_A represents a pure state, ρ_B^A is the same as $\rho_B(1)$, so (C.2) holds, with the same ρ_B, for all pure states of A and, therefore, for all mixtures as well. This completes the proof of the theorem.

Appendix D

Time evolution of the two qubit system

Here we outline the steps that went into computing the state $\mathcal{R}_t$ of the two qubit system at time t that is given in Eq. (3.5). The starting point is to use the properties of the Pauli matrices to write the unitary time evolution operator corresponding to the Hamiltonian in Eq. (3.4) as

$$U(t) = e^{-iHt} = \cos(\omega t/2)\mathbf{1} - i\sigma_3 \otimes \tau_3 \sin(\omega t/2) \tag{D.1}$$

and

$$U^\dagger(t) = e^{iHt} = \cos(\omega t/2)\mathbf{1} + i\sigma_3 \otimes \tau_3 \sin(\omega t/2). \tag{D.2}$$

We have to find the action of U and $U^\dagger$ on each of the terms in the initial state of the two qubit system,

$$\mathcal{R}_0 = \frac{1}{4}\left(\mathbf{1} \otimes \mathbf{1} + a_i\sigma_i \otimes \mathbf{1} + b_j\mathbf{1} \otimes \tau_j + c_{ij}\sigma_i \otimes \tau_j\right) \tag{D.3}$$

Using the commutation relations between the Pauli matrices,

$$[\sigma_i\,,\,\sigma_j] = i\epsilon_{ijk}\sigma_k \quad ; \quad [\tau_i\,,\,\tau_j] = i\epsilon_{ijk}\tau_k$$

we obtain the following results:

$$
\begin{aligned}
U\ \mathbf{1}\otimes\mathbf{1}\ U^\dagger &= \mathbf{1}\otimes\mathbf{1}\\
U\ a_1\sigma_1\otimes\mathbf{1}\ U^\dagger &= a_1\cos\omega t\ \sigma_1\otimes\mathbf{1} + a_1\sin\omega t\ \sigma_2\otimes\tau_3\\
U\ a_2\sigma_2\otimes\mathbf{1}\ U^\dagger &= a_2\cos\omega t\ \sigma_2\otimes\mathbf{1} - a_2\sin\omega t\ \sigma_1\otimes\tau_3\\
U\ a_3\sigma_3\otimes\mathbf{1}\ U^\dagger &= a_3\ \sigma_3\otimes\mathbf{1}\\
U\ b_1\mathbf{1}\otimes\tau_1\ U^\dagger &= b_1\cos\omega t\ \mathbf{1}\otimes\tau_1 + b_1\sin\omega t\ \sigma_3\otimes\tau_2\\
U\ b_2\mathbf{1}\otimes\tau_2\ U^\dagger &= b_2\cos\omega t\ \mathbf{1}\otimes\tau_2 - b_2\sin\omega t\ \sigma_3\otimes\tau_1\\
U\ b_3\mathbf{1}\otimes\tau_3\ U^\dagger &= b_3\ \mathbf{1}\otimes\tau_3\\
U\ c_{11}\sigma_1\otimes\tau_1\ U^\dagger &= c_{11}\ \sigma_1\otimes\tau_1\\
U\ c_{12}\sigma_1\otimes\tau_2\ U^\dagger &= c_{12}\ \sigma_1\otimes\tau_2\\
U\ c_{13}\sigma_1\otimes\tau_3\ U^\dagger &= c_{13}\cos\omega t\ \sigma_1\otimes\tau_3 + c_{13}\sin\omega t\ \sigma_2\otimes\mathbf{1}\\
U\ c_{21}\sigma_2\otimes\tau_1\ U^\dagger &= c_{21}\ \sigma_2\otimes\tau_1\\
U\ c_{22}\sigma_2\otimes\tau_2\ U^\dagger &= c_{22}\ \sigma_2\otimes\tau_2\\
U\ c_{23}\sigma_2\otimes\tau_3\ U^\dagger &= c_{23}\cos\omega t\ \sigma_2\otimes\tau_3 - c_{23}\sin\omega t\ \sigma_1\otimes\mathbf{1}\\
U\ c_{31}\sigma_3\otimes\tau_1\ U^\dagger &= c_{31}\cos\omega t\ \sigma_3\otimes\tau_1 + c_{31}\sin\omega t\ \mathbf{1}\otimes\tau_2\\
U\ c_{32}\sigma_3\otimes\tau_2\ U^\dagger &= c_{32}\cos\omega t\ \sigma_3\otimes\tau_2 - c_{32}\sin\omega t\ \mathbf{1}\otimes\tau_1\\
U\ c_{33}\sigma_3\otimes\tau_3\ U^\dagger &= c_{33}\ \sigma_3\otimes\tau_3
\end{aligned}
$$

Collecting together like terms we get Eq. (3.5).

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