

**Geometry of unital quantum maps and locally maximally
mixed bipartite states.**

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Abstract

In this thesis, we consider the geometry of the set of unital quantum maps and the geometry of the set of bipartite states with maximally mixed marginals. By the map-state duality, these two sets are isomorphic and can be considered by using the same mathematical formalism. When considering the geometry of unital quantum maps we encounter one crucial difference between two-dimensional systems and systems of higher dimensions. Unital qubit maps can be decomposed in terms of unitary maps. However, non-unitary maps need to be considered to decompose other unital qudit maps. To consider the geometry of unital quantum maps in higher dimensions, we construct a novel family of maps that includes both unitary and non-unitary unital quantum maps. For this family, we derive a criterion determining whether a given map of the family corresponds to an extreme point of the set of unital quantum maps. By applying the Choi-Jamiołkowski isomorphism over the family of maps, we consider the geometry of the set of locally maximally mixed bipartite states. In particular, we consider the problem of entanglement classification for the elements of this family of bipartite states. To do this, we find a set of invariants determining local unitary classes for our family. We also consider this family of bipartite states for qutrit systems. Remarkably, in this scenario, the chosen set of invariants can be used for the entanglement classification of the states of the family. For qutrit states, we consider the solutions of the equations giving unital quantum maps and locally maximally mixed bipartite states for the families previously considered. To do this, we construct an algorithm based on numerical methods to solve these equations. We also provide a graphical representation of the solutions given by the algorithm. Finally, we consider a constraint in the parameters of the equations allowing us to obtain solutions with analytical methods.

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Declaration

I declare that the research contained in this thesis, unless otherwise formally indicated within the text, is the original work of the author. The thesis has not been previously submitted to this or any other university for a degree and does not incorporate any material already submitted for a degree.

Signed: 22-09-2023

A handwritten signature in black ink, appearing to read 'C. Ramos', with a long horizontal stroke extending to the right.

Constantino Rodriguez Ramos

Contents

1	Introduction	7
2	Basic concepts in quantum mechanics	11
2.1	Introduction to quantum information theory	11
2.1.1	Axioms of quantum mechanics	12
2.1.2	Density operators	17
2.2	Quantum maps	18
2.2.1	Representations of quantum maps	19
2.3	Bipartite states	25
2.3.1	Entanglement as a resource	26
2.3.2	Entanglement characterisation	27
2.4	Channel-state duality	34
3	Unital quantum maps and locally maximally mixed states	37
3.1	Introduction	37
3.2	UCTP qubit maps	38
3.2.1	UCTP qubit maps and doubly-stochastic matrices	41
3.3	LMM bipartite qubit states	42
3.4	Higher dimensional case	48

<i>CONTENTS</i>	6
4 The convex set of unital quantum maps	50
4.1 Introduction	50
4.2 Convex characterisation of UCPT maps	51
4.3 A family of UCPT-extremal maps	52
4.4 Qutrit case	59
4.4.1 Rank-four UCPT-extremal qutrit maps	62
4.4.2 Evaluating extremal conditions	63
4.5 Conclusion	67
5 On the entanglement classification of locally maximally mixed states	68
5.1 Introduction	68
5.2 A family of locally maximally mixed bipartite states	69
5.3 Local unitary invariants	71
5.4 Bipartite qutrit state LU classification	77
5.5 Conclusion	79
6 Solving UCPT/LMM equations in qutrit systems	81
6.1 Introduction	81
6.2 Expressing UCPT/LMM equations in terms of real parameters	82
6.3 Numerical solutions	83
6.4 Analytical solutions	87
6.5 Conclusions	88
7 Conclusions	89
7.1 Future work	91

Chapter 1

Introduction

The study of the geometrical structure of the quantum state space is usually of great help in understanding novel features of quantum systems and developing new measures and algorithms with potential applications. In this thesis, we consider the geometry of the set of unital complete positive trace-preserving (UCPT) maps and the geometry of the set of locally maximally mixed (LMM) bipartite states. The advantage of considering these two sets is that the techniques developed for describing bipartite states can be directly applied to describe quantum maps and vice-versa. There are several good reasons to consider unital quantum maps instead of general quantum maps. For low-dimensional systems, the additional constraint required by unitality often simplifies problems and allows for a geometrical intuition of the state space. For example, for qubit maps, the set of UCPT maps can be associated with a 3-simplex in the Euclidean space.

This thesis aims to investigate the geometry of the set of UCPT maps/LMM states for systems of dimensions higher than two. There exists a crucial difference between qubit maps and maps based on systems of higher dimensions. As opposed to the qubit case, there are examples of maps based on higher dimensional systems that are not mixed-unitary (they cannot be expressed as convex combinations of unitary maps). From a theoretical perspective, the existence of such maps implies that Birkhoff's theorem does not extend to cases other than the qubits. The initial mission of this research is to investigate the rationale behind the failure of the quantum analogue of Birkhoff's

theorem in high-dimensional systems. Many of the results presented are valid for arbitrary qudit systems. However, during this work, we focus on the qutrit setup, the simplest case for which the quantum analogue of Birkhoff's theorem is no longer valid.

Some relevant works considered geometrical aspects of the set of UCPT maps/LMM states. Audenaert *et al.*, considered the distance between the set of mixed-unitary maps and the set of unital quantum maps [1]. Another contribution to this area was made by Mendl and Wolf who provided computable criteria for the separation of both sets [2]. More recently, the complexity of the problem of detecting whether a given map is mixed-unitary was determined to be an NP-hard problem [3]. For locally maximally mixed states, Baumgartner *et al.*, considered the set of bipartite states obtained as convex mixtures of maximally-mixed pure states [4-6]. In this series of papers, the entanglement characterisation of this class of bipartite states was considered both for two-qutrit systems and arbitrary dimension systems. The approach used in this thesis to consider UCPT maps/LMM states differs from previous works on the same topic. The crucial step in this approach is to construct novel families of UCPT maps which extends the set of mixed-unitary maps. Just as mixed-unitary channels correspond to all possible convex combinations of rank-one maps (unitary channels), we consider the class of unital maps arising from mixing a restricted set of UCPT maps that are extreme in the whole set of UCPT maps (analogously for LMM states).

To achieve the thesis aims, we determine the following research objectives.

1. Create a novel framework generalising the construction of UCPT maps. Such a framework should include both unitary maps and maps that are not convex mixtures of unitary maps.
2. Describe the geometry of the maps constructed with this novel framework by determining a separation criterion between these maps and the set of mixed-unitary maps.
3. Investigate properties of the bipartite states associated through the state-duality to the constructed maps. In particular, consider the degree of entanglement of the bipartite states and classify them in terms of their entanglement properties.
4. Verify numerically the construction methods developed as well as the characterisation of the resulting maps and states for low dimensional systems

The results of this thesis, are organised into three different chapters. Here, we outline their contents, pointing out the main contributions in each chapter.

In Chapter 4, we consider the convex characterisation of UCPT maps. The contents of this chapter are partially included in [7]. The main contribution of this chapter is the definition of a novel family of maps $\mathcal{E} : \mathcal{D}_d \rightarrow \mathcal{D}_d$ of rank $k \leq d$ generalising previously known UCPT-extremal maps. A similar family of trace-preserving (not unital) maps was considered in [8] in the context of quantum circuit decomposition. For this family of maps, the constraints that guarantee that such maps are unital and trace-preserving are derived as well as the conditions which determine whether the elements of the family correspond to extreme points of the set of UCTP maps. However, we acknowledge that the family of maps introduced does not span the whole set of UCPT-extremal maps. While the family of maps is given in terms of $2d^2 - 3d + 1$ real parameters, a general description of UCTP-extremal maps would require $2d^3 - 3d^2$ real parameters [9, 10]. Finally, we consider the particular case of qutrit maps. For this dimension, we show that the family of UCTP maps presented contains the set of unitary qutrit maps but also the antisymmetric Werner-Holevo channel of dimension three, a well-studied example of UCTP-extremal map [11].

In Chapter 5, we consider the geometry of the set of locally maximally mixed bipartite states and the problem of entanglement classification for a particular set of bipartite states. First, we obtain the family of LMM states associated with the family of UCPT maps introduced in Chapter 4. Then, the classification of the elements of this family is made in terms of local unitary equivalence classes. We use three different sets of LU invariants for entanglement classification. These are the set of invariants given by the eigenvalues of the density matrix, the set of invariants given by the eigenvalues of the partially transposed matrix and, finally, the set of invariants given by the singular values of the correlation matrix. We find that for the family introduced, the diagonalisation of the mentioned matrices is faster than for a general bipartite state. Finally, the particular case of two qutrit states is considered.

In Chapter 6, we consider the solutions of the equations giving the families UCTP maps and LMM bipartite states for qutrit systems and an approximate algorithm based to find solutions for these equations. A graphical representation of the equations is provided allowing to visualise the

space of solutions. Finally, we consider a constraint in the parameters of the equations. For this constraint, the solutions of the equations giving UCTP and LMM states can be solved analytically. For this particular set of solutions, the LU invariants considered in Chapter 5 are used for entanglement classification.

Chapter 2

Basic concepts in quantum mechanics

This chapter serves as an introduction to the area of knowledge of this thesis, quantum information theory. We start by introducing a set of axioms establishing the basic mathematical framework to describe quantum systems. This mathematical framework will be used to define the two different descriptions of quantum systems which we will consider in this thesis: Quantum maps, describing the evolution of open quantum systems and bipartite states, describing two-party composite quantum systems. Finally, we introduce a useful relationship that links both descriptions.

2.1 Introduction to quantum information theory

Quantum information theory is the area of science describing the manipulation of information by means of quantum systems. Before a proper introduction to the subject, we may ask what do we mean when we talk about ‘information’ and when we talk about ‘quantum’. Information can be identified as the most general thing which must propagate from a cause to an effect. Quantum science is the area of physics describing systems, such as electrons or photons, which cannot be described in terms of classical mechanics. It was soon acknowledged that information could be

transmitted, stored and processed by quantum systems [12]. Quantum information science appears precisely to describe the manipulation of information from the perspective of quantum physics. Many introductory texts in quantum information theory use an axiomatic approach [12, 13]. Quantum axioms or postulates are based on empirical evidence and provide the basic framework to construct quantum theory. These axioms characterise the mathematical objects used to describe quantum systems.

2.1.1 Axioms of quantum mechanics

The first axiom establishes the mathematical description of the state space of quantum systems.

Axiom 1. *The state space of a quantum mechanical system is represented by a complex vector space V equipped with a Hermitian inner product.*

The Hermitian inner product is defined as follows.

Definition 1. *A Hermitian inner product on a complex vector space is a map*

$$\langle \cdot | \cdot \rangle : V \times V \rightarrow \mathbb{C} \quad (2.1)$$

with the following properties

- *Conjugate symmetry. For $x, y \in V$*

$$\langle x | y \rangle = \langle y | x \rangle^* \quad (2.2)$$

where ‘ $*$ ’ denotes the complex conjugate operation.

- *Anti-linearity in the first argument and linearity in the second. For $x, y, z \in V$ and $\alpha, \beta \in \mathbb{C}$*

$$\langle \alpha x + \beta y | z \rangle = \alpha^* \langle x | z \rangle + \beta^* \langle y | z \rangle \quad (2.3)$$

and

$$\langle z | \alpha x + \beta y \rangle = \alpha \langle z | x \rangle + \beta \langle z | y \rangle. \quad (2.4)$$

- *Positive-definiteness. For $x \neq 0 \in V$,*

$$\langle x | x \rangle > 0. \quad (2.5)$$

The vector space V together with the Hermitian inner product is complete with respect to the norm induced by the inner product and, by definition, it is a Hilbert space. With a slight abuse of notation, we will use the term Hilbert space as synonym of the particular state space used to describe quantum systems.

Depending on the quantum system, its associated Hilbert space can be finite dimensional or infinite dimensional. For example, the space of positions or the space of momentums of a particle are infinite dimensional. However, the possible spins of a electron or the polarisations of a photon are given by finite dimensional vector spaces. In this thesis, we will consider only Hilbert spaces of finite dimension $\mathcal{H} := \mathbb{C}^n$ where $n \in \mathbb{N}$ denotes the dimension of the Hilbert space. The vector space \mathbb{C}^n is formed by all n -tuples of complex numbers and a vector $x \in \mathbb{C}^n$ is represented as

$$x = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}, \quad (2.6)$$

where $\alpha_1 \dots \alpha_n \in \mathbb{C}$. Consider a set of vectors $y_1, \dots, y_n \in \mathbb{C}^n$ such that any vector $x \in \mathbb{C}^n$ can be expressed as the linear combination

$$x = \beta_1 y_1 + \dots + \beta_n y_n, \quad (2.7)$$

where $\beta_1, \dots, \beta_n \in \mathbb{C}$. Then, the set y_1, \dots, y_n is a spanning set of \mathbb{C}^n . For example, the set $\left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$ is a spanning set of \mathbb{C}^2 and, in this case, a vector $x \in \mathbb{C}_2$ is expressed in terms of this spanning set as

$$x = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \alpha_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.8)$$

To represent the vector space describing a quantum system, we use the standard notation in quantum information theory, Dirac's notation. In this notation, the elements of the Hilbert space are given by 'kets' expressed as $|\psi\rangle \in \mathbb{C}^n$. For the finite space \mathbb{C}^n , there is always a spanning set of orthonormal vectors $|\phi_1\rangle \dots |\phi_n\rangle \in \mathbb{C}^n$ satisfying

$$\langle \phi_i | \phi_j \rangle = \delta_{i,j}, \quad (2.9)$$

where $\delta_{i,j}$, the Kroneker delta, is defined as

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases} \quad (2.10)$$

In this case, the spanning set $|\phi_1\rangle \dots |\phi_n\rangle \in \mathbb{C}^n$ forms an orthonormal basis of \mathbb{C}^n and each element of the vector space has a unique representation in terms of the same orthonormal basis. The particular orthonormal basis given by vectors with all zeros except one term is denoted as the computational basis of \mathbb{C}^n . In Dirac's notation the elements of the computational basis of \mathbb{C}^n are denoted by kets labelled with natural numbers $|0\rangle, \dots, |n-1\rangle$. For example, for \mathbb{C}^2 , the elements of the computational basis are denoted by

$$|0\rangle =: \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (2.11)$$

and

$$|1\rangle =: \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.12)$$

A fundamental components in Dirac's notation is the so called 'bra', denoted by $\langle\theta|$. In this notation, a bra corresponds to a linear map from the space of 'kets' $|\phi\rangle \in \mathbb{C}^n$ to a number in the complex plane. The map given by $\langle\theta|$ is formally defined as

$$\theta : |\phi\rangle \rightarrow \langle\phi|\theta\rangle \in \mathbb{C}. \quad (2.13)$$

Using Dirac's notation, we can also define linear operators acting on the Hilbert space. A linear operator A acts on the space of kets as

$$A : |\phi\rangle \rightarrow A|\phi\rangle \in \mathcal{H}. \quad (2.14)$$

For a given basis, an operator can always be expressed as a matrix. For example, for \mathbb{C}^2 , an operator can be expressed on the computational basis as

$$A = a_{00} |0\rangle \langle 0| + a_{01} |0\rangle \langle 1| + a_{10} |1\rangle \langle 0| + a_{11} |1\rangle \langle 1| \quad (2.15)$$

where $a_{ij} \in \mathbb{C}$ for $i, j \in \{0, 1\}$. In this basis, the operator A corresponds to the matrix

$$A = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix}. \quad (2.16)$$

We denote the space of $n \times m$ matrices by $\mathcal{M}_{n \times m}$. In the case of square matrices, $n = m$, we denote them by $\mathcal{M}_n := \mathcal{M}_{n \times n}$. The following axiom describes how information can be extracted from quantum systems by means of observables.

Axiom 2. *The observables of a quantum mechanical system are given by hermitian operators acting on the state space \mathcal{H} .*

An operator A is hermitian if it is equal to its adjoint

$$A = A^\dagger \quad (2.17)$$

where ‘ \dagger ’, the adjoint operation, represents the combination of conjugation and transposition operations, $A^\dagger := (A^*)^T$. Observables represent physical quantities that can be measured. Consider an observable O and consider the state $|\psi\rangle$ which can be expressed in the basis spanned by the eigenvectors of the observable O as

$$|\psi\rangle = \sum_{i=1}^n |\phi_i\rangle \langle \phi_i | \psi \rangle \quad (2.18)$$

where

$$O |\phi_i\rangle = \lambda_i |\phi_i\rangle. \quad (2.19)$$

The possible outcomes of the measurement are given by the set of eigenvalues of O , $\lambda_1, \dots, \lambda_n$. The Born rule says that the probability of obtaining an eigenvalue λ_i as the outcome of a measurement is given by the squared modulus of the projection of the state on the i th eigenstate of the observable

$$P(\lambda_i) = |\langle \psi | \phi_i \rangle|^2. \quad (2.20)$$

Note that the outcomes of the measurements have a physical interpretation because the observables are Hermitian operators and consequently, they have a real spectrum.

We introduce now the axiom that describes how quantum states evolve in time.

Axiom 3. *The evolution of a closed quantum system is given by unitary operators acting on the state,*

$$|\psi\rangle \rightarrow U|\psi\rangle \quad (2.21)$$

where an unitary operator is defined as the matrix $U \in \mathcal{M}_n$ such that

$$U^\dagger U = UU^\dagger = \mathbb{I}_n. \quad (2.22)$$

There are two equivalent interpretations of how quantum systems evolve in time: The Heisenberg picture and the Schrödinger picture. In the Schrödinger picture, states change over time. However, in the Heisenberg picture, states are static and observables evolve in time. In this work, we will consider the first approach in which the evolution of quantum systems is given by the states.

Until this point we have considered only single quantum systems. However, there are numerous physical situations in which the joint description of several systems is necessary. For example, composite systems appear in many-body physics or communication theory where the usual set-up is two distant systems transmitting information. The following axiom provides the description of the state space for composite quantum systems.

Axiom 4. The state space of a composite physical system is the tensor product of the state spaces of the component physical systems.

The tensor product of two Hilbert spaces \mathcal{H} of dimension m and \mathcal{G} of dimension n and is another Hilbert space $\mathcal{H} \otimes \mathcal{G}$ which has dimension mn . The elements of $\mathcal{H} \otimes \mathcal{G}$ are given by linear combinations of ‘tensor products’ $|\psi\rangle \otimes |\phi\rangle$ such that $|\psi\rangle \in \mathcal{H}$ and $|\phi\rangle \in \mathcal{G}$. As an example, consider a system of two two-dimensional systems denoted as A and B , respectively. The Hilbert space of the joint system is given by $\mathcal{H}_A \otimes \mathcal{H}_B = C^2 \otimes C^2$. Any state of the joint system can be written in the computational basis as

$$|\phi_{AB}\rangle = a_0 |0\rangle \otimes |0\rangle + a_1 |0\rangle \otimes |1\rangle + a_2 |1\rangle \otimes |0\rangle + a_3 |1\rangle \otimes |1\rangle \quad (2.23)$$

Usually, the tensor product is not explicitly written and $|\phi_{AB}\rangle$ is usually expressed as

$$|\phi_{AB}\rangle = a_0 |0\rangle |0\rangle + a_1 |0\rangle |1\rangle + a_2 |1\rangle |0\rangle + a_3 |1\rangle |1\rangle \quad (2.24)$$

where the tensoring of adjacent kets is assumed.

2.1.2 Density operators

Axioms 1 to 4 provide the mathematical formalism used to describe closed quantum systems. By closed systems, we refer to systems not interacting with their environment for which all the variables can be controlled. This description of a quantum system is far from practical. In reality, it is impossible to have total control over all the variables affecting a system. Even the most controlled quantum state is affected by external variables. For example, in modern quantum computers, memory qubits are susceptible to interaction with the environment and error-correcting techniques are necessary to correctly run codes. For this reason, open quantum systems are the reference framework in quantum information theory.

The general description of open quantum systems is given by probability ensembles (statistical mixtures) of multiple states. In this description, we can not longer assume that a system is in a certain state, instead, we can only assign probabilities of finding the system in a given set of states. The mathematical description of probability ensembles is made with operators. In particular, the description of the state of an open quantum system is given by the so-called, density operators. Using Dirac's notation, a density operator ρ can be expressed as a matrix in terms of the computational basis of $\mathbb{C}_n \{|0\rangle \dots |n-1\rangle\}$ as

$$\rho = \sum_{i,j=0}^{n-1} p_{ij} |i\rangle \langle j| \quad (2.25)$$

with $p_{ij} \in \mathbb{R}$. However, not all matrices represent probability ensembles of quantum states. The matrix $\rho \in \mathcal{M}_n$ represents a probability ensemble of states if it satisfies the following two conditions:

- Positive-semidefinite: The matrix ρ has non-negative eigenvalues,

$$\rho \geq 0. \quad (2.26)$$

- Unit trace: The trace of a density matrix needs to be equal to one.

$$\text{tr } \rho = 1. \quad (2.27)$$

We denote the set of density matrices by $\mathcal{D}_n \subset \mathcal{M}_n$. Based on the rank of the density matrix, there are two types of states. A state ρ is pure if $\text{rank}(\rho) = 1$. Conversely, ρ is mixed if $\text{rank}(\rho) > 1$.

A special type of state is the maximally-mixed state represented by the density matrix $\rho = \frac{1}{n} \mathbb{I}_n$ where \mathbb{I}_n corresponds to the identity operator acting on the Hilbert space. Pure states represent states with total certainty about the state of the system and maximally states represent states with maximal noise and complete uncertainty about the state of the system.

2.2 Quantum maps

In this section, we introduce the description of the evolution of open quantum systems. Axiom 3 states that the evolution of closed systems is given by unitary transformations on the state space. The state evolution formalism given by axiom 3 can also be extended to open quantum systems [12, 13]. The most general evolution of an open system is given by a linear map Ψ transforming an initial density operator $\rho \in \mathcal{D}_n$ into a final density operator,

$$\Psi : \rho \rightarrow \Psi(\rho) \in \mathcal{D}_n. \quad (2.28)$$

However, not every linear map can be used to represent the evolution of an open quantum system. To see this, we will consider the two conditions required by quantum maps. The first condition is given by the fact that the matrix obtained after the application of the linear maps needs to be a density matrix, so it needs to be positive, semi-definite and normalised (trace one). This means that a quantum map must preserve the positivity and the trace of the output matrix. For the second condition, consider the space of density matrices $\mathcal{D}_n \otimes \mathcal{D}_m$ and the set of linear maps $\Psi \otimes \mathbb{I}_m$ acting on the first subspace while ignoring the second. The form of the linear map Ψ is constrained by the fact $\Psi \otimes \mathbb{I}_m(\rho)$ is also a density matrix. The linear maps that transform positive semi-definite matrices to positive semi-definite matrices $\Psi : \mathcal{D}_n \mapsto \mathcal{D}_m$ are denoted as positive maps. On top of that, if $\Psi \otimes \mathbb{I}_n$ is also positive for $n \in \mathbb{Z}$, the map Ψ is completely positive. We conclude that the evolution of quantum maps is given by completely positive and trace-preserving (CPT) linear maps.

2.2.1 Representations of quantum maps

The action of a linear map $\Psi : \mathcal{M}_n \rightarrow \mathcal{M}_m$ can always be expressed, as the product of an operator $O_\Psi \in \mathcal{M}_{n^2 \times m^2}$ action on the vectorised form of a density matrix as

$$\text{vec}(\Psi(\rho)) = O_\Psi \text{vec}(\rho), \quad (2.29)$$

where the action of vec on a matrix corresponds to arranging the rows of the matrix in vector form. The matrix O_Ψ corresponds to the super-operator representation of the map Ψ . This representation is not very practical as the conditions for a map to be completely positive and trace-preserving can not be easily expressed in terms of the operator O_Ψ . For this reason, other representations are more suitable to represent quantum maps.

In [14], Jamilokowski established a correspondence between the space of linear maps from \mathcal{M}_n to \mathcal{M}_m and the operators in the tensor product space $\mathcal{M}_n \otimes \mathcal{M}_m$. This correspondence is stated by the following theorem.

Theorem 1. *For every linear map $\Psi : \mathcal{M}_n \rightarrow \mathcal{M}_m$, there is an operator $C_\Psi \in \mathcal{M}_m \otimes \mathcal{M}_n$ given by*

$$C_\Psi = (\Psi \otimes \mathbb{I}_n) |\psi\rangle \langle \psi| \quad (2.30)$$

where $|\psi\rangle$ corresponds to $|\psi\rangle = \sum_{i=0}^{n-1} |i\rangle |i\rangle$.

The operator C_Ψ is denoted as the Choi operator. The action of the mapping Ψ can be recovered from C_Ψ by means of the equation

$$\psi(\rho) = \text{tr}_B [(\mathbb{I}_m \otimes \rho^T) C_\Psi] \quad (2.31)$$

where $\text{tr}_A(\text{tr}_B)$ denotes the operator applying a partial trace over the first (second) subsystem. This equation completes the bijection between operators and maps usually referred as the Choi-Jamilokowski isomorphism. To see that this is the right expression for $\psi(\rho)$, we may insert C_Ψ in the expression given by 2.31. We obtain that

$$\text{tr}_B [(\mathbb{I}_m \otimes \rho^T) C_\Psi] = \frac{1}{n} \sum_{i,j=0}^{n-1} \text{tr}_B [(\mathbb{I}_m \otimes \rho^T)(\Psi(|i\rangle \langle j|) \otimes |i\rangle \langle j|)]$$

$$\begin{aligned}
&= \frac{1}{n} \sum_{i,j=0}^{n-1} \text{tr}_B [\Psi(|i\rangle\langle j|) \otimes \rho^T |i\rangle\langle j|] \\
&= \frac{1}{n} \sum_{i,j,l=0}^{n-1} \Psi(|i\rangle\langle j|) \otimes \langle l|\rho^T|i\rangle\langle j|l\rangle \\
&= \frac{1}{n} \sum_{i,j,l=0}^{n-1} \Psi(|i\rangle\langle j|) p_{i,l} \delta_{j,l} \\
&= \frac{1}{n} \sum_{i,j} p_{i,j} \Psi(|i\rangle\langle j|) \\
&= \psi(\rho).
\end{aligned} \tag{2.32}$$

The following theorem originally introduced in [15] states the condition on C_Ψ to represent a completely positive map.

Theorem 2. *The linear map $\Psi : \mathcal{M}_n \rightarrow \mathcal{M}_m$ is completely positive iff C_Ψ is positive semi-definite,*

$$C_\Psi \geq 0. \tag{2.33}$$

The original proof of this theorem is given by [15]. The following theorem states the condition on C_Ψ to represent a trace-preserving map.

Theorem 3. *The linear map $\Phi : \mathcal{M}_n \rightarrow \mathcal{M}_m$ is trace-preserving iff the following condition on C_Ψ is satisfied,*

$$\text{tr}_A(C_\Psi) = \mathbb{I}_n. \tag{2.34}$$

Proof. The map is trace-preserving if $\text{tr}(\Psi(\rho)) = \text{tr}(\rho) \forall \rho \in \mathcal{M}_n$. We take the trace over equation (2.30) as

$$\text{tr}(\psi(\rho)) = \text{tr}(\text{tr}_B(C_\Psi(\mathbb{I}_m \otimes \rho^T))). \tag{2.35}$$

Consider the sets of density matrices $\{\mu_i\}_{i \in \mathbb{Z}}$ and $\{\nu_j\}_{j \in \mathbb{Z}}$ spanning \mathcal{M}_m and \mathcal{M}_n , respectively. We have that the Choi matrix $C_\Psi \in \mathcal{M}_m \otimes \mathcal{M}_n$ can be expressed in terms of the elements of the set

$\{\mu_i \otimes \nu_j\}_{i \in \mathbb{Z}_m, j \in \mathbb{Z}_n}$ as

$$C_\Psi = \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} p_{ij} \mu_i \otimes \nu_j \tag{2.36}$$

where $\{p_{ij} \in \mathbb{C}\}_{i,j \in \mathbb{Z}}$. However, C_Ψ is hermitian so a basis can always be found such that $p_{ij} \in \mathbb{R}$.

We express the trace of $\psi(\rho)$ as

$$\begin{aligned}
\text{tr}(\psi(\rho)) &= \text{tr}[(\mathbb{I}_m \otimes \rho^T)C_\Psi] \\
&= \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} p_{ij} \text{tr}[(\mathbb{I}_m \otimes \rho^T)\mu_i \otimes \nu_j] \\
&= \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} p_{ij} \text{tr}[\mu_i \otimes \rho^T \nu_j] \\
&= \sum_{i=0}^{m-1} \text{tr} \left[\rho^T \sum_{j=0}^{n-1} p_{ij} \nu_j \right] \\
&= \text{tr}[\rho^T \text{tr}_A(C_\psi)]
\end{aligned} \tag{2.37}$$

and consequently, we require $\text{tr}_A(C_\psi) = \mathbb{I}_n$ which yields

$$\text{tr}(\psi(\rho)) = \text{tr}(\rho^T) \quad \forall \rho \in \mathcal{M}_n. \tag{2.38}$$

□

Theorems 2 and 3 establish the conditions for a map to be completely positive and trace-preserving, respectively, in terms of the Choi matrix C_Ψ . The following theorem establish the conditions for a map to be unital [16], a map which leaves the maximally-mixed state unchanged.

Theorem 4. [16] *The linear map $\Phi : \mathcal{M}_m \rightarrow \mathcal{M}_n$ is unital iff*

$$\text{tr}_B(C_\Psi) = \mathbb{I}_m. \tag{2.39}$$

Proof. The map ψ applied to the maximally mixed state \mathbb{I}_n gives as a result

$$\begin{aligned}
\psi(\mathbb{I}_n) &= \text{tr}_B[(\mathbb{I}_m \otimes \mathbb{I}_n)C_\Psi] \\
&= \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} p_{ij} \text{tr}_B[(\mathbb{I}_m \otimes \mathbb{I}_n)\mu_i \otimes \nu_j] \\
&= \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} p_{ij} \text{tr}_B[\mu_i \otimes \nu_j] \\
&= \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} p_{ij} \mu_i = \text{tr}_B(C_\Psi)
\end{aligned} \tag{2.40}$$

and, consequently, the identity operator is mapped to the identity operator iff $\text{tr}_B(C_\Psi) = \mathbb{I}_m$. \square

One can obtain a different representation of a quantum map deriving from the properties of the Choi matrix of a completely positive map. By theorem 2.33, the Choi matrix representing completely positive map is a positive matrix and consequently it can be expressed as

$$C_\Psi = \sum_i |A_i\rangle \langle A_i| \quad (2.41)$$

where $\{|A_i\rangle\}_{i \in \mathbb{Z}}$ are state vectors in the Hilbert space $\mathcal{H} = \mathbb{C}^{mn}$. A state vector can always be expressed in terms of operators $A_i \in \mathcal{M}_{m \times n}$ as

$$|A_i\rangle = (\mathbb{I}_n \otimes A_i) |\psi\rangle \quad (2.42)$$

where $|\psi\rangle = \sum_{i=0}^{n-1} |i\rangle |i\rangle$. The set of operators $\{A_i\}_{i \in \mathbb{Z}}$ provides the representation of a completely positive map known as operator-sum representation. This representation was first introduced by Kraus in [17] and A_0, \dots, A_{n-1} are denoted as Kraus operators in his honour. The action of a map in terms of the Kraus operators can be obtained by expressing the Choi matrix of the map as

$$\begin{aligned} C_\Psi &= \sum_i |A_i\rangle \langle A_i| \\ &= \sum_i (A_i \otimes \mathbb{I}_n) |\psi\rangle \langle \psi| (A_i^\dagger \otimes \mathbb{I}_n) \\ &= \sum_{ijk} (A_i \otimes \mathbb{I}_n) (|j\rangle \langle k| \otimes |j\rangle \langle k|) (A_i^\dagger \otimes \mathbb{I}_n). \end{aligned} \quad (2.43)$$

We introduce the expression of C_Ψ in equation (2.31). We get that

$$\begin{aligned} \psi(\rho) &= \text{tr}_B [(\mathbb{I}_m \otimes \rho^T) C_\Psi] \\ &= \sum_{ijk} \text{tr}_B [(\mathbb{I}_m \otimes \rho^T) (A_i \otimes \mathbb{I}_n) (|j\rangle \langle k| \otimes |j\rangle \langle k|) (A_i^\dagger \otimes \mathbb{I}_n)] \\ &= \sum_{ijk} \text{tr}_B [(A_i |j\rangle \langle k| A_i^\dagger \otimes \rho^T |j\rangle \langle k|)] \\ &= \sum_{ijkl} A_i |j\rangle \langle k| A_i^\dagger \otimes \langle l| \rho^T |j\rangle \langle k| l\rangle \\ &= \sum_{ijk} p_{j,k} A_i |j\rangle \langle k| A_i^\dagger \end{aligned}$$

$$= \sum_i A_i \rho A_i^\dagger \quad (2.44)$$

which is the action of the map on a density matrix in terms of its operator-sum representation. As we did with the Choi matrix, we evaluate the conditions in terms of the Kraus operators that guarantee that a map is trace-preserving and unital. In order to get the trace-preserving and unital conditions, we express the partial traces of the Choi matrix in terms the Kraus operators $\{A_i\}_{i \in \mathbb{Z}}$. The partial trace with respect of the first subsystem can be expressed as

$$\begin{aligned} \text{tr}_A [C_\Psi] &= \sum_{ijk} \text{tr}_A \left[(A_i \otimes \mathbb{I}_n) (|j\rangle \langle k| \otimes |j\rangle \langle k|) (A_i^\dagger \otimes \mathbb{I}_n) \right] \\ &= \sum_{ijk} \text{tr}_A \left[A_i |j\rangle \langle k| A_i^\dagger \otimes |j\rangle \langle k| \right] \\ &= \sum_{ijk} \text{tr}_A \left[A_i^\dagger A_i |j\rangle \langle k| \otimes |j\rangle \langle k| \right] \\ &= \sum_{ijkl} \langle l| A_i^\dagger A_i |j\rangle \langle k|l\rangle |j\rangle \langle k| \\ &= \sum_{ijk} \langle k| A_i^\dagger A_i |j\rangle |j\rangle \langle k| \\ &= \sum_i (A_i^\dagger A_i)^T. \end{aligned} \quad (2.45)$$

By theorem 3, we have that a map is trace preserving if $\text{tr}_A [C_\Psi] = \mathbb{I}_m$. In terms of the Kraus operators representing a map, we require that

$$\sum_i A_i^\dagger A_i = \mathbb{I}_m. \quad (2.46)$$

Similarly, the partial trace of the Choi matrix with respect to the second subsystem is given by

$$\begin{aligned} \text{tr}_B [C_\Psi] &= \sum_{ijk} \text{tr}_B \left[(A_i \otimes \mathbb{I}_n) (|j\rangle \langle k| \otimes |j\rangle \langle k|) (A_i \otimes \mathbb{I}_n) \right] \\ &= \sum_{ijk} \text{tr}_B \left[A_i |j\rangle \langle k| A_i^\dagger \otimes |j\rangle \langle k| \right] \\ &= \sum_{ijkl} A_i |j\rangle \langle k| A_i^\dagger \langle l|j\rangle \langle k|l\rangle \\ &= \sum_i A_i \left(\sum_l |l\rangle \langle l| \right) A_i^\dagger \end{aligned}$$

$$= \sum_i A_i A_i^\dagger. \quad (2.47)$$

In this case, by theorem 4, a map is unital if $\text{tr}_B [C_\Psi] = \mathbb{I}_n$. In terms of the operator-sum representation, this condition corresponds to

$$\sum_i A_i A_i^\dagger = \mathbb{I}_n. \quad (2.48)$$

A Choi matrix representing a completely positive map can always be expressed as a convex sum of pure states as in (2.41). However, for a given matrix this decomposition is not unique. The following theorem provides the relation between two different convex pure decompositions of the same operator

Theorem 5 ([18]). *Consider two different decompositions of the same positive operator $O \in \mathcal{M}_{d \times d}$ given by*

$$O = \sum_i^N a_i |A_i\rangle \langle A_i|, \quad \sum_i a_i = c, \quad a_i \geq 0 \quad (2.49)$$

and

$$O = \sum_i^M b_i |B_i\rangle \langle B_i|, \quad \sum_i b_i = c, \quad b_i \geq 0 \quad (2.50)$$

$c \in \mathbb{R}$. Then, $\{|A_i\rangle\}_{i \in \mathbb{Z}_N}$ and $\{|B_i\rangle\}_{i \in \mathbb{Z}_M}$ are related through the following equation

$$B_i = \frac{1}{\sqrt{b_i}} \sum_j^N u_{ij} \sqrt{a_j} |A_j\rangle, \quad (2.51)$$

where $U = (u_{ij})_{i,j \in \mathbb{Z}_M}$ is unitary $U^\dagger U = U U^\dagger = \mathbb{I}_M$.

One consequence of this theorem is that the operator-sum representation of a CP map is not unique. To see this, we can express the sets of state vectors $\{|A_i\rangle\}_{i \in \mathbb{Z}_N}$ and $\{|B_i\rangle\}_{i \in \mathbb{Z}_M}$ in theorem 5 in terms of operators as in (2.42). The two sets of operators $(A_i)_{i \in \mathbb{Z}_N}$ and $(B_j)_{j \in \mathbb{Z}_M}$ representing the same CP map are necessarily related by the following equation

$$(\mathbb{I}_n \otimes B_j) |\psi\rangle = \frac{1}{\sqrt{b_j}} \sum_i^N u_{ij} \sqrt{a_i} (\mathbb{I}_n \otimes A_i) |\psi\rangle. \quad (2.52)$$

and, consequently,

$$B_j = \sum_i^N u_{ij} A_i. \quad (2.53)$$

Note that two sets of Kraus operators with different cardinality $M \neq N$ represent the same map if by appending zero operators to the set with fewer elements, equation (2.53) maintains. From all the pure decompositions of the Choi matrix representing a CP map the spectral decomposition has the particularity that the states are orthonormal

$$C_\Psi = \sum_i^c \lambda_i |\kappa_i\rangle \langle \kappa_i|, \quad \langle \kappa_i | \kappa_j \rangle = \delta_{i,j} \quad (2.54)$$

In this case, c is the rank of the Choi matrix and is denoted as the Choi (or Kraus) rank of a map. Sets of Kraus operators associated with orthogonal eigenvectors of a given matrix provide representations of the map for which the Kraus rank is minimal. We will use this idea to construct a family of maps in Chapter 3.

2.3 Bipartite states

Axiom 4 states that the vector space of a composite closed quantum system is the tensor product of the vector spaces of the individual subsystems. This property is a characteristic of quantum mechanics and establishes a significant difference with respect to classical mechanics. We will consider those differences and their consequences on the understanding of nature using a quantum mechanics. We shall consider joint systems composed of two individual subsystems which we denote by A and B . The state space of systems A and B are given by the Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , respectively. By axiom 4, the state space of the joint system is given by the set of states $\mathcal{H}_A \otimes \mathcal{H}_B$.

Consider that \mathcal{H}_A and \mathcal{H}_B have dimension m and n , respectively. In the previous section, we saw that an orthonormal basis can be found for each one of the Hilbert spaces. If the set of vectors $\{|e_i\rangle_A\}_{i \in \mathbb{Z}}$ is an orthonormal base of \mathcal{H}_A and the set $\{|f_i\rangle_B\}_{i \in \mathbb{Z}}$ is an orthonormal base of \mathcal{H}_B , then, the set $\{|e_i\rangle_A \otimes |f_j\rangle_B\}_{i,j \in \mathbb{Z}}$ is a basis of the tensor space $\mathcal{H}_A \otimes \mathcal{H}_B$. Any density operator representing the state of the composite system can be expressed as a complex matrix $\rho_{AB} \in \mathcal{M}_{mn \times mn}$ acting on the state space $\mathcal{H}_A \otimes \mathcal{H}_B$.

The fact that the state space of the system is mn -dimensional establishes a crucial difference in relation to a classical description of the system. In a classical description, all the information

of a composite system can always be reconstructed from the characterisation of its parts. However, this is not the case for quantum systems. If all the information of a compound system was contained in its parts the state space of the system could only have $m + n$ dimensions. In reality, for quantum systems the state space is mn -dimensional, and the majority of the states cannot be described by classical means. Schrödinger summarised this fact stating that in quantum mechanics the description of the whole is larger than the description of the parts.

We differentiate bipartite states which can be described by classical means from those which do not admit such description. A bipartite pure state admits a classical description if it can be expressed as a product state

$$|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle. \quad (2.55)$$

Similarly, a bipartite mixed state admits a classical description if it can be expressed as an probabilistic ensemble of product states

$$\rho_{AB} = \sum_{i=0}^{d-1} \rho_i^{(A)} \otimes \rho_i^{(B)}. \quad (2.56)$$

Those states that can be expressed as equation (2.56) (or as equation (2.55) for the particular case of pure states) are said to be separable. In general, the state of a bipartite system is not separable and in those cases, the state is said to be entangled. In other words, entangled bipartite states are those which can only be described using quantum mechanics.

2.3.1 Entanglement as a resource

In 1935, Schrödinger was the first to consider entangled states in a response letter to the famous paper by Einstein, Podolski and Rosen [19, 20]. For many years, entanglement was seen as a mathematical artefact with no practical use. However, this vision changed in the early nineties when several groups showed that entangled states could be used to perform useful tasks. Bennett *et al.* created protocols using entangled states for dense coding [21], they also showed that entanglement could be used for teleportation [22]. Similarly, Ekert showed that entanglement in states could be used quantum cryptography [23] and also in quantum computing [23]. Since then, more applications of entanglement appeared and some of them were experimentally carried out. Entanglement

emerged as a rich field of study both for theoretical and experimental research and today it is a key ingredient of the so-called second quantum revolution which aims to bring to the people applications of quantum information theory such as the future quantum internet [24]. A protocol using entanglement usually starts with the generation of entangled pairs between systems A and B by the direct interaction of the two systems or by the interaction of systems A and B with a third system. As a result of applying a protocol entangled pairs are consumed and, as a consequence, the entanglement between the systems is lost. In this scenario, entanglement can be seen a resource in the same way that energy is as a resource in thermodynamics.

2.3.2 Entanglement characterisation

In many applications, it is usually important to characterise entanglement between two systems. Intuitively, characterising a state in terms of its entanglement corresponds to determining whether the state is indeed entangled or not. In the case it is entangled, the characterisation consists of determining the degree of entanglement of the state or, in other words, how far is the state from not being entangled. To do this, we need to determine which operations can be performed over ρ_{AB} without increasing its entanglement. As previously stated, operations acting locally on subsystems A and B do not increase the entanglement of the system. A local operation on ρ_{AB} can be expressed as

$$\Psi_A \otimes \Psi_B(\rho_{AB}) \tag{2.57}$$

where Ψ_A is a quantum operation applied only A and Ψ_B is a quantum operation applied on B . However, local operations are not the only operations that do not increase the entanglement of the system. The parts of a certain system may be classical correlated without being entangled. This type of correlation can be established via classical communication between A and B which may perform measurements on their respective states, communicate their results and apply an operation based on information they receive from the other part. The operations result from applying successive rounds of local operations and classical communication (LOCC operations) transform the initial state ρ_{AB} as

$$\rho_{AB} \xrightarrow{\text{LOCC}} \rho'_{AB} \tag{2.58}$$

where the state ρ'_{AB} is, as much, as entangled as the original state ρ_{AB} .

We may also consider the class of operations which maintain the degree of entanglement of ρ_{AB} . Such operations are necessarily local because they do not increase entanglement. In this case, they also need to be reversible (no measurements) so that entanglement does not decrease either. This type of operations are called local unitary (LU). In this case, Ψ_A and Ψ_B represent unitary operations so the initial state ρ_{AB} is reversely transformed as

$$\rho_{AB} \xleftrightarrow{\text{LU}} \rho'_{AB} \quad (2.59)$$

where

$$\rho'_{AB} = (U_A \otimes U_B) \rho_{AB} (U_A^\dagger \otimes U_B^\dagger) \quad (2.60)$$

and U_A and U_B are unitary operators. In this case, the degree of entanglement is maintained after applying the LU operation. Local unitary operations determine entanglement classes of equivalent states. Determining all the LU classes of a system is usually hard and it can only be done for some certain states such as pure states or two-dimensional mixed states. The LU classification of these states can be obtained as follows.

Pure states

One of the cases where LU classification is possible is the set of pure states. Consider the pure state $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ where d_A and d_B are the dimensions of \mathcal{H}_A and \mathcal{H}_B , respectively. This state can always be expressed in terms of a product basis as

$$|\psi_{AB}\rangle = \sum_{i=0}^{d_A-1} \sum_{j=0}^{d_B-1} t_{i,j} |i\rangle \otimes |j\rangle, \quad (2.61)$$

where $t_{i,j} \in \mathbb{C}$. The LU equivalence class of $|\psi_{AB}\rangle$ is given by all the states of the form $(U \otimes V) |\psi_{AB}\rangle$ such that U and V are unitary matrices. By expressing U and V in terms of the computational

basis as $U = \sum_{i,j=0}^{d_A-1} u_{ij} |i\rangle \langle j|$ and $V = \sum_{i,j=0}^{d_B-1} v_{ij} |i\rangle \langle j|$, we get that

$$\begin{aligned} (U \otimes V) |\psi_{AB}\rangle &= \sum_{i,j,k=0}^{d_A-1} \sum_{l,m,n=0}^{d_B-1} u_{i,j} t_{k,l} v_{m,n} |i\rangle \langle j|k\rangle \otimes |l\rangle \langle m|n\rangle \\ &= \sum_{i,j=0}^{d_A-1} \sum_{k,l=0}^{d_B-1} u_{i,j} t_{j,m} v_{m,l} |i\rangle \otimes |l\rangle. \end{aligned} \quad (2.62)$$

Therefore, a LU operation on $|\psi_{AB}\rangle$ corresponds to applying two changes of basis on the matrix of coefficients $T = (t_{i,j})_{i=1,\dots,d_A, j=1,\dots,d_B}$. This transformation in matrix form is expressed as $T' = UTV^T$.

We are interested in finding a state representative for each of the LU classes. For any matrix T , one can always find matrices U and V such that UTV^T is diagonal. Suppose that $d_A \geq d_B$, then $|\psi_{AB}\rangle$ can be brought by means of LU operations to the following form

$$|\psi_{AB}\rangle = \sum_{i=0}^{d_A-1} \lambda_{i+1} |i\rangle \otimes |i\rangle. \quad (2.63)$$

The expression above corresponds to the Schmidt decomposition of the state $|\psi_{AB}\rangle$ [25]. The coefficients of the decomposition λ_i correspond to the singular values of the matrix T . They form the Schmidt vector $\vec{\lambda} = (\lambda_i)_{i=1,\dots,d_A}$ determining the entanglement properties of any pure state. The number of non-zero elements of the Schmidt vector is denoted as Schmidt rank. Because of the normalisation condition $\langle \psi_{AB} | \psi_{AB} \rangle = 1$ the Schmidt vector elements satisfy $\sum_{i=1}^{d_A} \lambda_i^2 = 1$. Equivalently, the coefficients λ_i can be evaluated as the square root of the eigenvalues of the partially reduced states $\rho_A = \text{tr}_B |\psi_{AB}\rangle \langle \psi_{AB}|$ and $\rho_B = \text{tr}_A |\psi_{AB}\rangle \langle \psi_{AB}|$ which may differ by $d_A - d_B$ zero valued eigenvalues.

We can discriminate between separable and entangled states by using the Schmidt decomposition. For pure separable states, the Schmidt decomposition is a product state and therefore has only one term. Therefore, we can determine whether a pure state is entangled by evaluating its Schmidt rank. In the case that the Schmidt rank is one the state is separable. Otherwise the state is entangled. Schmidt decomposition can also be used to determine the degree of entanglement of a pure state. In this context, Nielsen introduced a theorem used to compare the degree of entanglement of two states. Before presenting this theorem we need to define vector majorisation.

Definition 2. Consider two positive vectors with the same length $\vec{u} = (u_1, \dots, u_d)$ and $\vec{v} = (v_1, \dots, v_d)$ where their elements add up to the same number $\sum_{i=1}^d u_i = \sum_{i=1}^d v_i$. The elements in \vec{u} and \vec{v} can be ordered in decreasing order, we denote the ordered versions of these vectors by \vec{u}^\downarrow and \vec{v}^\downarrow , respectively. The vector \vec{u} majorises \vec{v} , written as $\vec{u} \succ \vec{v}$, if and only if

$$\sum_{i=1}^k u_i^\downarrow \geq \sum_{i=1}^k v_i^\downarrow \quad \text{for } k = 1, \dots, d. \quad (2.64)$$

The following theorem can be used to compare the degree of entanglement of two pure states.

Theorem 6 ([26]). The state $|\psi_{AB}\rangle$ can be transformed into $|\phi_{AB}\rangle$ by a LOCC operation if the Schmidt vector $\vec{\lambda}_\phi$ majorises the Schmidt vector $\vec{\lambda}_\psi$

$$|\psi_{AB}\rangle \xrightarrow{\text{LOCC}} |\phi_{AB}\rangle \quad \Leftrightarrow \quad \vec{\lambda}_\psi \prec \vec{\lambda}_\phi. \quad (2.65)$$

We refer to the original paper by Nielsen for the proof of the theorem. Theorem 6 provides a hierarchy for the degree of entanglement of pure states. We may ask if there are states on the top of that hierarchy, states that can be transformed into any other using LOCC operations. This class of states are characterised by a uniform Schmidt vector and they are usually denoted as maximally entangled pure states (MEPS),

$$|\psi_{MEPS}\rangle \quad \Leftrightarrow \quad \vec{\lambda}_{MEPS} = \left\{ \sqrt{\frac{1}{d_A}}, \dots, \sqrt{\frac{1}{d_A}} \right\}. \quad (2.66)$$

By theorem 6, maximally entangled states can be transformed to any other by means of LOCC operations. A well-known example of two-dimensional maximally entangled states, $d_A = 2$ and $d_B = 2$, are the four Bell states $|\psi^+\rangle$, $|\psi^-\rangle$, $|\phi^+\rangle$ and $|\phi^-\rangle$ which in the computational basis are expressed as

$$|\psi^\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle|1\rangle \pm |1\rangle|0\rangle) \quad \text{and} \quad |\phi^\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle|0\rangle \pm |1\rangle|1\rangle). \quad (2.67)$$

The degree of entanglement of a state can be quantified using entanglement measures. An entanglement measure is a real and positive function quantifying the degree of entanglement of a given state. Despite there is not a universally accepted definition of entanglement measure,

there are commonly accepted properties that entanglement measure should satisfy. Namely, one of these commonly accepted properties is monotonicity proposed by Vidal in [27]. An entanglement monotone is a magnitude which does not increase, on average, under probabilistic LOCC operations. Probabilistic LOCC operations generalise of LOCC operations by allowing the preparation probabilistic outcomes in the rounds of classical communication between the subsystems. Another commonly accepted property is that entanglement measures must discriminate between entangled and separable states. This means that the result of applying an entanglement measure on a state is zero if and only if the state is separable. Besides these two commonly accepted properties, there are some desirable properties for entanglement measures such as additivity or normalisation.

In the case of pure states, we can find well-behaved entanglement measures. One example of an entanglement measure of pure states is the entropy of entanglement $E(|\psi_{AB}\rangle)$ which was first introduced in [28]. Entropy of entanglement is defined as the Von Neumann entropy of the partially traced state

$$E(|\psi_{AB}\rangle) := S(\text{tr}_B |\psi_{AB}\rangle) \quad (2.68)$$

where the Von Neuman entropy of a density state ρ is given by

$$S(\rho) = - \sum_{i=0}^{d-1} e_i \log(e_i) \quad (2.69)$$

where e_0, \dots, e_{d-1} are the eigenvalues of ρ . Following the fact that Schmidt coefficients correspond to the square root of the eigenvalues of the partially traced states, the entropy of entanglement of $|\psi_{AB}\rangle$ can be obtained as

$$E(|\psi_{AB}\rangle) = - \sum_{i=1}^d \lambda_i^2 \log(\lambda_i^2), \quad (2.70)$$

where $\{\lambda_1, \dots, \lambda_d\}$ are the Schmidt coefficients of $|\psi_{AB}\rangle$. For example, the entropy of entanglement of a maximally entangled pure state is given by

$$\begin{aligned} E(|\psi_{MEPS}\rangle) &= - \sum_{i=1}^d \frac{1}{d} \log\left(\frac{1}{d}\right) \\ &= \log(d) \end{aligned} \quad (2.71)$$

and, in the case of separable states

$$E(|\psi_{SEP}\rangle) = \log(1) = 0. \quad (2.72)$$

For two-qudit states $d_A = d_B = d$ so the Schmidt vector has d elements. Due to the normalisation the Schmidt vector, $d - 1$ degrees of freedom are required to characterise the entanglement of the system. For example, for a two-qubit system, we only require one entanglement measure (such as entropy of entanglement) to characterise completely the entanglement of the system.

Mixed states

Pure state entanglement can be detected and quantified by using the Schmidt decomposition. Unfortunately, there is not an analogous tool for the characterisation of the entanglement of mixed states. One of the objectives of entanglement characterisation is detecting whether a given bipartite system is entangled. This is known as the separability problem. In the case of mixed states of arbitrary dimension, the separability problem is known to be NP-hard [29].

The best technique so far to determine whether a given mixed state is separable is by using entanglement witnesses [30]. Horodecki *et al.* proved the following result

Theorem 7 ([31]). *For every entangled state ρ_{AB} , there exists a Hermitian operator W such that*

$$\text{tr}(W\rho_{AB}) < 0 \quad (2.73)$$

and

$$\text{tr}(W\sigma_{AB}) \geq 0 \quad (2.74)$$

for all separable states σ_{AB} .

An operator W which fulfils the conditions in theorem 7 is an entanglement witness for the state ρ_{AB} . Therefore, a given state can be determined to be entangled if a witness is found. However, finding the entanglement witness is usually hard and on top of that, a witness is only valid to detect the entanglement of a limited set of states. For these reasons, more practical methods are to be developed to detect entanglement.

One possibility for detecting entanglement is via entanglement tests or criteria. One of the most used tests to detect the entanglement is the so-called Peres–Horodecki criterion which was proposed in [32]. The Peres–Horodecki criterion, also known as the partial positive transpose (PPT) criterion, says that for separable states, their partially transpose necessarily have a positive spectrum,

$$\rho_{AB}^{T_B} \geq 0. \quad (2.75)$$

It can be shown that the Peres–Horodecki criterion is necessary and sufficient for qubit-qubit and qubit-qutrit states [33] and consequently it can be used to detect entanglement in those systems. However, for arbitrary dimensional systems, the Peres–Horodecki criterion despite still being necessary, is not sufficient. In other words, this means that there are entangled states which pass the PPT criterion. This class of entangled states are known as PPT-bound entangled states.

As in the case of pure states, entanglement measures may be used to quantify the degree of entanglement of a state. In the case of mixed states, finding an entanglement measure is a compromise between possessing desirable properties (such as monotonicity or additivity) and being easy to compute. In what follows, we introduce several examples of entanglement measures and we discuss their advantages and disadvantages.

Negativity is an easy to compute entanglement measure. Negativity was first introduced in [34] and is defined as the trace norm of the partially transposed density matrix minus one,

$$N(\rho_{AB}) := \|\rho_{AB}^{T_A}\|_1 - 1 \quad (2.76)$$

where the trace norm of a density matrix, written $\|\rho\|_1$, is defined as the sum of its singular values or, equivalently

$$\|\rho\|_1 = \text{tr} \sqrt{\rho \rho^\dagger}. \quad (2.77)$$

Negativity measures the degree to which the partial transposed matrix fails to be positive, and therefore it can be regarded as a quantitative version of the PPT criterion. As mentioned, one of the advantages of negativity is its ease to compute. However, one problem of negativity is that it fails to discriminate entangled states from separable ones. For example, bound PPT states have zero negativity despite being entangled.

One of the most used entanglement measures is the entanglement of formation (EoF), first introduced in [35]. Entanglement of formation is defined as

$$E_F(\rho) := \min_{\mathcal{E}_b} \sum_{i=1}^M p_i E_i(|\psi_i\rangle) \quad (2.78)$$

where the minimisation is performed over all possible decompositions

$$\mathcal{E}_b = \{p_i, |\psi_i\rangle\}_{i=1}^M : \quad \rho = \sum_{i=1}^M p_i |\psi\rangle \langle\psi| \quad (2.79)$$

where $p_i > 0$ and $\sum_{i=1}^M p_i = 1$. Entanglement of formation can be interpreted as the minimal degree of entanglement from pure states required to construct a given mixed state.

Unlike pure states, there is not a hierarchy in the degree of entanglement of mixed states. It was shown that the forms of the maximally entangled mixed states can vary with the measures chosen [36].

2.4 Channel-state duality

In section 2.2, we considered the Choi-Jamilkowski isomorphism as a tool to represent a quantum map in terms of an operator. However, the implications of this isomorphism go beyond quantum maps representation theory. In this section, we see that Choi-Jamilkowski's isomorphism can be used to establish a duality between the set of quantum maps and the set of bipartite states. This duality is of extreme usefulness in quantum information theory as it allows the employment of the measures normally used with bipartite states to characterise quantum maps and vice-versa.

The Choi-Jamilkowski isomorphism establishes a correspondence between the space of linear maps from \mathcal{M}_n to \mathcal{M}_m and the space operators in the tensor product space $\mathcal{M}_n \otimes \mathcal{M}_m$. The condition on a Choi operator to represent a complete positive map corresponds to C_Ψ be positive semi-definite. Thus, by choosing the correct normalisation, every Choi matrix $C_\Psi \in \mathcal{M}_n \otimes \mathcal{M}_m$ representing a complete positive map can be associated with a density matrix representing the state of a bipartite system. In particular

$$C_\Psi = n\rho_{AB} \quad (2.80)$$

is the relation that guarantees that $\text{tr}[\rho_{AB}] = 1$. By using this relation, we consider different classes of maps and their corresponding classes of bipartite states.

In section 2.2, we considered trace-preserving CP maps which were those representing physical evolutions of quantum systems. In terms of the Choi representation, a map is trace-preserving if equation $\text{tr}_A [C_\Psi] = \mathbb{I}_n$ holds. In the case of bipartite states, this condition is equivalent to obtaining the maximally mixed state if we trace ρ_{AB} with respect to system A . Note that, contrary to the case of quantum maps, physically realisable bipartite states do not require to fulfil this condition.

In section 2.2, we also considered the set of maps which were unital on top of being trace-preserving. In terms of the Choi representation of the map, this condition is equivalent to the equation $\text{tr}_B [C_\Psi] = \mathbb{I}_m$. Similarly, unital and trace-preserving maps correspond to bipartite states in which the maximally mixed state is obtained after partial tracing with respect to any of the subsystems. Unital quantum channels and locally maximally mixed bipartite states will be deeply considered in this thesis and an introduction to these classes of maps and their equivalent class of bipartite states will be given in the following chapter. For the moment, we will consider the relation between other classes of maps and bipartite states given by the channel-state duality.

A subclass of unital and trace-preserving maps is the class of unitary maps. In terms of the action over the density matrix, unitary maps correspond to conjugations of ρ given by

$$\Psi(\rho) = U\rho U^\dagger. \quad (2.81)$$

Equivalently, they are represented by rank-one Choi matrices. By the map-state duality, the class of bipartite states corresponding to unitary maps is the class of maximally entangled pure states. For these states the Schmidt decomposition is given by

$$|\psi\rangle_{AB} = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} |e_j\rangle_A \otimes |f_j\rangle_B \quad (2.82)$$

with the Schmidt coefficients $\alpha_i = \frac{1}{\sqrt{n}}$.

Finally, we may consider another interesting association between maps and states. In section 2.3, we considered the class of separable states. In [37], the authors introduce entanglement breaking channels, the class of quantum maps associated, by the map-state duality, with separable states.

A bipartite entangled bipartite state is separable if an entanglement breaking channel is applied to any of the two subsystems.

Chapter 3

Unital quantum maps and locally maximally mixed states

3.1 Introduction

In the previous chapter, we introduced quantum maps which are the mathematical representation used in quantum information science to describe open quantum systems. We also introduced bipartite states describing two-part compound systems. We saw that dualism can be established between quantum maps and bipartite states which is given by the so-called Choi-Jamilkowski isomorphism.

In this chapter, we will consider the particular type of quantum maps which are trace-preserving and unital (UTCP maps). We will also consider the same object represented by UTCP maps in the space of bipartite states which are the so-called locally maximally mixed (LMM) bipartite states. These two mathematical objects are the main focus of this thesis. In particular, we consider the convex geometry of UTCP maps and the entanglement classification of LMM states. To do this, first, we will review the simplest setup of these problems which is given by qubit systems. Second, we will consider the case in which the dimension of the quantum system is higher than two and we will review some problems appearing when dealing with such systems.

3.2 UCTP qubit maps

The set of qubit maps (not necessarily unital) can be parametrised [38–41]. We will follow a well-known method to obtain such parametrisation which is based on the Bloch state representation. We start by defining the Bloch decomposition of a density matrix.

Definition 3 (Bloch decomposition). *Any density matrix $\rho \in \mathcal{M}_d$ can be expressed as*

$$\rho = \frac{\mathbb{I}_2}{2} + \sum_{i=1}^{d^2-1} \tau_i \lambda_i \quad (3.1)$$

where $\tau_i \in \mathbb{C}$ and $\lambda_1, \dots, \lambda_{d^2-1}$ form a basis of traceless matrices.

In the case of qubit systems, $\rho \in \mathcal{M}_2$, we can choose this basis to be the set of Pauli matrices, denoted as $\{\sigma_1, \sigma_2, \sigma_3\}$ where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.2)$$

The elements of the Pauli basis are Hermitian and unitary. As a consequence of the hermiticity, the coefficients of the Bloch decomposition in (3.1) are real and they can be represented graphically as points in \mathbb{R}^3 . If we do this for all qubit states, we obtain a graphical representation of the whole set denoted as the Bloch ball which, by convention, is given by a sphere of radius one. In this picture, the pure states correspond to points on the surface of the sphere and the mixed states correspond to points in the interior. The maximally-mixed state locates at the centre of the sphere.

Consider the qubit map $\phi(\rho) : \mathcal{M}_2 \rightarrow \mathcal{M}_2$. The super-operator representation of $\phi(\rho)$ is expressed in the Pauli basis as the 4×4 real matrix \mathcal{T} . In the case that the map is trace-preserving

$$\mathcal{T} = \begin{pmatrix} 1 & \vec{0} \\ \vec{\kappa} & T \end{pmatrix} \quad (3.3)$$

where $\vec{\kappa}, \vec{0} \in \mathbb{R}^3$ and T is a 3×3 matrix. In this basis, the action of a map on the Bloch representation of the state can be expressed as

$$\vec{\tau} \rightarrow \vec{\tau}' = \phi(\vec{\tau}) = \vec{\kappa} + T\vec{\tau}. \quad (3.4)$$

The maximally-mixed in the Pauli basis corresponds to the zero vector and the action of ϕ on this state is given by

$$\phi(\vec{0}) = \vec{\kappa}. \quad (3.5)$$

Unital maps are those sending the maximally-mixed state to itself $\phi(\vec{0}) = \vec{0}$, so $\vec{\kappa} = \vec{0}$ for these types of maps.

A crucial towards the parametrisation of qubit maps is made in [39]. In this work, it is shown that for any qubit map ϕ , the matrix \mathcal{T} can be brought to the form

$$\mathcal{T} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \kappa_1 & \eta_1 & 0 & 0 \\ \kappa_2 & 0 & \eta_2 & 0 \\ \kappa_3 & 0 & 0 & \eta_3 \end{pmatrix} \quad \text{with } \kappa_i, \eta_i \in \mathbb{R}, \quad (3.6)$$

by applying two unitary conjugations on the map as

$$\phi_{UV}(\rho) = U\phi(V\rho V^\dagger)U^\dagger \quad (3.7)$$

where U and V are unitary matrices. In the Bloch representation of two dimensional systems, unitary conjugations correspond to rotations of the Bloch ball. The action of all maps $\phi_{UV}(\rho)$ given by the same matrix \mathcal{T} are equal up to two rotations of the Bloch ball, one before the action of the map and another one after it. A unital map ($\vec{\kappa} = \vec{0}$) given by a matrix \mathcal{T} as in (3.6) can be characterised solely in terms of the vector $\vec{\eta} = (\eta_1, \eta_2, \eta_3)$, usually denoted as the distortion vector. The action of such maps on Bloch vector can be expressed in terms of the distortion vector as $\vec{\tau}' = \vec{\eta}\vec{\tau}$. By considering this equation, the set of pure states $|\tau|=1$, corresponding to the exterior of the Bloch ball, is mapped into the ellipsoid given by the following equation

$$\left(\frac{\tau'_1}{\eta_1}\right)^2 + \left(\frac{\tau'_2}{\eta_2}\right)^2 + \left(\frac{\tau'_3}{\eta_3}\right)^2 = 1. \quad (3.8)$$

We conclude that the parameters in the distortion vector determine the way in which the Bloch ball is squeezed along the three principal axis.

Now we can identify all the parameters of a qubit map and determine their action on the Bloch ball. Firstly, we have the three parameters of the vector $\vec{\kappa}$ corresponding to a displacement of

the whole Bloch ball which in the case of unital maps is zero. Secondly, we have another three parameters corresponding to the rotation in the Bloch ball induced by the conjugation of the map with V as in (3.7). Thirdly, we have the action of the distortion vector converting the Bloch sphere into an ellipsoid. Finally, we have another three parameters corresponding to a rotation of the squeezed ball.

However, not all ellipsoids in the Bloch picture represent physically allowed transformations between maps. In Chapter 1, we saw that physically realizable maps are necessary completely positive. We may obtain the conditions for complete positive maps in terms of the parametrisation of unital qubit maps. Given a unital qubit map, its Choi matrix is expressed in terms of the distortion vector as

$$C_\phi = \frac{1}{2} \begin{pmatrix} 1 + \eta_3 & 0 & 0 & \eta_1 + \eta_2 \\ 0 & 1 - \eta_3 & \eta_1 - \eta_2 & 0 \\ 0 & \eta_1 - \eta_2 & 1 - \eta_3 & 0 \\ \eta_1 + \eta_2 & 0 & 0 & 1 + \eta_3 \end{pmatrix}. \quad (3.9)$$

By Choi's Theorem, a map is completely positive iff the Choi matrix of the map has positive eigenvalues. The eigenvalues of C_ϕ in (3.9) are given by

$$\begin{aligned} e_1 &= (1 + \eta_3 + (\eta_1 + \eta_2))/2 \\ e_2 &= (1 + \eta_3 - (\eta_1 + \eta_2))/2 \\ e_3 &= (1 - \eta_3 + (\eta_1 - \eta_2))/2 \\ e_4 &= (1 - \eta_3 - (\eta_1 - \eta_2))/2 \end{aligned} \quad (3.10)$$

and are all positive iff the following four conditions are satisfied

$$(1 \pm \eta_3)^2 \geq (\eta_1 \pm \eta_2)^2. \quad (3.11)$$

The four conditions given by (3.11), first introduced in [38], define a 3-simplex in the space of distortion vectors in which the extreme points are given by

$$\vec{\eta}_0 = (1, 1, 1), \vec{\eta}_1 = (1, -1, -1), \vec{\eta}_2 = (-1, 1, -1) \text{ and } \vec{\eta}_3 = (-1, -1, 1). \quad (3.12)$$

The action of these four maps over a state can be expressed as

$$\rho \rightarrow \rho' = \sigma_i \rho \sigma_i \quad \text{for } i = 0, 1, 2, 3 \quad (3.13)$$

where $\sigma_0 = \mathbb{I}$ and $\{\sigma_i\}_{i=1,2,3}$ is the set of Pauli matrices. We can identify all UCTP qubit maps with a point of the tetrahedron with Pauli maps as vertices. We just need to express the Choi matrix of the map in terms of the Pauli basis and evaluate its eigenvalues which correspond to the parameters of the distortion vector. Similarly, the set of UCTP qubit maps correspond to all possible convex combinations of unitary channels. We will see that this is no longer true for higher dimensions.

3.2.1 UCTP qubit maps and doubly-stochastic matrices

We saw that any UCTP qubit map can be expressed as a convex combination of unitary maps. As a consequence, the set UCTP qubit maps has the geometry of a 3-simplex for which the vertices are given by unitary maps. This property of UCTP qubit maps relates to Birkhoff's theorem, a well-known result in matrix theory which we consider in what follows.

The map $\phi(\rho) = \sum_{i=0}^{d-1} K_i \rho K_i^\dagger$ is doubly-stochastic (UCTP) if it is trace-preserving, $\sum_{i=0}^{d-1} K_i^\dagger K_i = \mathbb{I}$, and unital, $\sum_{i=0}^{d-1} K_i K_i^\dagger = \mathbb{I}$. Similarly, the matrix $M = (m_{ij})_{i,j=0,\dots,d-1}$ with $m_{ij} \geq 0$ is doubly-stochastic if $\sum_{i=0}^{d-1} m_{ij} = 1$ for $j = 0, \dots, d-1$ and $\sum_{j=0}^{d-1} m_{ij} = 1$ for $i = 0, \dots, d-1$. This is, the rows and the columns of a doubly-stochastic matrix add up to one. In a similar fashion, unitary maps $\phi_U(\rho) = U\rho U^\dagger$ correspond to permutation matrices in the space of real matrices. Permutation matrices P are doubly-stochastic matrices that have exactly just one entry equal to one in each row and each column and zeros elsewhere. Now we are in position to state Birkhoff's theorem which characterises the convex structure of doubly-stochastic matrices.

Theorem 8. *Any doubly-stochastic matrix M of dimension d admits a decomposition in terms of the possible permutation matrices of dimension d , $P_0, \dots, P_{d!-1}$. Such decomposition is given by*

$$M = \sum_{i=0}^{d!-1} t_i P_i \quad (3.14)$$

where $t_0, \dots, t_{d!-1}$ are positive scalars such that $t_1 + \dots + t_{d!-1} = 1$.

For the proof of this theorem, we refer to the original paper by Birkhoff [42]. By this theorem, the set of doubly-stochastic matrices can be associated with a the $d!$ dimensional polytope (usually known as Birkhoff polytope) in which the vertices correspond to permutation matrices. This geometrical picture of the set of doubly-stochastic matrices agrees with the representation of UCPT qubit maps. Interestingly, as mentioned, this common property of doubly-stochastic matrices and UCPT qubit maps is lost when the sets of UCPT maps of higher dimensions are considered.

3.3 LMM bipartite qubit states

As we saw the set of locally maximally mixed bipartite qubit states is isomorphic to the set of unital and trace-preserving quantum maps. In this section, we will discuss the classification of LMM qubit states in terms of their entanglement [43, 44]. We will see that the entanglement classification of this set allows for a geometrical representation that, unsurprisingly, is completely equivalent to the geometrical representation of UCPT maps. As in pure states, the degree of entanglement of LMM qubit bipartite states can be characterised by using local unitary equivalent classes.

Consider a density matrix ρ_{AB} acting on the product space $\mathcal{H}_A \otimes \mathcal{H}_B$ in which both spaces have the same dimension $d_A = d_B = d$. In the previous section, we considered the Bloch decomposition of a density state. For bipartite states, the elements of the Bloch basis can be chosen to be product states. The Fano decomposition of ρ_{AB} [45] is given by

$$\rho_{AB} = \frac{1}{d^2} \left(\mathbb{I}_d \otimes \mathbb{I}_d + \sum_{i=1}^{d^2-1} s_i \lambda_i \otimes \mathbb{I}_d + \sum_{i=1}^{d^2-1} t_i \mathbb{I}_d \otimes \lambda_i + \sum_{i,j=1}^{d^2-1} r_{ij} \lambda_i \otimes \lambda_j \right) \quad (3.15)$$

where $s_i = \text{tr}(\rho_{AB} \lambda_i \otimes \mathbb{I}_d)$, $t_i = \text{tr}(\rho_{AB} \mathbb{I}_d \otimes \lambda_i)$, $r_{ij} = \text{tr}(\rho_{AB} \lambda_i \otimes \lambda_j)$ and $\{\lambda_i\}_{i \in \mathbb{Z}_{d^2-1}}$ is a base of traceless matrices. In the particular case of LMM states, the Fano form can be further simplified.

By taking the partial trace of ρ_{AB} with respect to the first subsystem we get that

$$\text{tr}_A(\rho_{AB}) = \frac{1}{d} \left(\mathbb{I}_d + \sum_{i=1}^{d^2-1} t_i \lambda_i \right). \quad (3.16)$$

The vector $\vec{t} = \{t_i\}_{i \in \mathbb{Z}_{d^2-1}}$ corresponds to the coefficients of the Bloch decomposition of one of the reduced states. Similarly, if we take the partial trace of the same state with respect with the second

subsystem we get that

$$\mathrm{tr}_B(\rho_{AB}) = \frac{1}{d} \left(\mathbb{I}_d + \sum_{i=1}^{d^2-1} s_i \lambda_i \right). \quad (3.17)$$

In this case, the vector $\vec{s} = \{s_i\}_{i \in \mathbb{Z}_{d^2-1}}$ corresponds to the coefficients of the Bloch decomposition of the other reduced state. In the case of LMM states, $\mathrm{tr}_A(\rho_{AB}) = \mathrm{tr}_B(\rho_{AB}) = \frac{1}{d} \mathbb{I}_d$, so it follows that $\vec{t} = \vec{s} = \vec{0}$. LMM states are expressed in the Fano form as

$$\rho_{AB} = \frac{1}{d^2} \left(\mathbb{I}_d \otimes \mathbb{I}_d + \sum_{i,j=1}^{d^2-1} r_{ij} \lambda_i \otimes \lambda_j \right). \quad (3.18)$$

The matrix $R = \{r_{ij}\}_{i,j \in \mathbb{Z}_{d^2-1}}$ is usually denoted as the correlation matrix and it encodes non-local information about the state. As we saw, LMM states can be described solely in terms of their correlation matrix. We will introduce a theorem that establishes a set of LU invariants in terms of the correlation matrix. To prove this theorem we will make use of the following lemma.

Lemma 1. *Let $U \in SU(d)$ and let $\{\lambda_m\}_{m \in \mathbb{Z}_{d^2-1}}$ denote an orthonormal basis of traceless matrices.*

Then

$$U \lambda_m U^\dagger = \sum_{n=1}^{d^2-1} v_{mn} \lambda_n, \quad \text{for } m = 1, \dots, d^2 - 1 \quad (3.19)$$

where $V = (v_{mn})_{n,m \in \mathbb{Z}_{d^2-1}} \in SU(d^2 - 1)$.

Proof. Let $\overline{\mathcal{M}}_d$ denote the set of all $d \times d$ traceless matrices. Since $\{\lambda_m\}_{m \in \mathbb{Z}_{d^2-1}}$ is a basis of $\overline{\mathcal{M}}_d$ over \mathbb{C} , we can write any matrix $A \in \overline{\mathcal{M}}_d$ as

$$A = \sum_{m=1}^{d^2-1} v_m \lambda_m, \quad (3.20)$$

where $v_m \in \mathbb{C}$. All the matrices which are unitarily similar to A are also traceless and can be expressed as

$$A' = U A U^\dagger = \sum_{m=0}^{d-1} v'_m \lambda_m. \quad (3.21)$$

The product of two matrices given by the left hand side of equation (3.19) can be expressed as

$$\begin{aligned}
\langle U\lambda_i U^\dagger, U\lambda_j U^\dagger \rangle &= \left\langle \sum_{m=1}^{d^2-1} v_{mi} \lambda_m, \sum_{n=1}^{d^2-1} v_{nj} \lambda_n \right\rangle \\
&= \sum_{m,n=1}^{d^2-1} v_{mi}^* v_{nj} \langle \lambda_m, \lambda_n \rangle \\
&= \sum_{m=1}^{d^2-1} v_{mi}^* v_{mj} \tag{3.22}
\end{aligned}$$

where $\langle \lambda_i, \lambda_j \rangle = \delta_{i,j}$. Since unitary similar transformations preserve the normalisation and orthogonality between elements of the basis,

$$\begin{aligned}
\langle U\lambda_i U^\dagger, U\lambda_j U^\dagger \rangle &= \text{tr}(U\lambda_i^\dagger U^\dagger U\lambda_j U^\dagger) \\
&= \text{tr}(\lambda_i^\dagger \lambda_j U^\dagger U) \\
&= \text{tr}(\lambda_i^\dagger \lambda_j) \\
&= \langle \lambda_i, \lambda_j \rangle = \delta_{i,j}, \tag{3.23}
\end{aligned}$$

we get that necessarily

$$\sum_{m=1}^{d^2-1} v_{mi}^* v_{mj} = \delta_{i,j} \tag{3.24}$$

which corresponds to the conditions that guarantee that $V = (v_{mn})_{m,n \in \mathbb{Z}_{d^2-1}}$ is a unitary matrix. \square

Now we are in a position to introduce the following theorem.

Theorem 9 ([43]). *Any state ρ_{AB} can be transformed by means of LU operations into a state ρ'_{AB} whose correlation matrix R' is in diagonal form.*

Proof. Let ρ_{AB} and ρ'_{AB} be two bipartite states related by a local unitary operation,

$$\rho'_{AB} = (U_A \otimes U_B) \rho_{AB} (U_A^\dagger \otimes U_B^\dagger). \tag{3.25}$$

We recall from the Bloch decomposition in (3.15) that the coefficients of the correlation matrix are given by

$$r_{ij} = \langle \rho_{AB}, \lambda_i \otimes \lambda_j \rangle. \tag{3.26}$$

The corresponding coefficients of ρ'_{AB} can be expressed as

$$\begin{aligned}
r'_{ij} &= \langle \rho'_{AB}, \lambda_i \otimes \lambda_j \rangle \\
&= \text{tr} \left((U_A \otimes U_B) \rho^\dagger (U_A^\dagger \otimes U_B^\dagger) \lambda_i \otimes \lambda_j \right) \\
&= \text{tr} \left(\rho^\dagger (U_A^\dagger \otimes U_B^\dagger) \lambda_i \otimes \lambda_j (U_A \otimes U_B) \right) \\
&= \text{tr} \left(\rho^\dagger U_A^\dagger \lambda_i U_A \otimes U_B^\dagger \lambda_j U_B \right) \\
&= \langle \rho, U_A^\dagger \lambda_i U_A \otimes U_B^\dagger \lambda_j U_B \rangle
\end{aligned} \tag{3.27}$$

and, by lemma 1,

$$\begin{aligned}
r'_{ij} &= \langle \rho, U_A^\dagger \lambda_i U_A \otimes U_B^\dagger \lambda_j U_B \rangle \\
&= \langle \rho, \sum_{m=1}^{d^2-1} v_{mi}^{(A)} \lambda_i \otimes \sum_{n=1}^{d^2-1} v_{nj}^{(B)} \lambda_j \rangle \\
&= \sum_{m,n=1}^{d^2-1} v_{mi}^{(A)} v_{nj}^{(B)} \langle \rho, \lambda_i \otimes \lambda_j \rangle.
\end{aligned} \tag{3.28}$$

If we express it in matrix form, then

$$R' = V_A R V_B \tag{3.29}$$

where $V_A, V_B \in SU(d^2 - 1)$. We can always find two special unitary matrices, V_A and V_B , such that $R' = \text{diag}(r'_1, \dots, r'_{d^2-1})$ where $r'_i \in \mathbb{R}$. \square

Note that we did not use the usual singular value decomposition (SVD) in the last step of the proof. As opposed to the usual SVD, in this case, the matrices V_A and V_B are restricted to the subset of unitary matrices with determinant one. To compensate for this constraint, the condition that the singular values are positive needs to be relaxed and accordingly the elements of the diagonal matrix R' may also take negative values. Regardless of this fact, the singular values of the correlation matrix can be used for entanglement classification as they correspond to the absolute values of the elements of R'

$$SVD(R) = |r'_1|, \dots, |r'_{d^2-1}|. \tag{3.30}$$

By using the mathematical tools introduced, we can discuss the particular case of two-qubit LMM states and their characterisation in terms of entanglement. Lemma 1 associates a unitary

matrix $V \in SU(d^2 - 1)$ to every unitary transformation given by the left-hand side of equation (3.19). For, $d = 2$, this association can be established in the other direction and for every decomposition given by the right-hand side of (3.19), one can find a unique conjugation in terms of a unitary matrix $U \in SU(2)$. To see this, it is useful to consider Pauli matrices as the elements of the Bloch basis. In this case, the matrix V is real and consequently $V \in SO(3)$. The sets $U \in SU(2)$ and $V \in SO(3)$ are both three-dimensional and a direct relationship exists between the elements from both Lie groups. In particular, $SU(2)$ is a double-cover of $SO(3)$.

Consider now a state $\rho'_{AB} \in \mathcal{M}_2$ for which R' is a diagonal matrix

$$R' = \begin{pmatrix} r'_1 & 0 & 0 \\ 0 & r'_2 & 0 \\ 0 & 0 & r'_3 \end{pmatrix}. \quad (3.31)$$

By Theorem 9, any state can be brought to this form by means of LU operations and consequently states like ρ'_{AB} are representatives of the entire LU class. All the LU classes of a two-qubit LMM state can be characterised by using three parameters r'_1, r'_2 and r'_3 . However, not all diagonal matrices R' correspond to density matrices with positive eigenvalues. To obtain the positive constraints, we express ρ'_{AB} in terms of r'_1, r'_2 and r'_3 and we evaluate its spectrum. We obtain that ρ'_{AB} is positive if the conditions given by

$$\begin{aligned} 1 - r'_1 - r'_2 - r'_3 &\geq 0 \\ 1 - r'_1 + r'_2 + r'_3 &\geq 0 \\ 1 + r'_1 - r'_2 + r'_3 &\geq 0 \\ 1 + r'_1 + r'_2 - r'_3 &\geq 0 \end{aligned} \quad (3.32)$$

are satisfied. In \mathbb{R}^3 , these conditions correspond to the points of the 3-simplex with vertices at $(1, 1, 1)$, $(1, -1, -1)$, $(-1, 1, -1)$ and $(-1, -1, 1)$ and correspond to the four bell states $|\Phi^+\rangle$, $|\Phi^-\rangle$, $|\Psi^+\rangle$ and $|\Psi^-\rangle$ introduced in the first chapter.

This geometrical representation of the LU classes of two-qubit LMM states is equivalent to the parametric representation of qubit UCPT maps. The Choi-Jamilokowsli isomorphism establishes a

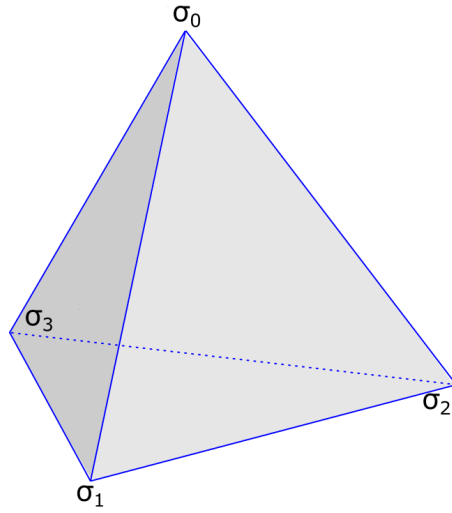


Figure 3.1: Tetrahedron representing the set of unital and trace-preserving qubit maps.

one-to-one correspondence between the set of LMM states and the set of UCPT maps. On top of that, Choi's theorem establishes that the conditions that guarantee the positivity of ρ'_{AB} correspond to the conditions for a map to be completely positive and, in this case, they are given by (3.11). The elements of the correlation matrix R' in the case of LMM states play the same role played by the distortion vector $\vec{\eta}$ for UCPT maps.

Now we can discuss the entanglement characterisation of the set of two-qubit LMM states in terms of the geometry of the set of LU classes. As we saw, the degree of entanglement is maximised by the four Bell states which lie at the vertices of the tetrahedron. We can consider the position of the separable states within this tetrahedron. To do that, we will use the PPT criterion which is necessary and sufficient for two-qubit states. If we take the partial transpose of ρ'_{AB} expressed in terms of r'_1, r'_2 and r'_3 and we evaluate the spectrum of the resulting matrix we obtain that PPT

states are those which fulfil the following conditions

$$\begin{aligned}
 1 + r'_1 + r'_2 + r'_3 &\geq 0 \\
 1 + r'_1 - r'_2 - r'_3 &\geq 0 \\
 1 - r'_1 + r'_2 - r'_3 &\geq 0 \\
 1 - r'_1 - r'_2 + r'_3 &\geq 0.
 \end{aligned} \tag{3.33}$$

In \mathbb{R}^3 , these conditions correspond to the 3-simplex obtained from inverting the 3-simplex representing the states in which ρ'_{AB} is positive. The set of separable states corresponds to the intersection of both figures. Geometrically, the intersection of these two figures is the octahedron with vertices at $(0, 0, \pm 1), (0, \pm 1, 0)$ and $(\pm 1, 0, 0)$.

3.4 Higher dimensional case

It is the case that qubit systems have some particularities which can not be extrapolated to higher-dimensional setups [46]. From an algebraic point of view, unitary conjugations correspond to rotations in the real space, $SU(d) \cong SO(d^2 - 1)$ only for $d = 2$. In a like manner, for higher dimensional systems the Bloch representation of the state space has a much richer structure than the Bloch ball used for qubit systems [47]. For example, for $d = 2$ the boundary of the state space corresponds only to pure states. In the higher dimension, every density state with at least one eigenvalue equal to zero is on the boundary of the state space, including those density states with more than one non-zero eigenvalues (mixed-states). In general, the problems appearing in higher-dimensional quantum systems are substantially harder than their qubit counterparts and many questions about such maps remain unanswered [48].

We saw unital qubit quantum maps possess a differential property compared to higher-dimensional maps. Namely, UCPT qubit maps always admit a decomposition in terms of convex combinations of unitary map [49]. This property of qubit maps allows the representation of the UCPT set as the 3-simplex with Pauli channels as vertices. However, this is no longer true for UCPT maps of higher dimensions. Various investigations introduced examples of maps which were neither uni-

tary channels nor could be decomposed in terms of convex combinations of unitary channels [50, 51]. One consequence of the existence of these types of maps is that there is not an analogue of Birkhoff's theorem for UCPT maps of dimension greater than two. Interestingly, it was found that the distance between a given UCPT map and the set of mixed-unitary maps was reduced by applying the tensor product with more copies of the same map [52]. Based on this observation, it was conjectured that Birkhoff's theorem could be restored in the asymptotic limit. However, Haagerup and Musat in [53] resolved this conjecture as negative.

Chapter 4

The convex set of unital quantum maps

4.1 Introduction

The objective of this chapter is to find families of UCPT-extremal maps generalising the set of rank-one maps (unitary maps) to maps of higher rank. Such maps are interesting from the point of view of the convex characterisation of UCPT maps. To see this, we consider the set of all possible convex mixtures of a family of UCPT-extremal maps including both rank one maps and other maps with a higher rank. Such a set of maps includes all mixed-unitary maps but also other maps which cannot be expressed as convex combinations of unitary maps. An extension of the mixed-unitary set like this could provide new insight into the failure of the quantum analogue of Birkhoff's theorem and it could also offer better classifications for UCPT maps. Figure 4.1 shows the relation between the set of all UCPT maps, the set of mix-unitaries and the set of maps which can be reached by considering convex combinations of families of UCPT-extremal maps including maps other than unitaries.

To do this, we present a family of CP maps which is defined in terms of a particular set of

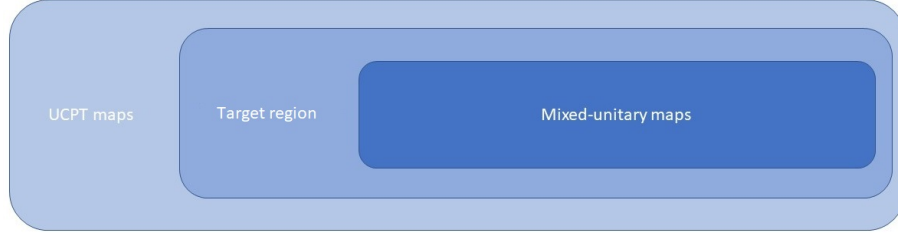


Figure 4.1: Schematic representation of the set of UCPT maps, the set of mixed-unitary maps and the set of all maps given by convex mixtures of rank-generalised families UCPT-extremal maps.

Kraus operators. We introduce a canonical parametrisation of the elements of this family and we discuss in terms of the parameters which elements of the family correspond to UCPT-extremal maps. As an application, we consider the particular case of qutrit maps. In this setting, we see that the family of maps introduced includes maps of rank three or less and we see explicit examples of those UCPT-extremal maps. However, it is well documented the existence of UCPT-extremal maps with rank four [2]. For this reason, we also introduce a different family of qutrit maps including rank-four UCPT-extremal maps. Finally, we consider the evaluation of the degree of extremality for the families of qutrit maps introduced.

4.2 Convex characterisation of UCPT maps

We start by introducing some results concerning the convex characterisation of UCPT maps. The set of trace-preserving maps and its adjoint, the set of unital maps, are convex sets. We denote those maps in a set which cannot be expressed as convex combinations of other elements of the same set as extremal maps. The concise characterisation of the extreme points of the set of unital maps (not trace-preserving) was provided by Choi with the following theorem.

Theorem 10 ([15]). *Consider the set of UCP maps $\mathcal{E} : \mathcal{D}_n \mapsto \mathcal{D}_m$ with minimal operator-sum representation $\mathcal{E}(\rho) = \sum_{i=1}^r K_i \rho K_i^\dagger$. Then, \mathcal{E} is an extreme point within the set of unital maps if and only if the set $\{K_i K_j^\dagger\}_{i,j \in \mathbb{Z}_r}$ is linearly independent.*

Choi's theorem has a natural extension provided that the set of CPT maps is the dual of the set of UCP maps with respect to the complex conjugation. The following theorem establishes when a

CPT map is extremal with respect to the CPT set.

Theorem 11. *Consider the set of CPT maps $\mathcal{E} : \mathcal{D}_n \mapsto \mathcal{D}_m$ with minimal operator-sum representation $\mathcal{E}(\rho) = \sum_{i=1}^r K_i \rho K_i^\dagger$. Then, \mathcal{E} is an extreme point of within the set of trace preserving maps if and only if the set $\{K_i^\dagger K_j\}_{i,j \in \mathbb{Z}_r}$ is linearly independent.*

Theorem 10 and theorem 11 establish bounds to the Kraus rank of the extreme points of the sets of unital maps and trace-preserving maps, respectively. The Kraus rank of an extreme point of the set of unital maps is upper bounded by m . This follows from the fact that at most m^2 matrices $K_i K_j^\dagger$ can be linearly independent as their size is $m \times m$. For the case of trace-preserving maps, we have it that the Kraus rank of an extreme point of the set is upper bounded by n . This follows from the fact that at most n^2 matrices $K_i^\dagger K_j \in \mathcal{M}_{n \times n}$ can be linearly independent. The set of unital and trace-preserving maps is also convex and the following theorem characterises the extreme points of the set.

Theorem 12 ([51]). *Consider the set of UCPT maps $\mathcal{E} : \mathcal{D}_d \rightarrow \mathcal{D}_d$ where $\mathcal{E}(\rho) := \sum_{i=1}^r K_i \rho K_i^\dagger$ and $\sum_{i=1}^r K_i K_i^\dagger = \sum_{i=1}^r K_i^\dagger K_i = \mathbb{I}_d$. Then we say that \mathcal{E} is UCPT-extremal if and only if the set of $2d \times 2d$ matrices*

$$\{K_i^\dagger K_j \oplus K_i K_j^\dagger\}_{i,j \in \mathbb{Z}_r} \quad (4.1)$$

is linearly independent.

From this theorem, it follows that the Kraus rank of UCPT-extremal maps is upper bounded by $\lfloor \sqrt{2d^2} \rfloor$. This follows from the fact that $2d^2$ is the maximum number of linearly independent matrices given by $K_i^\dagger K_j \oplus K_i K_j^\dagger$.

4.3 A family of UCPT-extremal maps

The objective of this section is to find a family of maps including both unitary maps and UCPT-extremal maps of higher rank. To do this, we look at a particular family of CP maps in which its Kraus operators have a special form with respect to the Heisenberg-Weyl basis. For this family

of maps, we select a canonical parametrisation and we discuss in terms of those parameters which elements of the family correspond to UCTP maps.

Let us consider the family of CP maps over dimension d , $\mathcal{E} : \mathcal{D}_d \mapsto \mathcal{D}_d$, whose operator-sum representation is given by

$$\mathcal{E}(\rho) = \sum_{i=0}^{d-1} K_i \rho K_i^\dagger \quad (4.2)$$

with the following Kraus operators

$$\begin{aligned} K_i &= \sum_j^{d-1} \alpha_{ij} X_i Z_j \\ &= \sum_{j,k=0}^{d-1} \alpha_{ij} \omega^{kj} |k+i\rangle \langle k| \end{aligned} \quad (4.3)$$

where $(\alpha_{ij})_{i,j \in \mathbb{Z}_d} \in \mathbb{C}^{d \times d}$ is a matrix of complex coefficients and $\omega = e^{\frac{2\pi}{d}i}$ is the d th primitive root of unity. The set $\{X_i Z_j = \sum_{k=0}^{d-1} \omega^{kj} |k+i\rangle \langle k|\}_{i,j \in \mathbb{Z}_d}$ corresponds to the Heisenberg-Weyl basis over dimension d , a set of orthonormal matrices that generalise the set of Pauli matrices to arbitrary dimension [54]. The sets of Kraus operators $\{K_i\}_{i=0,\dots,d-1}$ and $\{G_i\}_{i=0,\dots,d-1}$ represent the same map if

$$K_j = \sum_{ij=0}^{d-1} u_{ij} G_i \text{ for } j = 0, \dots, d-1 \quad (4.4)$$

where $U = (u_{ij})_{i,j \in \mathbb{Z}_d}$ is a unitary matrix. Now suppose that $\{K_i\}_{i=0,\dots,d-1}$ and $\{G_i\}_{i=0,\dots,d-1}$ are given respectively by the Kraus operators in (4.3). Because of the orthogonality of the sets, $\text{tr}(K_i^\dagger G_j) \propto \delta_{i,j}$ for $i, j = 0, \dots, d-1$, we have it that the unitary matrix in theorem 4.4 is given by

$$U = \begin{pmatrix} e^{i\phi_1} & & \\ & \ddots & \\ & & e^{i\phi_d} \end{pmatrix} \quad (4.5)$$

and this means that the only possible freedom corresponds to multiplying each one of the d Kraus operators by an arbitrary phase. In terms of group theory, this freedom is determined by the action of the group generated by taking the direct product of d copies of the unitary group $U(1)$, $\bigotimes_{i \in \mathbb{Z}_d} U(1)$. The different maps given by the Kraus operators in (4.3) can be divided in equivalence

classes determined by the action of $\bigotimes_{i \in \mathbb{Z}_d} U(1)$. We can represent each one of these classes of maps by fixing the phase of one of the columns of the matrix of coefficients $(\alpha_{ij})_{i,j \in \mathbb{Z}_d}$. To represent each class, we fix the phase of the first column of this matrix of coefficients to zero. We can discuss the properties of a given map of this family in terms of the coefficients α_{ij} . The following theorem establishes which maps are unital and trace preserving.

Theorem 13. *The map $\mathcal{E} : \mathcal{D}_d \mapsto \mathcal{D}_d$ given by the operator-sum representation $\mathcal{E}(\rho) = \sum_{i=0}^{d-1} K_i \rho K_i^\dagger$ where $K_i = \sum_{j,k=0}^{d-1} \alpha_{ij} \omega^{jk} |k+i\rangle \langle k|$ is trace-preserving if*

$$\sum_{i,j=0}^{d-1} \alpha_{ij} \alpha_{ij}^* = 1 \quad (4.6)$$

and

$$\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* = 0, \quad l = 1, \dots, d-1. \quad (4.7)$$

The map \mathcal{E} is unital if in addition to condition (4.6), we have it that

$$\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{-il} = 0 \quad l = 1, \dots, d-1. \quad (4.8)$$

Proof. The proof follows from the evaluation of the trace-preserving and unital conditions for the Kraus set given by (4.3). Let us consider the set $\{K_i^\dagger K_i\}_{i \in \mathbb{Z}_d}$ in the $\{|a\rangle \langle b|, a, b \in \mathbb{Z}_d\}$ basis as

$$\begin{aligned} K_i^\dagger K_i &= \left(\sum_{k,j=0}^{d-1} \alpha_{ij}^* \omega^{-kj} |k\rangle \langle k+i| \right) \left(\sum_{m,n=0}^{d-1} \alpha_{im} \omega^{mn} |n+i\rangle \langle n| \right) \\ &= \sum_{k,j,m,n=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{mn-kj} |k\rangle \langle k+i|n+i\rangle \langle n| \\ &= \sum_{k,j,m=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{k(m-j)} |k\rangle \langle k|. \end{aligned} \quad (4.9)$$

To satisfy the trace-preserving condition $\sum_{i=0}^{d-1} K_i^\dagger K_i = \mathbb{I}_d$, it necessarily follows that

$$\sum_{i,j,m=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{k(m-j)} = 1 \text{ for } k = 0, \dots, d-1. \quad (4.10)$$

By the change of index, $m - j = l$, (4.10) can be expressed as

$$\sum_{i,l=0}^{d-1} \sum_{j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{kl} = 1 \text{ for } k = 0, \dots, d-1 \quad (4.11)$$

and using the change of variable $\beta_{il} = \sum_{j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^*$, we get that

$$\sum_{i,l=0}^{d-1} \beta_{il} \omega^{kl} = 1 \text{ for } k = 0, \dots, d-1. \quad (4.12)$$

The unique solution to this system of d linearly independent equations in terms of the set of variables $\{\beta_{il}\}_{i,l \in \mathbb{Z}_d}$ corresponds to $\sum_{i=0}^{d-1} \beta_{i0} = 1$ and $\sum_{i=0}^{d-1} \beta_{il} = 0$ for $l = 1, \dots, d-1$. By expressing the solution of the system in terms of the original variables $\{\alpha_{ij}\}_{i,k \in \mathbb{Z}_d}$ we get precisely the equations (4.6) and (4.7).

Similarly, we can obtain the conditions required by a map to be unital. Let us consider the set $\{K_i K_i^\dagger\}_{i \in \mathbb{Z}_d}$ as

$$\begin{aligned} K_i K_i^\dagger &= \left(\sum_{m,n=0}^{d-1} \alpha_{im} \omega^{mn} |n+i\rangle \langle n| \right) \left(\sum_{k,j=0}^{d-1} \alpha_{ij}^* \omega^{-kj} |k\rangle \langle k+i| \right) \\ &= \sum_{k,j,m,n=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{mn-kj} |k+i\rangle \langle k|n\rangle \langle n+i| \\ &= \sum_{k,j,m,n=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{mn-kj} \delta_{k,n} |k+i\rangle \langle n+i| \\ &= \sum_{k,j,m=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{(k-i)(m-j)} |k\rangle \langle k|. \end{aligned} \quad (4.13)$$

To satisfy the unital condition $\sum_{i=0}^{d-1} K_i K_i^\dagger = \mathbb{I}_d$, it follows that

$$\sum_{i,j,m=0}^{d-1} \alpha_{im} \alpha_{ij}^* \omega^{(k-i)(m-j)} = 1 \text{ for } k = 0, \dots, d-1. \quad (4.14)$$

By the change of index, $m - j = l$, equation (4.14) can be written as

$$\sum_{i,l=0}^{d-1} \sum_{j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{(k-i)l} = 1 \text{ for } k = 0, \dots, d-1 \quad (4.15)$$

and using now the change of variable $\beta_{il} = \sum_{j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^*$ we get that

$$\sum_{i,l=0}^{d-1} \beta_{ik} \omega^{(k-i)l} = 1 \text{ for } k = 0, \dots, d-1. \quad (4.16)$$

We get again a system of d equations in terms of $\{\beta_{ik}\}_{i,k \in \mathbb{Z}_d}$. The solution of this system is given by $\sum_{i,l=0} \beta_{i0} = 1$ and $\sum_i \beta_{il} \omega^{-l} = 0$ for $l = 1, \dots, d-1$. If we express the solution of the system in terms of the elements of the set $\{\alpha_{ij}\}_{i,j \in \mathbb{Z}_d}$ we get precisely the equations (4.6) and (4.8) which completes the proof. \square

Equations (4.6), (4.7) and (4.8) represent $2(d-1)+1$ real constraints. To see this, we notice that (4.6) corresponds to one real constraint while (4.7) and (4.8) correspond to $(d-1)$ real constraints each. The following theorem establishes whether a UCPT map given by the Kraus set in (4.3) corresponds to a UCPT-extremal map.

Theorem 14. *A unital and trace-preserving map given by $\mathcal{E} : \mathcal{D}_d \mapsto \mathcal{D}_d$ with operator-sum representation $\mathcal{E}(\rho) = \sum_{i=0}^{d-1} K_i \rho K_i^\dagger$ where $K_i = \sum_{j,k=0}^{d-1} \alpha_{ij} \omega^{jk} |k+i\rangle \langle k|$ corresponds to an extreme point of the set unital and trace-preserving maps iff the matrices $(M_l | N_l)$ are full-rank for $l = 0, \dots, d-1$ where*

$$M_l = \left(\left(\sum_{j=0}^{d-1} \alpha_{i+l,j} \omega^{j(k-l)} \right) \left(\sum_{j=0}^{d-1} \alpha_{i,j}^* \omega^{-jk} \right) \right)_{i,k \in \mathbb{Z}_d} \quad (4.17)$$

and

$$N_l = \left(\left(\sum_{j=0}^{d-1} \alpha_{i+l,j} \omega^{(k-i)j} \right) \left(\sum_{j=0}^{d-1} \alpha_{i,j}^* \omega^{-(k-i)j} \right) \right)_{i,k \in \mathbb{Z}_d}. \quad (4.18)$$

Proof. By theorem 12, we have it that a map is an extreme point of $\Xi_{d,d}^{UT}$ if the set $\{K_i^\dagger K_j \oplus K_i K_j^\dagger\}_{i,j \in \mathbb{Z}_d}$ is linear independent. First, let us consider $K_i^\dagger K_{i+l}$ as

$$\begin{aligned} K_i^\dagger K_{i+l} &= \left(\sum_{k,j=0}^{d-1} \alpha_{i,j}^* \omega^{-kj} |k\rangle \langle k+i| \right) \left(\sum_{j,n=0}^{d-1} \alpha_{i+l,j} \omega^{jn} |n+i+l\rangle \langle n| \right) \\ &= \sum_{k,n=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i+l,j} \omega^{jn} \right) \left(\sum_{j=0}^{d-1} \alpha_{i,j}^* \omega^{-kj} \right) |k\rangle \langle k+i|n+i+l\rangle \langle n| \end{aligned}$$

$$\begin{aligned}
&= \sum_{k,n=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i+l_j} \omega^{j(n-l)} \right) \left(\sum_{j=0}^{d-1} \alpha_{i_j}^* \omega^{-kj} \right) |k\rangle \langle k+i|n+i\rangle \langle n-l| \\
&= \sum_k^{d-1} \left(\sum_j^{d-1} \alpha_{i+l_j} \omega^{j(k-l)} \right) \left(\sum_j^{d-1} \alpha_{i_j}^* \omega^{-jk} \right) |k\rangle \langle k-l|. \tag{4.19}
\end{aligned}$$

The matrices in (4.19) can be expressed in vector form if we use $|k\rangle \langle k-l| \sim |k, k-l\rangle$ so that

$$K_i^\dagger K_{i+l} \cong \sum_{k=0}^{d-1} \gamma_{ikl} |k, k-l\rangle. \tag{4.20}$$

We take the inner product of two arbitrary vectors as

$$\langle K_j^\dagger K_{j+n} | K_i^\dagger K_{i+l} \rangle = \sum_{km}^{d-1} \gamma_{ikl} \gamma_{jmn}^* \langle m, m-n | k, k-l \rangle. \tag{4.21}$$

We see that $\langle K_j^\dagger K_{j+n} | K_i^\dagger K_{i+l} \rangle = 0$ if $l \neq n$ for $k, l, m, n \in \mathbb{Z}_d$. The non-zero coefficients of $\{K_i^\dagger K_{i+l}\}_{i \in \mathbb{Z}_d}$ can be expressed in matrix form as M_l for $l = 0, \dots, d-1$. Second, we consider $K_{i+l} K_i^\dagger$ as

$$\begin{aligned}
K_{i+l} K_i^\dagger &= \left(\sum_{j,n=0}^{d-1} \alpha_{i+l_j} \omega^{nj} |n+i+l\rangle \langle n| \right) \left(\sum_{j,k=0}^{d-1} \alpha_{i_j}^* \omega^{-jk} |k\rangle \langle k+i| \right) \\
&= \sum_{n,k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i+l_j} \omega^{jn} \right) \left(\sum_{j=0}^{d-1} \alpha_{i_j}^* \omega^{-jk} \right) |n+i+l\rangle \langle n|k\rangle \langle k+i| \\
&= \sum_{k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i+l_j} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{i_j}^* \omega^{-jk} \right) |k+i+l\rangle \langle k+i| \\
&= \sum_{k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i+l_j} \omega^{(k-i)j} \right) \left(\sum_{j=0}^{d-1} \alpha_{i_j}^* \omega^{-(k-i)j} \right) |k+l\rangle \langle k|. \tag{4.22}
\end{aligned}$$

As we did before, we may vectorise these matrices by using $|k+l\rangle \langle k| \sim |k+l, k\rangle$ so that

$$K_{i+l} K_i^\dagger \cong \sum_{k=0}^{d-1} \gamma_{ikl} |k+l, k\rangle \tag{4.23}$$

The inner product of two arbitrary vectors is expressed as

$$\langle K_{j+n} K_j^\dagger | K_{i+l} K_i^\dagger \rangle = \sum_{km}^{d-1} \gamma_{ikl} \gamma_{jmn}^* \langle m+n, m | k+l, k \rangle \tag{4.24}$$

and we note that $\langle K_{j+n}K_j^\dagger | K_{i+l}K_i^\dagger \rangle = 0$ in the case that $n \neq l$. In this case, the non-zero coefficients of the sets $\{K_{i+l}K_i^\dagger\}_{i \in \mathbb{Z}_d}$ are given by the matrices N_l with $l = 0, \dots, d-1$. As we saw, two elements of $\{K_{i+l}K_i^\dagger \oplus K_iK_{i+l}^\dagger\}_{i, l \in \mathbb{Z}_d}$ with different l are linear independent so we just require that the all the matrices $(M_l | N_l)$ with $l = 0, \dots, d-1$ to be full-rank as stated by the theorem. \square

The following theorem characterises the set of maps given in terms of the operator-sum representation in (4.3) which are extremal with respect to the set of UCPT maps.

Theorem 15. *Consider the set of matrices given by*

$$\mathcal{A}(d) = \left\{ (\alpha_{ij})_{i, j \in \mathbb{Z}_d} \in \mathbb{C}^{d \times d} : \begin{array}{l} \sum_{i, j=0}^{d-1} \alpha_{ij} \alpha_{ij}^* = 1 \\ \sum_{i, j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* = 0 \text{ for } l = 1, \dots, d-1 \\ \sum_{i, j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{-il} = 0 \text{ for } l = 1, \dots, d-1 \end{array} \right\} \quad (4.25)$$

where $\omega = e^{\frac{2\pi}{d}i}$ and further consider the set

$$\mathcal{B}_l(d) = \{(\alpha_{ij})_{i, j \in \mathbb{Z}_d} \in \mathbb{C}^{d \times d} : \det((M_l | N_l)(M_l | N_l)^\dagger) = 0\} \text{ for } l = 0, \dots, d-1 \quad (4.26)$$

where the matrices $\{M_l\}_{l=0, \dots, d-1}$ and $\{N_l\}_{l=0, \dots, d-1}$ are given by (4.17) and (4.18), respectively.

Then we have it that the set

$$\mathcal{X}(d) = \left(\mathcal{A}(d) - \left(\mathcal{A}(d) \cap \left(\bigcup_{l \in \mathbb{Z}_d} \mathcal{B}_l(d) \right) \right) \right) / \bigotimes_{i \in \mathbb{Z}_d} U(1) \quad (4.27)$$

corresponds to the set of all quantum maps defined by the Kraus operators in (4.3) which are extreme points of the set of unital and trace-preserving maps.

Proof. This theorem follows directly from the consideration of theorems 13 and 14. Let π denote the map that sends complex matrices to quantum maps as

$$\pi(\alpha_{ij}) = \mathcal{E} \quad (4.28)$$

where the action of the quantum map \mathcal{E} on a density operator is given by

$$\mathcal{E}(\rho) = \sum_{i=0}^{d-1} \left(\sum_{j, k=0}^{d-1} \alpha_{ij} \omega^{kj} |k+i\rangle \langle k| \right) \rho \left(\sum_{j, k=0}^{d-1} \alpha_{ij}^* \omega^{-kj} |k\rangle \langle k+i| \right). \quad (4.29)$$

On the one hand, by theorem 13, we have it that if we apply the map π to $\mathcal{A}(d)$ we get as a result the set of maps which are trace-preserving and unital. On the other hand, if we apply the map π to the elements of the sets $\mathcal{B}_l(d)$ for $l = 0, \dots, d-1$ we get maps where the matrices $(M_l|N_l)$ are not full-rank. Therefore, by theorem 14, the map π applied over the set $\mathcal{A}(d) \cap (\bigcup_{l \in \mathbb{Z}_d} \mathcal{B}_l(d))$ corresponds to the maps which are not UCPT-extremal. Note that the theorem is enunciated in terms of its complementary, the maps that are extreme within the set. Finally, it remains to consider the freedom in the choice of Kraus operators to obtain an injection between the set $\mathcal{A}(d)$ and the set of unital and trace-preserving maps. In this case, the freedom in the choice of Kraus operators is given by the action of the group $\prod_{i \in \mathbb{Z}_d} U(1)$ and therefore to get a one-to-one correspondence we take the quotient space of the set $\mathcal{A}(d)$ with respect to the action of this group. \square

Corollary 1. *The set of unital and trace-preserving maps given by the Kraus operators defined by (4.3) has dimension $2d^2 - 3d + 1$.*

Proof. This lemma follows from the evaluation of the dimension of the set given by (4.27). We have it that

$$\dim(\mathcal{X}(d)) = \dim(\mathcal{A}(d)) - \dim\left(\bigotimes_{i \in \mathbb{Z}_d} U(1)\right) \quad (4.30)$$

Since $\mathcal{A}(d)$ is a $2d^2$ dimensional set with $2(d-1) + 1$ real constraints and $\bigotimes_{i \in \mathbb{Z}_d} U(1)$ is a d dimensional group. We conclude that

$$\dim(\mathcal{X}(d)) = 2d^2 - (2(d-1) + 1) - d = 2d^2 - 3d + 1 \quad (4.31)$$

\square

4.4 Qutrit case

In the previous section, we introduced a family of UCPT-extremal maps to extend the well-known set of mixed-unitary channels. The simplest set of UCPT maps for which the existence of non-unitary extremal maps is known is the set of qutrit maps. For qutrit maps, by theorem 12, the rank of UCPT-extremal maps is bounded by $\lfloor \sqrt{18} \rfloor \approx \lfloor 4.24 \rfloor$. While all rank one UCTP maps are

UCPT-extremal (unitary maps), it is the case that all rank-two maps admit a decomposition in terms of other UCTP qutrit maps [51]. Rank-three and rank-four UCTP-extremal maps are key to characterising the convex structure of the set of UCPT qutrit maps. However, the rank of the maps of the family is bounded by d and consequently, for qutrit maps, this family only includes maps with a rank of three or less. In this section, we will see some examples of UCTP-extremal qutrit maps of this family. In particular, we will present examples of unitary maps but also one example of a rank-three UCTP-extremal map.

Let $\mathcal{E} : \mathcal{D}_3 \mapsto \mathcal{D}_3$ be the map $\mathcal{E}(\rho) = \sum_{i=0}^2 K_i \rho K_i^\dagger$ where the Kraus operators are given by

$$K_0 = \begin{pmatrix} \alpha_{00} & 0 & 0 \\ 0 & \alpha_{00} & 0 \\ 0 & 0 & \alpha_{00} \end{pmatrix} + \begin{pmatrix} \alpha_{01} & 0 & 0 \\ 0 & \alpha_{01}\omega & 0 \\ 0 & 0 & \alpha_{01}\omega^2 \end{pmatrix} + \begin{pmatrix} \alpha_{02} & 0 & 0 \\ 0 & \alpha_{02}\omega^2 & 0 \\ 0 & 0 & \alpha_{02}\omega \end{pmatrix}, \quad (4.32)$$

$$K_1 = \begin{pmatrix} 0 & 0 & \alpha_{10} \\ \alpha_{10} & 0 & 0 \\ 0 & \alpha_{10} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \alpha_{11}\omega^2 \\ \alpha_{11} & 0 & 0 \\ 0 & \alpha_{11}\omega & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \alpha_{12}\omega \\ \alpha_{12} & 0 & 0 \\ 0 & \alpha_{12}\omega^2 & 0 \end{pmatrix} \quad (4.33)$$

and

$$K_2 = \begin{pmatrix} 0 & \alpha_{20} & 0 \\ 0 & 0 & \alpha_{20} \\ \alpha_{20} & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \alpha_{21}\omega & 0 \\ 0 & 0 & \alpha_{21}\omega^2 \\ \alpha_{21} & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \alpha_{22}\omega^2 & 0 \\ 0 & 0 & \alpha_{22}\omega \\ \alpha_{22} & 0 & 0 \end{pmatrix} \quad (4.34)$$

where $\omega = e^{\frac{2\pi i}{3}}$ denotes the third root of unity. Theorem 13 maintains that a map given by this Kraus set is unital and trace-preserving if it satisfies the equations

$$\sum_{i,j=0}^2 \alpha_{ij} \alpha_{ij}^* = 1, \quad (4.35)$$

$$\sum_{i,j=0}^2 \alpha_{ij+1} \alpha_{ij}^* = 0 \quad (4.36)$$

and

$$\sum_{i,j=0}^2 \alpha_{i,j+1} \alpha_{ij}^* \omega^{-i} = 0. \quad (4.37)$$

We note that, for the case of qutrit maps, equations (4.36) and (4.37) can be expressed as the simple condition

$$\omega^i \sum_{j=0}^{d-1} \alpha_{i,j+1} \alpha_{ij}^* = \beta \quad \text{for } i = 0, 1, 2 \quad (4.38)$$

where $\beta \in \mathbb{C}$. The family of maps given by the Kraus set in (4.3) includes the nine unitary Heisenberg-Weyl channels,

$$\mathcal{E}_{mn}^{HW}(\rho) = X_m Z_n \rho (X_m Z_n)^\dagger \quad \text{for } m, n \in \mathbb{Z}_3. \quad (4.39)$$

These maps can be obtained from the Kraus operators in (4.3) by fixing the coefficients

$$\alpha_{ij} = \begin{cases} 1 & \text{if } i = m, j = n \\ 0 & \text{if } i \neq m, j \neq n \end{cases} \quad (4.40)$$

for $m, n \in \mathbb{Z}_3$. The family of maps introduced includes also UCPT-extremal maps of rank three and to see that, we present an example of such map. We also show that this example corresponds to a unitary transformation of the well-known antisymmetric qutrit Werner-Holevo channel \mathcal{E}_{WH} [11].

Example 4.4.1. We define the map \mathcal{E}_a by the Kraus set in (4.3) where, in this case, the defining coefficients are given by the matrix

$$(\alpha_{ij}) = \frac{\sqrt{2}}{6} \begin{pmatrix} 2 & e^{\frac{5\pi}{3}i} & e^{\frac{\pi}{3}i} \\ 2 & e^{\pi i} & e^{\pi i} \\ 2 & e^{\frac{\pi}{3}i} & e^{\frac{5\pi}{3}i} \end{pmatrix}. \quad (4.41)$$

To see the relation between \mathcal{E}_a and \mathcal{E}_{WH} , we consider $\mathcal{E}_a(\rho) = \sum_{i=0}^2 K_i \rho K_i^\dagger$ where

$$K_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, K_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad K_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} \quad (4.42)$$

and the unitary matrix

$$U = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (4.43)$$

The conjugation of \mathcal{E}_a with U results in the map

$$\begin{aligned} U\mathcal{E}_a(\rho)U^\dagger &= \sum_{i=0}^2 UK_i\rho K_i^\dagger U^\dagger \\ &= \sum_{i=0}^2 UK_i\rho(UK_i)^\dagger \end{aligned} \quad (4.44)$$

where the Kraus operators are

$$UK_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, UK_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \text{ and } UK_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (4.45)$$

This Kraus set corresponds precisely to the anti-symmetric Werner–Holevo channel of dimension three. One peculiarity of this map is that it maximises the distance from the set of mixed-unitaries [2]. We also note that the Landau–Streater channel over dimension three can be obtained as a unitary conjugation of the Werner–Holevo channel [55] and consequently, it can also be recovered as a unitary conjugation of the map \mathcal{E}_a .

4.4.1 Rank-four UCPT-extremal qutrit maps

Theorem 12, establishes that the rank of UCPT-extremal qutrit maps is bounded by four. However, the family of maps we introduced in the previous section only includes maps of rank three or less. To provide a better characterisation of the set UCPT-extremal qutrit maps, rank-four maps need to be considered too. We construct a family of rank-four qutrit maps given also in terms of the operator-sum representation which is nothing but a modification of the structure of the Kraus set given by 4.2 to include also rank-four qutrit maps.

Let $\mathcal{F} : \mathcal{D}_3 \mapsto \mathcal{D}_3$ be the map $\mathcal{F}(\rho) = \sum_{i=0}^3 K_i \rho K_i^\dagger$ where the Kraus operators are given by

$$K_0 = \begin{pmatrix} \alpha_{00} & 0 & 0 \\ 0 & \alpha_{00} & 0 \\ 0 & 0 & \alpha_{00} \end{pmatrix} + \begin{pmatrix} \alpha_{01} & 0 & 0 \\ 0 & \alpha_{01}\omega & 0 \\ 0 & 0 & \alpha_{01}\omega^2 \end{pmatrix} + \begin{pmatrix} \alpha_{02} & 0 & 0 \\ 0 & \alpha_{02}\omega^2 & 0 \\ 0 & 0 & \alpha_{02}\omega \end{pmatrix}, \quad (4.46)$$

$$K_1 = \begin{pmatrix} 0 & 0 & 0 \\ \alpha_{10} & 0 & 0 \\ 0 & \alpha_{10} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ \alpha_{11} & 0 & 0 \\ 0 & \alpha_{11}\omega & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ \alpha_{12} & 0 & 0 \\ 0 & \alpha_{12}\omega^2 & 0 \end{pmatrix}, \quad (4.47)$$

$$K_2 = \begin{pmatrix} 0 & 0 & \alpha_{10} \\ 0 & 0 & 0 \\ \alpha_{20} & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \alpha_{11}\omega^2 \\ 0 & 0 & 0 \\ \alpha_{21} & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \alpha_{12}\omega \\ 0 & 0 & 0 \\ \alpha_{22} & 0 & 0 \end{pmatrix} \quad (4.48)$$

and

$$K_3 = \begin{pmatrix} 0 & \alpha_{20} & 0 \\ 0 & 0 & \alpha_{20} \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \alpha_{21}\omega & 0 \\ 0 & 0 & \alpha_{21}\omega^2 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \alpha_{22}\omega^2 & 0 \\ 0 & 0 & \alpha_{22}\omega \\ 0 & 0 & 0 \end{pmatrix} \quad (4.49)$$

where $\omega = e^{\frac{2\pi i}{3}}$ denotes the primitive cube root of unity.

4.4.2 Evaluating extremal conditions

Now we present the conditions which determine whether these maps correspond to extreme points of the set of UCTP maps. For the case of the family of rank-three qutrit maps, these particular conditions are established by Theorem 14. However, for the case of the family of rank-four qutrit maps the same result does not hold. To overcome this issue, we construct a set of matrices which determine whether the maps of the family correspond to extreme points of the set of UCTP maps.

Rank-three qutrit maps

Theorem 14 states that a map with the given Kraus form is an extreme point of the set of UCTP maps if the matrices $(M_l|N_l)$ are full-rank for $l = 0, \dots, d-1$. In the case of dimension $d = 3$, we write the explicit form of these matrices. Letting $\omega = e^{\frac{2\pi i}{3}}$ we have it that for $l = 0$

$$M_0 = \begin{pmatrix} \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-2j}\right) \\ \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) & \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{2j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-2j}\right) \\ \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{1j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-2j}\right) \end{pmatrix} \quad (4.50)$$

and

$$N_0 = \begin{pmatrix} \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^j\right) \\ \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{2j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) \\ \left(\sum_j^2 \alpha_{1j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) \end{pmatrix}. \quad (4.51)$$

Simiraly, for $l = 1$, we have it that

$$M_1 = \begin{pmatrix} \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{2j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{1j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{0j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) & \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) \end{pmatrix} \quad (4.52)$$

and

$$N_1 = \begin{pmatrix} \left(\sum_j^2 \alpha_{2j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{1j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^j\right) \\ \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) \end{pmatrix}. \quad (4.53)$$

Finally, for $l = 2$, we have

$$M_2 = \begin{pmatrix} \left(\sum_j^2 \alpha_{1j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\right) \\ \left(\sum_j^2 \alpha_{0j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\right) \\ \left(\sum_j^2 \alpha_{2j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\right) \end{pmatrix} \quad (4.54)$$

and

$$N_2 = \begin{pmatrix} \left(\sum_j^2 \alpha_{1j} \omega^{-j}\right) \left(\sum_j^2 \alpha_{2j}^* \omega^j\right) & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) & \left(\sum_j^2 \alpha_{1j} \omega^j\right) \left(\sum_j^2 \alpha_{2j}^* \omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{0j} \omega^j\right) \left(\sum_j^2 \alpha_{1j}^* \omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j} \omega^{-j}\right) \left(\sum_j^2 \alpha_{1j}^* \omega^j\right) \\ \left(\sum_j^2 \alpha_{2j} \omega^j\right) \left(\sum_j^2 \alpha_{0j}^* \omega^{-j}\right) & \left(\sum_j^2 \alpha_{2j} \omega^{-j}\right) \left(\sum_j^2 \alpha_{0j}^* \omega^j\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) \end{pmatrix}. \quad (4.55)$$

Theorem 14 states that a map with the given Kraus form in 4.3 is an extreme point of the set of UCTP maps if the matrices $(M_l|N_l)$ are full-rank for $l = 0, \dots, d-1$. The matrix M_1 corresponds to the conjugate of M_2 and the matrix N_1 corresponds to the conjugate of N_2 . Therefore, it suffices to establish the rank of $(M_0|N_0)$ and $(M_1|N_1)$ in order to determine whether the given map corresponds to an extreme point of the set of UCPT maps. Noting that the rank of a matrix is given by the number of non-zero singular values, we shall consider the specific case of the map \mathcal{E}_a . For this map we get that

$$(M_0|N_0) = \frac{1}{2} \left(\begin{array}{ccc|ccc} 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 \end{array} \right) \quad (4.56)$$

and

$$(M_1|N_1) = \frac{1}{2} \left(\begin{array}{ccc|ccc} 0 & -1 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 \end{array} \right). \quad (4.57)$$

The singular values of the matrix $(M_0|N_0)$ are given by $\sigma(M_0|N_0) = \{\sqrt{2}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$ and the singular values of the matrix $(M_1|N_1)$ are given by $\sigma(M_1|N_1) = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$.

Rank-four qutrit maps

For the case of rank-four qutrit maps, Theorem 14 cannot be applied. However, a similar result can be derived for this particular family of maps. We have that a map given by the Kraus operators (4.46), (4.47), (4.48) and (4.49) is an extreme point of the set of UCTP maps if the matrices $(M'_l|N'_l)$ are full-rank for $l = 0, \dots, 3$. The specific form of these matrices is given as follows. Letting $\omega = e^{\frac{2\pi i}{3}}$ we have it that for $l = 0$ we obtain

$$M'_0 = \begin{pmatrix} \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-2j}\right) \\ \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) & 0 \\ \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) & 0 & \left(\sum_j^2 \alpha_{1j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-2j}\right) \\ 0 & \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{2j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-2j}\right) \end{pmatrix} \quad (4.58)$$

and

$$N'_0 = \begin{pmatrix} \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^j\right) \\ 0 & \left(\sum_j^2 \alpha_{2j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) \\ \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & 0 & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{1j}\omega^{-j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^j\right) & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & 0 \end{pmatrix}. \quad (4.59)$$

Similarly, for the case in which $l = 1$, we have that

$$M'_1 = \begin{pmatrix} \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-2j}\right) \\ \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-j}\right) & 0 \\ 0 & \left(\sum_j^2 \alpha_{2j}\omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-2j}\right) \\ \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-2j}\right) \end{pmatrix} \quad (4.60)$$

and

$$N'_1 = \begin{pmatrix} \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{1j}\omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-j}\right) \\ 0 & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) \\ \left(\sum_j^2 \alpha_{2j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-2j}\right) & 0 \\ \left(\sum_j^2 \alpha_{0j}\omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-j}\right) & \left(\sum_j^2 \alpha_{0j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-2j}\right) \end{pmatrix}. \quad (4.61)$$

For $l = 2$, we have it that

$$M'_2 = \begin{pmatrix} \left(\sum_j^2 \alpha_{1j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\omega^{-2j}\right) \\ \left(\sum_j^2 \alpha_{2j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & 0 \\ \left(\sum_j^2 \alpha_{0j}\omega^{2j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) & \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{1j}^*\omega^{-2j}\right) \\ 0 & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{2j}^*\omega^{-2j}\right) \end{pmatrix} \quad (4.62)$$

and

$$N'_2 = \begin{pmatrix} \left(\sum_j^2 \alpha_{1j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{0j}^* \omega^{-2j}\right) & \left(\sum_j^2 \alpha_{2j}\right) \left(\sum_j^2 \alpha_{0j}^*\right) \\ \left(\sum_j^2 \alpha_{2j} \omega^j\right) \left(\sum_j^2 \alpha_{1j}^* \omega^{-j}\right) & 0 \\ \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) & \left(\sum_j^2 \alpha_{0j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{1j}^* \omega^{-2j}\right) \\ 0 & \left(\sum_j^2 \alpha_{1j}\right) \omega^j \left(\sum_j^2 \alpha_{2j}^* \omega^{-j}\right) \end{pmatrix}. \quad (4.63)$$

Finally, for $l = 3$, we have it that

$$M'_3 = \begin{pmatrix} \left(\sum_j^2 \alpha_{0j} \omega^j\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{0j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{1j}^* \omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{1j} \omega^j\right) \left(\sum_j^2 \alpha_{2j}^*\right) & 0 \\ 0 & \left(\sum_j^2 \alpha_{1j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{2j}^* \omega^{-j}\right) \\ \left(\sum_j^2 \alpha_{2j} \omega^j\right) \left(\sum_j^2 \alpha_{0j}^*\right) & \left(\sum_j^2 \alpha_{2j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{0j}^* \omega^{-2j}\right) \end{pmatrix} \quad (4.64)$$

and

$$N'_3 = \begin{pmatrix} \left(\sum_j^2 \alpha_{0j}\right) \left(\sum_j^2 \alpha_{1j}^*\right) & \left(\sum_j^2 \alpha_{0j} \omega^j\right) \left(\sum_j^2 \alpha_{1j}^* \omega^{-j}\right) \\ 0 & \left(\sum_j^2 \alpha_{1j}\right) \left(\sum_j^2 \alpha_{2j}^*\right) \\ \left(\sum_j^2 \alpha_{1j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{2j}^* \omega^{-2j}\right) & 0 \\ \left(\sum_j^2 \alpha_{2j} \omega^j\right) \left(\sum_j^2 \alpha_{0j}^* \omega^{-j}\right) & \left(\sum_j^2 \alpha_{2j} \omega^{2j}\right) \left(\sum_j^2 \alpha_{0j}^* \omega^{-2j}\right) \end{pmatrix}. \quad (4.65)$$

The specific form of the matrices $\{(M'_l|N'_l)\}_{l \in \mathbb{Z}_4}$ can be obtained just as we did for rank-three maps.

4.5 Conclusion

In this chapter, we introduced a family of UCPT-extreme defined in terms of its operator-sum representation. To do so, we constructed a family of CP maps for which the set Kraus operators have a special form with respect to the Heisenberg-Weyl basis of matrices. We derived firstly the equations needed to establish that the maps of the family are unital and trace-preserving. Secondly, we established the conditions which determine whether a given map corresponds to an extreme point of the set of unital and trace-preserving maps. As an application, we considered the case of maps of dimension three. For the qutrit case, we showed that the family of maps introduced contains examples of rank one and rank-three maps. In this setting, we also presented a different family of UCPT-extreme maps which includes also maps with rank four.

Chapter 5

On the entanglement classification of locally maximally mixed states

5.1 Introduction

The Choi–Jamiolkowski (CJ) isomorphism establishes a correspondence between quantum maps and bipartite states [14]. By the CJ isomorphism, unital quantum channels correspond to bipartite states with maximally-mixed partially traced states. In Chapter 4, we constructed a family of d -dimensional UCPT-extremal maps of rank $r \leq d$ to study the convex structure of the set of UCPT maps.

In this chapter, we consider the family of bipartite states which are CJ-isomorphic to the family of UCPT-extremal maps introduced in Chapter 4. For pure states, maximally entangled states correspond to those states for which the marginals are maximally mixed. However, universally maximally entangled mixed bipartite states cannot be defined for qutrit systems as different states may maximize different entanglement measures. The family of bipartite states we consider includes not only the set of maximally entangled pure states, but also mixed states with maximally mixed marginals. For this reason, our family of bipartite states is a good candidate to investigate entan-

lement classification in systems of dimension higher than two. In this chapter, we consider the local unitary classification for our family of states.

5.2 A family of locally maximally mixed bipartite states

In this section, we consider the bipartite states $\rho_{AB} \in \mathcal{M}_d$ associated to the family of completely positive maps for which the Kraus operators are given by equation 4.3. Through the Choi-Jamilkowski isomorphism we can find the corresponding set of bipartite states which are given by

$$\rho_{AB} = \frac{1}{d}(\Phi \otimes \mathbb{I}_d) |\psi\rangle \langle\psi| \quad (5.1)$$

where $|\psi\rangle$ represents a maximally entangled pure state i.e. $|\psi\rangle = \sum_{m=0}^{d-1} |m\rangle |m\rangle$ and

$$\phi(\rho) = \sum_{i=0}^{d-1} K_i \rho K_i^\dagger \quad (5.2)$$

represents the quantum operation in which the Kraus operators are given by

$$K_i = \sum_{j,k=0}^{d-1} \alpha_{ij} \omega^{jk} |k+i\rangle \langle k| \quad (5.3)$$

and ω is the d th root of unity. We have it that $K_i \otimes \mathbb{I}_d = \sum_{j,k,l=0}^{d-1} \alpha_{ij} \omega^{jk} |k+i\rangle |l\rangle \langle k| \langle l|$ so the density operator of the bipartite state can be expressed as

$$\begin{aligned} \rho_{AB} &= \frac{1}{d} \sum_{i=0}^{d-1} (K_i \otimes \mathbb{I}_d) |\psi\rangle \langle\psi| (K_i^\dagger \otimes \mathbb{I}_d) \\ &= \frac{1}{d} \sum_{i=0}^{d-1} \left(\sum_{k,j=0}^{d-1} \alpha_{ij} \omega^{jk} |k+i\rangle |k\rangle \right) \left(\sum_{k,j=0}^{d-1} \alpha_{ij}^* \omega^{-jk} \langle k+i| \langle k| \right) \\ &= \frac{1}{d} \sum_{i,k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jl} \right) |k+i\rangle |k\rangle \langle l+i| \langle l|. \end{aligned} \quad (5.4)$$

Sometimes it will be useful to express ρ_{AB} in terms of $c_{i,k} = \frac{1}{\sqrt{d}} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right)$ so that

$$\rho_{AB} = \sum_{i,k,l=0}^{d-1} c_{i,k} c_{i,l}^* |k+i\rangle |k\rangle \langle l+i| \langle l|. \quad (5.5)$$

We are interested in the set of locally maximally mixed states, those in which $\text{tr}_A(\rho_{AB}) = \frac{\mathbb{1}_d}{d}$ and $\text{tr}_B(\rho_{AB}) = \frac{\mathbb{1}_d}{d}$. We can express the LMM conditions in terms of the defining parameters $\{\alpha_{ij}\}_{i,j \in \mathbb{Z}_d}$ obtaining exactly the same set of equations. For our family of LMM states, we have that $\text{tr}_A(\rho_{AB}) = \frac{\mathbb{1}_d}{d}$ if

$$\sum_{i,j=0}^{d^2-1} \alpha_{ij} \alpha_{ij}^* = 1 \quad (5.6)$$

and

$$\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* = 0 \quad \text{for } l \neq 0. \quad (5.7)$$

On the other hand, we have that $\text{tr}_B(\rho_{AB}) = \frac{\mathbb{1}_d}{d}$ if condition (6.1) is satisfied and

$$\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{-il} = 0 \quad \text{for } l \neq 0. \quad (5.8)$$

To verify the correctness of the equations, we may evaluate the partial traces of the bipartite state ρ_{AB} as

$$\begin{aligned} \text{tr}_A(\rho_{AB}) &= \frac{1}{d} \text{tr}_A \left(\sum_{i,k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jl} \right) |k+i\rangle |k\rangle \langle l+i| \langle l| \right) \\ &= \frac{1}{d} \sum_{i,k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jk} \right) |k\rangle \langle k| \\ &= \frac{1}{d} \sum_{k,l=0}^{d-1} \left(\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{lk} \right) |k\rangle \langle k| \end{aligned} \quad (5.9)$$

By equation (6.2), we get that all the elements of the last sum in (5.9) with $l \neq 0$ cancel out and consequently we obtain that

$$\text{tr}_A(\rho_{AB}) = \frac{1}{d} \sum_{i,k=0}^{d-1} \left(\sum_j \alpha_{ij} \alpha_{ij}^* \right) |k\rangle \langle k| \quad (5.10)$$

and, by equation (6.1), we obtain that

$$\text{tr}_A(C_\phi) = \frac{1}{d} \sum_{k=0}^{d-1} |k\rangle \langle k|. \quad (5.11)$$

We may also evaluate the second partial trace which is given by

$$\begin{aligned}
\mathrm{tr}_B(\rho_{AB}) &= \frac{1}{d} \mathrm{tr}_B \left(\sum_{i,k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jl} \right) |k+i\rangle |k\rangle \langle l+i| \langle l| \right) \\
&= \frac{1}{d} \sum_{i,k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jk} \right) |k+i\rangle \langle k+i| \\
&= \frac{1}{d} \sum_{i,k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{j(k-i)} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-j(k-i)} \right) |k\rangle \langle k| \\
&= \frac{1}{d} \sum_{k,l=0}^{d-1} \left(\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{l(k-i)} \right) |k\rangle \langle k| \\
&= \frac{1}{d} \sum_{k,l=0}^{d-1} \left(\sum_{i,j=0}^{d-1} \alpha_{ij+l} \alpha_{ij}^* \omega^{-il} \right) \omega^{kl} |k\rangle \langle k|. \tag{5.12}
\end{aligned}$$

By equation (5.8), we get that all the elements of the sum in (5.12) with $l \neq 0$ cancel out and consequently we obtain that

$$\mathrm{tr}_B(\rho_{AB}) = \frac{1}{d} \sum_{i,k=0}^{d-1} \left(\sum_j \alpha_{ij} \alpha_{ij}^* \right) |k\rangle \langle k| \tag{5.13}$$

and, by equation (6.1),

$$\mathrm{tr}_B(\rho_{AB}) = \frac{1}{d} \sum_{k=0}^{d-1} |k\rangle \langle k|. \tag{5.14}$$

5.3 Local unitary invariants

In this section, we search for magnitudes invariant under local unitary transformations on ρ_{AB} . In principle, if we could find local unitary invariants for each one of the degrees of freedom of the family of states, we could obtain a complete characterisation of the family in terms of entanglement. We start by defining LU invariance. We have that $\kappa \in \mathbb{R}$ is an local unitary (LU) invariant of $\rho_{AB} \in \mathcal{M}_d$ if

$$\kappa(\rho_{AB}) = \kappa(\rho'_{AB}) \tag{5.15}$$

where

$$\rho'_{AB} = (U \otimes V) \rho_{AB} (U \otimes V)^\dagger \tag{5.16}$$

and $U, V \in SU(d)$. From this definition of LU invariant, we can see that the eigenvalues of ρ_{AB} are LU invariants of the state. This follows from the fact that a unitary transformation on the density matrix as the one given in (5.16) does not change the spectrum. To obtain the spectrum of ρ_{AB} , we find a unitary operator that leaves the density matrix into a block diagonal form. Such unitary operation leaves the spectrum unchanged and the eigenvalues of ρ_{AB} correspond exactly to the eigenvalues of the blocks of the transformed matrix. In particular, we have that the unitary operator

$$U = \sum_{q,j=0}^{d-1} |j-q\rangle\langle q| \langle j| \langle q| \quad (5.17)$$

is the one block diagonalizing ρ_{AB} . To see that we apply the unitary transformation τ_U on the density matrix so that the transformed matrix can be expressed as

$$\begin{aligned} \tau_U(\rho_{AB}) &= U\rho_{AB}U^{-1} \\ &= \frac{1}{d} \sum_{i=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} |i\rangle\langle k| \right) \left(\sum_{j,k=0}^{d-1} \alpha_{ij}^* \omega^{-jk} \langle i| \langle k| \right) \end{aligned} \quad (5.18)$$

The matrix $\tau_U(\rho_{AB})$ is block diagonal

$$\tau_U(\rho_{AB}) = \begin{pmatrix} P_0 & & \\ & \ddots & \\ & & P_{d-1} \end{pmatrix} \quad (5.19)$$

and the blocks P_0, \dots, P_{d-1} are given by

$$P_i = \frac{1}{d} \left(\sum_{k=0}^{d-1} \sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} |k\rangle \right) \left(\sum_{k=0}^{d-1} \sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jk} \langle k| \right). \quad (5.20)$$

We observe that the matrices P_0, \dots, P_{d-1} are can be expressed as a projector $P_i = |p_i\rangle\langle p_i|$ where

$$|p_i\rangle = \frac{1}{\sqrt{(d)}} \sum_{k=0}^{d-1} \sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} |k\rangle \quad (5.21)$$

and consequently P_0, \dots, P_{d-1} are rank one and each eigenvalue is given by

$$\begin{aligned}
\langle p_i | p_i \rangle &= \frac{1}{d} \sum_{k=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jk} \right) \\
&= \frac{1}{d} \sum_{k,j,l=0}^{d-1} \alpha_{i,j+l} \alpha_{ij}^* \omega^{lk} \\
&= \frac{1}{d} \sum_{k,j=0}^{d-1} \left(\alpha_{ij} \alpha_{ij}^* + \sum_{l=1}^{d-1} \alpha_{i,j+l} \alpha_{ij}^* \omega^{lk} \right) \\
&= \sum_{j=0}^{d-1} |\alpha_{ij}|^2.
\end{aligned} \tag{5.22}$$

We obtain a first set of LU invariants $\kappa_i^{(1)}, \dots, \kappa_{d-1}^{(1)}$ for our family of maps based on the spectrum of ρ_{AB} . These LU invariants are given by

$$\kappa_i^{(1)} = \sum_{j=0}^{d-1} |\alpha_{ij}|^2. \tag{5.23}$$

A different set of LU invariants is given the spectrum of the partially transposed matrix ρ_{AB}^T . Zhang *et al.* established that two states are local unitary equivalent iff their respective partially transposed matrices are local unitary equivalent too (Theorem 2 in [56]). Therefore, we have that the eigenvalues of the partially transposed matrix are also invariant under LU transformations.

To obtain this second set of LU invariants we proceed in the same way we did to obtain the eigenvalues of the density matrix: We define a unitary transformation that block diagonalises ρ_{AB}^T . To obtain $\rho_{AB}^{T_B}$ we apply the partial transposition over system B as

$$\rho_{AB}^{T_B} = \frac{1}{d} \sum_{i,k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jl} \right) |k+i\rangle |l\rangle \langle l+i| \langle k|. \tag{5.24}$$

Now we apply a unitary transformation τ_U on the partially transposed matrix where in this case the unitary is given by the unitary operator

$$U = \sum_{q,j=0}^{d-1} |j+q\rangle |q\rangle \langle j| \langle q|. \tag{5.25}$$

We get that the transformed matrix can be expressed as

$$\begin{aligned}\tau_U(\rho_{AB}^{T_B}) &= U\rho_{AB}^{T_B}U^{-1} \\ &= \frac{1}{d} \sum_{i,k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{ij}^* \omega^{-jl} \right) |k+l+i\rangle |l\rangle \langle l+k+i| \langle k|. \end{aligned} \quad (5.26)$$

To obtain the blocks we make use of the change of variable $i \rightarrow i - l - k$

$$\tau_U(\rho_{AB}^{T_B}) = \frac{1}{d} \sum_{i,k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i-l-k;j} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{i-l-k;j}^* \omega^{-jl} \right) |i\rangle |l\rangle \langle i| \langle k|. \quad (5.27)$$

This state can be written as

$$\tau_U(\rho_{AB}^{T_B}) = \begin{pmatrix} Q_0 & & \\ & \ddots & \\ & & Q_{d-1} \end{pmatrix} \quad (5.28)$$

where the blocks Q_0, \dots, Q_{d-1} are given by

$$Q_i = \frac{1}{d} \sum_{k,l=0}^{d-1} \left(\sum_{j=0}^{d-1} \alpha_{i-l-k;j} \omega^{jk} \right) \left(\sum_{j=0}^{d-1} \alpha_{i-l-k;j}^* \omega^{-jl} \right) |l\rangle \langle k|. \quad (5.29)$$

The eigenvalues of $Q_i \dots$ matrices are also eigenvalues of the partially transposed matrix $\rho_{AB}^{T_B}$ which are LU invariants. The second set of LU invariants $\kappa_0^{(2)}, \dots, \kappa_{d^2-1}^{(2)}$ is given by

$$\kappa_i^{(2)} = e_i \in \{E(Q_0) \cup \dots \cup E(Q_{d-1})\}. \quad (5.30)$$

where $E(Q_i)$ corresponds to the set of eigenvalues of Q_i .

We can obtain a third set of LU invariants for the states of our family based on their correlation matrix. In Chapter 2, we considered the singular values of the correlation matrix for bipartite state entanglement classification. By theorem 9, we have that the correlation matrix of a given state can be diagonalised by means of LU operations acting on the state. The elements of the diagonalized correlation matrix correspond to the singular values of the original matrix up to a sign. Consequently, the set of singular values of the correlation matrix are invariants under local unitary operations. The correlation matrix ρ_{AB} is given by

$$R = \{r_{ij}\}_{i,j \in \mathbb{Z}_{d^2-1}} \quad (5.31)$$

where

$$r_{ij} = \langle \rho_{AB}, \lambda^i \otimes \lambda^j \rangle := \text{tr}(\rho_{AB} \lambda_i \otimes \lambda_j) \quad (5.32)$$

and $\lambda_1, \dots, \lambda_{d^2-1}$ form a basis for the set of traceless matrices. To evaluate the correlation matrix, we select the particular basis $\lambda_1, \dots, \lambda_{d^2-1}$ defined as follows. We define the elements of this basis in terms of d collections of matrices which we denote by $\{\Lambda^{(k)}\}_{k=0, \dots, d-1}$. We have that $\Lambda^{(0)}$ contains $d-1$ elements while the rest of collections, $\Lambda^{(k)}$ for $k = 1, \dots, d-1$, contain d elements each. The matrices $\{\lambda_i^{(0)} \in \Lambda^{(0)}\}_{i=1, \dots, d-1}$ are given by

$$\lambda_i^{(0)} = \sum_{m=0}^{d-1} |m\rangle \langle m| \omega^{im} \quad \text{where } i = 1, \dots, d-1 \quad (5.33)$$

and ω is a d th root of unity. The rest of matrices $\{\lambda_i^{(k)} \in \Lambda^{(k)}\}_{i=0, \dots, d-1}$ for $k = 1, \dots, d-1$ are given by

$$\lambda_i^{(k)} = |i+k\rangle \langle i| \quad \text{where } i = 0, \dots, d-1. \quad (5.34)$$

Now we will relabel the elements of the correlation with taking into account the collection of the element of the basis. We have in this case that

$$R = \{r_{i,j}^{(k,l)}\} \quad \text{where } k, l \in \mathbb{Z}_d \quad \text{and} \quad \begin{cases} i \in \mathbb{Z}_{d-1} & \text{if } k = 0 \\ j \in \mathbb{Z}_{d-1} & \text{if } l = 0 \\ i, j \in \mathbb{Z}_d & \text{otherwise} \end{cases} \quad (5.35)$$

where the indexing in expression above has the exceptions that $i \in \mathbb{Z}_{d-1}$ if $k = 0$ and $j \in \mathbb{Z}_{d-1}$ if $l = 0$. To obtain all the elements of the correlation matrix, we evaluate first the projections of ρ_{AB} as given in (5.5) over the elements of the computational basis. We get that

$$\begin{aligned} \langle \rho_{AB}, |a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2| \rangle &= \text{tr} \left(\sum_{i,k,l=0}^{d-1} c_{i,k,l} |k+i\rangle \langle k| \langle l+i| \langle l| \cdot |a_1\rangle \langle b_1| \langle a_2| \langle b_2| \right) \\ &= \sum_{i,k,l=0}^{d-1} c_{i,k} c_{i,l}^* \langle a_2|k+i\rangle \langle b_2|k\rangle \langle l+i|a_1\rangle \langle l|b_1\rangle \\ &= \sum_{i=0}^{d-1} c_{i,b_2} c_{i,b_1}^* \langle a_2|b_2+i\rangle \langle b_1+i|a_1\rangle \end{aligned} \quad (5.36)$$

where $a_1, a_2, b_1, b_2 \in \mathbb{Z}_d$. We can see that only those terms in which $a_2 - b_2 = b_1 - a_1$ are different from zero so the projections can be expressed as

$$\langle \rho_{AB}, |a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2| \rangle = c_{a_1-b_1, b_2} c_{a_1-b_1, b_1}^* \langle a_2 + b_1 | b_2 + a_1 \rangle. \quad (5.37)$$

Consider the elements of the correlation matrix $r_{i,j}^{(k,l)}$ such that $k \neq l$. In that case, one can check that all the projections of the state in the computational basis are zero. We conclude that for this choice of basis the correlation matrix is block diagonal

$$R = \begin{pmatrix} R_0 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & R_{d-1} \end{pmatrix} \quad (5.38)$$

where each block R_0, \dots, R_{d-1} corresponds to each one of the collections $\Lambda^{(k)}$ of elements of the basis for $k = 0, \dots, d-1$. We shall evaluate their elements by using (5.37). In the case $k = l = 0$, we have that

$$R_0 = (r_{i,j}^{(0,0)})_{i,j=1,\dots,d-1} \quad (5.39)$$

where

$$\begin{aligned} r_{i,j}^{(0,0)} &= \langle \rho_{AB}, \lambda_i^{(0)} \otimes \lambda_j^{(0)} \rangle \\ &= \langle \rho_{AB}, \sum_{m=0}^{d-1} \omega^{mi} |m\rangle \langle m| \otimes \sum_{p=0}^{d-1} \omega^{pj} |p\rangle \langle p| \rangle \\ &= \sum_{m,p=0}^{d-1} \omega^{mi+pj} \langle \rho_{AB}, |m\rangle \langle m| \otimes |p\rangle \langle p| \rangle \\ &= \sum_{m,p=0}^{d-1} \omega^{mi+pj} c_{m-p,p} c_{m-p,p}^* \\ &= \frac{1}{d} \sum_{m,p=0}^{d-1} \omega^{mi+pj} \left(\sum_{s=0}^{d-1} \alpha_{m-p,s} \omega^{sp} \right) \left(\sum_{s=0}^{d-1} \alpha_{m-p,s}^* \omega^{-sp} \right). \end{aligned} \quad (5.40)$$

We can evaluate the rest of the blocks which are given by the elements of R for which $l = k \neq 0$. In this case, the blocks can be expressed as

$$R_k = (r_{i,j}^{(k,k)})_{i,j=0,\dots,d-1} \quad (5.41)$$

LU invariant	Set	Cardinality
$\kappa_i^{(1)}$	$\{\sum_{j=0}^{d-1} \alpha_{ij} ^2\}$	$i \in \mathbb{Z}_d$
$\kappa_i^{(2)}$	$\{E(Q_0) \cup \dots \cup E(Q_{d-1})\}$	$i \in \mathbb{Z}_{d^2}$
$\kappa_i^{(3)}$	$\{SV(R_0) \cup \dots \cup SV(R_{d-1})\}$	$i \in \mathbb{Z}_{d^2-1}$

Table 5.1: In this table we summarize all the different sets of LU invariants obtained for the bipartite state ρ_{AB} .

where

$$\begin{aligned}
r_{i,j}^{(k,k)} &= \langle \rho_{AB}, \lambda_i^{(k)} \otimes \lambda_j^{(k)} \rangle \\
&= \langle \rho_{AB}, |i+k\rangle \langle i| \otimes |j+k\rangle \langle j| \rangle \\
&= c_{i-j,j} c_{i-j,j+k}^* \\
&= \frac{1}{d} \left(\sum_{s=0}^{d-1} \alpha_{i-j,s} \omega^{sj} \right) \left(\sum_{s=0}^{d-1} \alpha_{i-j,s}^* \omega^{-s(j+k)} \right). \tag{5.42}
\end{aligned}$$

The singular values of R_0, \dots, R_{d-1} are also eigenvalues of the correlation ρ_{AB}^{TB} which, as we saw, are LU invariants of the state. The third set of LU invariants $\kappa_1^{(3)}, \dots, \kappa_{d^2-1}^{(3)}$ is given by

$$\kappa_i^{(3)} = s_i \in \{SV(R_0) \cup \dots \cup SV(R_{d-1})\}. \tag{5.43}$$

5.4 Bipartite qutrit state LU classification

In the previous section we obtained sets LU invariants for the family of LMM states given by (5.4).

In this section we will consider the particular case of qutrit states. We fix $d = 3$ in (5.4), in this case, the density state is given by

$$\rho_{AB} = \frac{1}{3} \sum_{i,k,l=0}^2 \left(\sum_{j=0}^2 \alpha_{ij} \omega^{jk} \right) \left(\sum_{j=0}^{3-1} \alpha_{ij}^* \omega^{-jl} \right) |k+i\rangle |k\rangle \langle l+i| \langle l|. \tag{5.44}$$

where $\omega = e^{\frac{2\pi i}{3}}$. For $d = 3$, we saw that ρ_{AB} is locally maximally mixed provided that

$$\sum_{i,j=0}^2 \alpha_{ij} \alpha_{ij}^* = 1 \tag{5.45}$$

and

$$\sum_{j=0}^2 \omega^i \alpha_{ij+1} \alpha_{ij}^* = \beta \quad \text{for } i = 0, 1, 2 \quad (5.46)$$

where $\beta \in \mathbb{C}$ is a complex constant. The family of LMM states given by ρ_{AB} has $2d^2 - 3d + 1$ dimensions. For qutrit systems, this family of bipartite states is 10 dimensional and entanglement classification can be achieved finding as many independent local unitary invariants. For $d = 3$, the invariants $\kappa_1^{(1)}, \kappa_2^{(1)}$ and $\kappa_3^{(1)}$ are given by

$$\begin{aligned} \kappa_1^{(1)} &= \sum_{j=0}^2 \alpha_{0j} \alpha_{0j}^*, \\ \kappa_2^{(1)} &= \sum_{j=0}^2 \alpha_{1j} \alpha_{1j}^*, \\ \kappa_3^{(1)} &= \sum_{j=0}^2 \alpha_{2j} \alpha_{2j}^*. \end{aligned} \quad (5.47)$$

We can also obtain $\kappa_1^{(2)}, \dots, \kappa_9^{(2)}$ which are given by the eigenvalues of the matrices

$$\begin{aligned} Q_0 &= \begin{pmatrix} c_{0,0} c_{0,0}^* & c_{2,0} c_{2,1}^* & c_{1,0} c_{1,2}^* \\ c_{2,1} c_{2,0}^* & c_{1,1} c_{1,1}^* & c_{0,1} c_{0,2}^* \\ c_{1,2} c_{1,0}^* & c_{0,2} c_{0,1}^* & c_{2,2} c_{2,2}^* \end{pmatrix}, \\ Q_1 &= \begin{pmatrix} c_{1,0} c_{1,2}^* & c_{0,1} c_{0,0}^* & c_{2,2} c_{2,1}^* \\ c_{0,0} c_{0,2}^* & c_{2,1} c_{2,0}^* & c_{1,2} c_{1,1}^* \\ c_{2,0} c_{2,2}^* & c_{1,1} c_{1,0}^* & c_{0,2} c_{0,1}^* \end{pmatrix}, \\ Q_2 &= \begin{pmatrix} c_{2,0} c_{2,2}^* & c_{1,1} c_{1,0}^* & c_{0,2} c_{0,1}^* \\ c_{1,0} c_{1,2}^* & c_{0,1} c_{0,0}^* & c_{2,2} c_{2,1}^* \\ c_{0,0} c_{0,2}^* & c_{2,1} c_{2,0}^* & c_{1,2} c_{1,1}^* \end{pmatrix}. \end{aligned} \quad (5.48)$$

where $c_{i,k} = \frac{1}{d} \left(\sum_{j=0}^{d-1} \alpha_{ij} \omega^{jk} \right)$. Finally, for qutrits, the LU invariants $\kappa_1^{(3)}, \dots, \kappa_8^{(3)}$ are given by the singular values of the matrices

$$R_0 = \sum_{m,p=0}^2 c_{m-p,p} c_{m-p,p}^* \begin{pmatrix} \omega^{m+p} & \omega^{2m+p} \\ \omega^{m+2p} & \omega^{2m+2p} \end{pmatrix},$$

$$\begin{aligned}
R_1 &= \begin{pmatrix} c_{0,0}c_{0,1}^* & c_{2,1}c_{2,2}^* & c_{1,2}c_{1,0}^* \\ c_{1,0}c_{1,1}^* & c_{0,1}c_{0,2}^* & c_{2,2}c_{2,0}^* \\ c_{2,0}c_{2,1}^* & c_{1,1}c_{1,2}^* & c_{0,2}c_{0,0}^* \end{pmatrix}, \\
R_2 &= \begin{pmatrix} c_{0,0}c_{0,2}^* & c_{2,1}c_{2,0}^* & c_{1,2}c_{1,1}^* \\ c_{1,0}c_{1,2}^* & c_{0,1}c_{0,0}^* & c_{2,2}c_{2,1}^* \\ c_{2,0}c_{2,2}^* & c_{1,1}c_{1,0}^* & c_{0,2}c_{0,1}^* \end{pmatrix}.
\end{aligned} \tag{5.49}$$

At this point, the evaluation of these invariants for qutrit systems depends on the specific choice of coefficients $\{\alpha_{ij}\}_{i,j \in \mathbb{Z}}$. For the moment, we can make some observations about the relation of the LU invariants in the qutrit case.

For the invariants $\kappa_1^{(1)}, \kappa_2^{(1)}, \kappa_3^{(1)}$, we have that only two of them are linearly independent. To see this, we may evaluate their sum as

$$\sum_{i=0}^2 \kappa_i^{(1)} = \sum_{ij=0}^2 \alpha_{ij} \alpha_{ij}^*. \tag{5.50}$$

If we use the condition satisfied by LMM states which is given by (5.45), we obtain that $\sum_{i=0}^2 \kappa_i^{(1)} = 1$. So one of the invariants can always be obtained from the other two. For the rest of the invariants, we also found that not all of them are linearly independent. In particular, the numerical analysis of the invariants suggests that for the $\kappa_1^{(2)}, \dots, \kappa_9^{(2)}$ at least three of them are linearly independent while for the invariants $\kappa_1^{(3)}, \dots, \kappa_8^{(3)}$, we also have that at least three of them are linearly independent. In total, we have that from all the LU invariants evaluated at least 8 of them are linearly independent.

5.5 Conclusion

In this chapter, we considered the set of bipartite states which are dual to the family of UCPT maps introduced in Chapter 4 in terms of the Choi-Jamilkowski isomorphism. For this family of bipartite states, we considered the problem of entanglement classification. To do this we used three known sets of invariants under local unitary operations corresponding to the spectra of three different matrices: the density matrix, the partially transposed matrix and the square of the correlation matrix. For the family of states considered, we found that the evaluation of these invariants is

greatly simplified. This follows from the fact the operators introduced can be expressed in block diagonal form by means of unitary transformations. We considered the particular case of bipartite states based on qutrit systems. In this setup, numerical evidence indicates that the set of invariants we derived provide full entanglement classification for the family of two qutrit states we studied. However, we acknowledge that a more robust analysis of the same problem should be carried out by considering analytical methods.

Chapter 6

Solving UCPT/LMM equations in qutrit systems

6.1 Introduction

In Chapter 4, we introduced a family of UCPT maps which served as an extension of the set of unitary maps in the context of convex set characterisation. In Chapter 5, we saw that this family had a dual in the set of LMM bipartite states which was interesting for state classification. To construct those maps/bipartite states, first, we considered matrices with a fixed structure whose elements were expressed in terms of a set of parameters. We found the equations in terms of these parameters representing UCPT maps and LMM bipartite states, respectively. In both cases, we considered the scenario of states based on qutrit systems. In this setup, we saw that the UCPT/LMM equations were simpler compared with the case of systems of higher dimensions. In this chapter, we will consider precisely the solutions to these equations. First, we will construct an algorithm solving the UCPT/LMM equations. Second, we will consider a particular simplification of these equations for which the solutions can be obtained analytically. Finally, for these solutions, we will evaluate explicitly the set of local unitary invariants we obtained in Chapter 5.

6.2 Expressing UCPT/LMM equations in terms of real parameters

Previously we considered the family of CP maps given by the Kraus set in (4.3) and also its dual in the set of bipartite states given by (5.4). In both cases, the elements of the families are given in terms of the same set of parameters $\{\alpha_{ij}\}_{ij \in \mathbb{Z}_d}$. In Chapter 4, we saw that for $d = 3$ a map given by (4.3) was unital and trace-preserving provided that

$$\sum_{i,j=0}^2 \alpha_{ij} \alpha_{ij}^* = 1 \quad (6.1)$$

and

$$\sum_{j=0}^2 \alpha_{ij+1} \alpha_{ij}^* \omega^i = \beta \quad \text{for } i = 0, 1, 2. \quad (6.2)$$

where $\beta \in \mathbb{C}$. Equivalently, in Chapter 5, we saw that a bipartite state given by (2.33) is locally maximally mixed if the same equations apply. The parameters α_{ij} can be arranged as the complex matrix $A = (\alpha_{ij})_{ij \in \mathbb{Z}_2}$ to represent the maps (or bipartite states) of the family. We saw that there is a freedom in the definition of maps in terms of A . To see this, consider a map represented in terms of A . The multiplication of any row of A by a constant complex phase factor preserves the map being represented. We can get rid of this arbitrariness in the choice of A by fixing the complex phases of the first column of the matrix to zero. For $d = 3$, by using complex exponents we have that A can be expressed in terms of 15 real parameters as

$$A = \begin{pmatrix} a_0 & b_0 e^{i\theta_0} & c_0 e^{i(\theta_0 + \phi_0)} \\ a_1 & b_1 e^{i\theta_1} & c_1 e^{i(\theta_1 + \phi_1)} \\ a_2 & b_2 e^{i\theta_2} & c_2 e^{i(\theta_2 + \phi_2)} \end{pmatrix} \quad (6.3)$$

where in this case $a_i, b_i, c_i, \theta_i, \phi_i \in \mathbb{R}$ for $i = 0, 1, 2$. We can rewrite the equations required by UCPT maps using these real parameters. We get that (6.1) is expressed as

$$a_0^2 + b_0^2 + c_0^2 + a_1^2 + b_1^2 + c_1^2 + a_2^2 + b_2^2 + c_2^2 = 1. \quad (6.4)$$

and (6.2) is given by

$$\begin{aligned}
 a_0 b_0 e^{i\theta_0} + b_0 c_0 e^{i\phi_0} + a_0 c_0 e^{-i(\theta_0 + \phi_0)} &= |\beta| e^{\arg(\beta)i} \\
 a_1 b_1 e^{i\theta_1} + b_1 c_1 e^{i\phi_1} + a_1 c_1 e^{-i(\theta_1 + \phi_1)} &= |\beta| e^{(\arg(\beta) + \frac{4\pi}{3})i} \\
 a_2 b_1 e^{i\theta_2} + b_2 c_2 e^{i\phi_2} + a_2 c_2 e^{-i(\theta_2 + \phi_2)} &= |\beta| e^{(\arg(\beta) + \frac{2\pi}{3})i}.
 \end{aligned} \tag{6.5}$$

We will consider two different approaches to solve this set of equations: First, we will introduce a numerical method to obtain the solutions to the equations. Second, we will show how analytical solutions can be obtained by considering an extra constraint on the set of parameters.

6.3 Numerical solutions

In this section we introduce an algorithm solving equations (6.4) and (6.5). This algorithm can be divided in two parts. The first part consists on selecting the modulus of the elements of A (a_i , b_i and c_i) such that equation (6.4) is satisfied. The second part of the algorithm consists on finding the phases of A (ϕ_i and θ_i) such that the set of equations (6.5) is satisfied too. This second part of the algorithm, in general, needs to be solved numerically. However, depending on the particular choice of parameters in the first part, solutions may exist or not. To understand why this is the case, we will consider a graphical representation of the equations. Consider the general form of the left hand side of (6.5) which can be expressed as the complex function

$$f(\phi, \theta) = abe^{i\theta} + bce^{i\phi} + ace^{-i(\theta + \phi)} \tag{6.6}$$

where a, b and c are fixed. We can always represent $f(\theta, \phi)$ in the complex plane with $\theta \in [0, 2\pi]$ and $\phi \in [0, 2\pi]$. If we do this for different combinations of parameters a, b and c , we obtain a variety of different representations of $f(\phi, \theta)$ in the complex plane (Fig. 6.1).

For fixed set of parameters $\{a_i, b_i, c_i\}_{\mathbb{Z}_3}$ a solution of the equation in (6.5) can be visualised as three points in the complex plane in $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and $f_2(\phi_2, \theta_2)$, respectively. The relation between the solution set of points is given by the right hand side of the equations in (6.5). We have that $f_0(\phi_0, \theta_0) = |\beta| e^{(\arg(\beta))i}$, So necessarily we have that the three points representing the solution

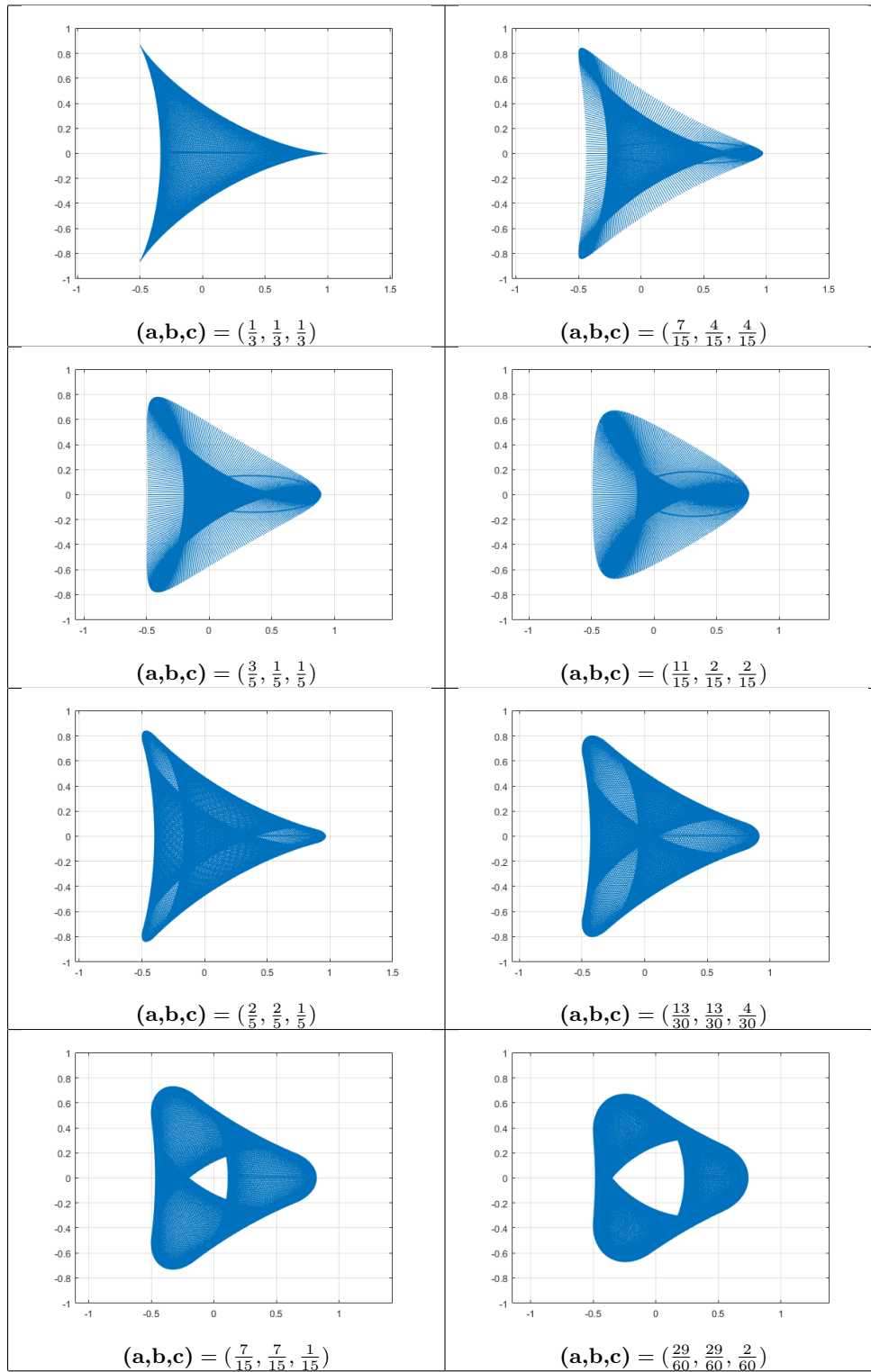


Figure 6.1: Representation in the complex plane of $f(\phi, \theta)$ for $\phi \in [0, 2\pi]$ and $\theta \in [0, 2\pi]$ and fixed a, b , and c such that $a + b + c = 1$.

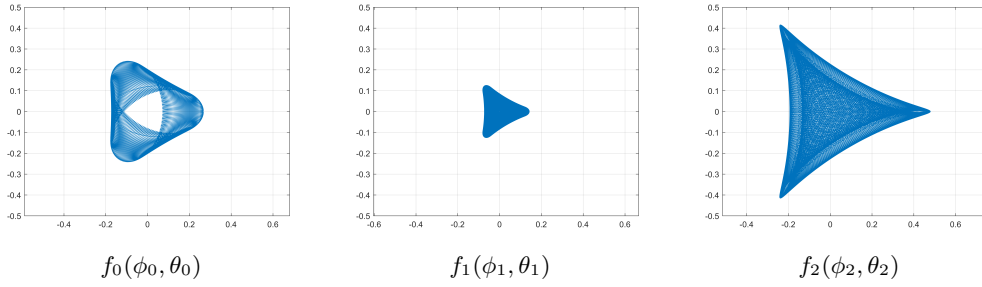


Figure 6.2: Representations in the complex plane of $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and $f_2(\phi_2, \theta_2)$ for the particular parameters given in 6.7

of the system lie in a circumference centred at the origin and have a relative phase of $\frac{2}{3}$ between them. We have now a geometrical intuition which allows us to know beforehand if for a given set of parameters $\{a_i, b_i, c_i\}_{i \in \mathbb{Z}_3}$ we can find a solution to the system of equations given by (6.5). In the following example, we show explicitly how the algorithm can be used to obtain a solution and the geometrical intuition we provided.

The objective of the algorithm is to obtain a matrix A such that the system of equations given by (6.4) and (6.5) is satisfied. By this algorithm, first we randomly choose a 3×3 matrix whose squared elements add up to one. We obtain the matrix

$$\begin{pmatrix} a_0 & b_0 & c_0 \\ a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \end{pmatrix} = \begin{pmatrix} 0.1196 & 0.4264 & 0.3976 \\ 0.2661 & 0.2711 & 0.1315 \\ 0.3873 & 0.3693 & 0.4449 \end{pmatrix}. \quad (6.7)$$

Before searching for the solutions we represent $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and $f_2(\phi_2, \theta_2)$ in the complex plane for particular choice of parameters in (6.7). The graphical representations of these functions in the complex plane are given in figure 6.2.

Any solution of the system is given by three points in $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and $f_2(\phi_2, \theta_2)$, respectively. The three points giving the solution lie in the same circumference centred at origin and have a relative phase between them of $\frac{2\pi}{3}$. Therefore, any solution is necessarily in the intersection of the representations of $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and $f_2(\phi_2, \theta_2)$. This intersection for this particular choice of parameters can be visualised in figure 6.3.

Finally, we randomly choose a complex number in the intersection of $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and

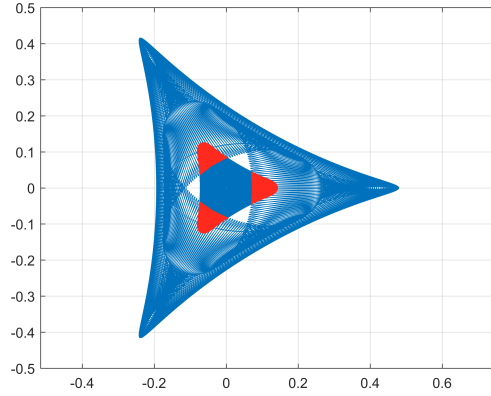


Figure 6.3: Representation of the superposition of $f_0(\phi_0, \theta_0)$, $f_1(\phi_1, \theta_1)$ and $f_2(\phi_2, \theta_2)$ in the same plot where the intersection of the three is shown in red.

$f_2(\phi_2, \theta_2)$. For example, we set

$$f_0(\phi_0, \theta_0) = -0.0485 + 0.0799i. \quad (6.8)$$

Then, we have that necessarily

$$f_1(\phi_1, \theta_1) = f_0(\phi_0, \theta_0)e^{\frac{4\pi i}{3}} = 0.0934 + 0.00205i \quad (6.9)$$

and

$$f_2(\phi_2, \theta_2) = f_0(\phi_0, \theta_0)e^{\frac{2\pi i}{3}} = -0.0449 - 0.0820i. \quad (6.10)$$

The three complex values are solutions of equations, now we need to obtain a set of parameters $\{\phi_i, \theta_i\}_{\mathbb{Z}_3}$ corresponding to that solution. To do this we solve numerically the three non-linear complex equations in (6.5). By substituting all the parameters in (6.3), we obtain the matrix

$$A = \begin{pmatrix} 0.1196 & 0.3984 - 0.1520i & -0.0696 + 0.3915i \\ 0.2661 & 0.2710 + 0.0068i & 0.0375 + 0.1261i \\ 0.3873 & 0.3498 - 0.1185i & -0.1792 + 0.4072i \end{pmatrix} \quad (6.11)$$

for which we can check that equations (6.4) and (6.5) are satisfied.

6.4 Analytical solutions

Consider the representation of maps/states in terms of the parameters of A in (6.3). As we did in the previous section, we will consider the solutions of the UCPT/LMM equations (6.4) and (6.5). In this case, instead of considering the general case, we will consider a particular constraint on A for which the UCPT/LMM equations can be solved analytically.

Consider a the matrix A such that $a_0 = a_1 = a_2 = a$, $b_0 = b_1 = b_2 = b$ and $c_0 = c_1 = c_2 = c$. In this case, to satisfy (6.4) we require that $a^2 + b^2 + c^2 = \frac{1}{3}$. One particularity of this A is that for every choice of a, b and c we can always find sets of $\theta_0, \phi_0, \theta_1, \phi_1, \theta_2$ and ϕ_2 solving the UCPT/LMM equations given by (6.5). An analytical solution of such system of equations is given by

$$\left| \begin{array}{l|l} \theta_0 = \theta & \phi_0 = \phi \\ \theta_1 = \theta - \frac{2\pi}{3} & \phi_1 = \phi - \frac{2\pi}{3} \\ \theta_2 = \theta - \frac{4\pi}{3} & \phi_2 = \phi - \frac{4\pi}{3} \end{array} \right|$$

In terms of A , this set of solutions is given by

$$A = \begin{pmatrix} a & be^{i\theta} & ce^{i(\theta+\phi)} \\ a & be^{i\theta-\frac{2\pi}{3}} & ce^{-i(\theta_1+\phi_1-\frac{4\pi}{3})} \\ a & be^{i\theta-\frac{4\pi}{3}} & ce^{-i(\theta_2+\phi_2-\frac{2\pi}{3})} \end{pmatrix}. \quad (6.12)$$

In this case, A represents a 4-dimensional family of UCTP maps/LMM states. Finally, for the family of bipartite states, we will compute the local unitary invariants derived in Chapter 5 in terms of the parameters of A . In this case, the first set of LU invariants corresponds to the spectrum of the density matrix. These invariants are given by

$$r_1^{(1)} = r_2^{(1)} = r_3^{(1)} = a^2 + b^2 + c^2 = \frac{1}{3}. \quad (6.13)$$

The second set consisting of nine LU invariants given by the eigenvalues of the partially transposed matrix. We get that

$$(r_{ij}^{(2)})_{i,j \in \mathbb{R}_3} = \begin{pmatrix} c + 2\sqrt{a}\sqrt{b}\cos(\theta) & c + 2\sqrt{a}\sqrt{b}\cos(\theta + \frac{2\pi}{3}) & c + 2\sqrt{a}\sqrt{b}\cos(\theta + \frac{4\pi}{3}) \\ a + 2\sqrt{b}\sqrt{c}\cos(\phi) & a + 2\sqrt{b}\sqrt{c}\cos(\phi + \frac{2\pi}{3}) & a + 2\sqrt{b}\sqrt{c}\cos(\phi + \frac{4\pi}{3}) \\ b + 2\sqrt{c}\sqrt{a}\cos(\theta + \phi) & b + 2\sqrt{c}\sqrt{a}\cos(\theta + \phi + \frac{2\pi}{3}) & b + 2\sqrt{c}\sqrt{a}\cos(\theta + \phi + \frac{4\pi}{3}) \end{pmatrix}. \quad (6.14)$$

Finally, the third set of invariants is represented by the eight singular values of the correlation matrix. However, for the particular family of states considered only four of them are distinct. These four eigenvalues can be evaluated as

$$\begin{aligned}
r_1^{(3)} &= \sqrt{a^2 + b^2 + c^2 - ab - bc - ac} \\
r_2^{(3)} &= \sqrt{ab + bc + ac - 2\sqrt{ab}\sqrt{c}\cos(\theta - \phi) - 2a\sqrt{b}\sqrt{c}\cos(-2\theta - \phi) - 2\sqrt{a}\sqrt{bc}\cos(\theta + 2\phi)} \\
r_3^{(3)} &= \sqrt{ab + bc + ac - 2\sqrt{ab}\sqrt{c}\cos(\theta - \phi + \frac{\pi}{3}) - 2a\sqrt{b}\sqrt{c}\cos(-2\theta - \phi + \frac{\pi}{3}) - 2\sqrt{a}\sqrt{bc}\cos(\theta + 2\phi + \frac{\pi}{3})} \\
r_4^{(3)} &= \sqrt{ab + bc + ac - 2\sqrt{ab}\sqrt{c}\cos(\theta - \phi - \frac{\pi}{3}) - 2a\sqrt{b}\sqrt{c}\cos(-2\theta - \phi - \frac{\pi}{3}) - 2\sqrt{a}\sqrt{bc}\cos(\theta + 2\phi - \frac{\pi}{3})}.
\end{aligned} \tag{6.15}$$

By inspecting these LU invariants we clearly see that more than four are linearly independent and consequently, they can be used to establish entanglement classification for the particular subfamily considered in this section.

6.5 Conclusions

In this chapter, we obtained explicit solutions to the equations producing families of unital and trace-preserving maps and locally maximally bipartite states which were previously considered in describing the geometry of the quantum state space. We considered the simplest setup ,the qutrit case, for which the convex decomposition of generic maps/bipartite states is still an open problem. Even in this setup, the family considered has 10 dimensions and numerical methods need to be used to solve the UCTP/LMM equations. We presented an algorithm obtaining the solutions to these equations. To gain insight about the high-dimensional space of solutions we introduced a geometrical representation of the equations which allows to determine which sets of parameters result in solvable equations. Finally, we considered a constraint on UCTP/LMM equations for which they can be solved analytically. The set of solutions for such equations represent a subset of the original family. For this subset of solutions, we evaluated explicitly the LU invariants provided in the previous chapter and we showed that these invariants can be use to establish a classification of the elements of this subfamily in terms of their entanglement.

Chapter 7

Conclusions

This thesis aims to improve the understanding of the geometry of the quantum state space. Such an improvement could lead to better characterisations of quantum systems. To do this, we develop novel tools to study the geometry of the set of unital quantum maps and the geometry of locally maximally mixed states. Despite the apparent differences between these sets, the map-state duality allows us to consider them using the same mathematical formalism. The geometry of unital qubit maps/LMM bipartite qubit states has the shape of a convex polytope in which the vertices correspond to unitary maps/pure bipartite quantum states. However, it is the case that the analogous geometry fails to describe the set of unital maps of higher dimensions. The description of unital qubit maps and LMM bipartite qubit states can be improved by considering polytopes whose vertices can be non-unitary maps and bipartite mixed quantum states, respectively. This thesis introduces the framework required to obtain and characterise novel families of unital quantum maps extreme with respect to the whole set of unital quantum maps. Following the aims of this work, we proposed a list of four objectives stated in the introduction. Here, we describe the main achievements associated with these research objectives.

In Chapter 4, we constructed a novel $(2d^2 - 3d + 1)$ -dimensional family of quantum unital maps containing both unitary maps and maps of higher rank (objective 1). To do this, we selected a particular set of Kraus operators representing a family of complete positive maps in terms of a list

of parameters. Then, we derived the equations for those parameters required by unital and trace-preserving conditions. For this family of unital and trace-preserving maps, we derived a criterion to determine whether a given map of the family corresponds to an extreme point of the set of unital and trace-preserving maps (objective 2). In the qutrit setup, the family of maps introduced cannot reproduce the rank-four maps for which set-extremal examples are known to exist. To consider this issue, we change the structure of the original set of Kraus operators. This change permits the description of rank-four qutrit maps (objective 1).

In Chapter 5, we considered the family of bipartite states isomorphic to the family of unital and trace-preserving maps constructed in Chapter 4. The main contribution of this chapter is the entanglement classification of the given family of bipartite states in terms of local unitary invariants (objective 3). To do this, we selected three sets of local unitary invariants whose evaluation is analytical. The selected sets invariants are the following: the eigenvalues of the density matrix, the eigenvalues of the partially transposed matrix and the singular values of the correlation matrix of the bipartite state. We evaluated the three sets of invariants for our family of bipartite states. Finally, we considered the particular case of two qutrit states. In this setup, we showed that not all invariants obtained are independent. However, numerical evidence supports the completeness of the invariants introduced for the entanglement classification of our family of locally maximally mixed two-qutrit states (objective 4).

In Chapter 6, we considered the solutions of the equations producing families of unital and trace-preserving qutrit maps and locally maximally two qutrit states considered in Chapter 4 and Chapter 5, respectively. The main contribution of this chapter is a numerical algorithm solving these equations (objective 4). To improve the parameter search by the algorithm, we presented a technique to visualise the 10-dimensional space of solutions. Finally, we derived the constraint on the equations used to find analytical solutions. For these constrained equations, we presented explicit solutions (objective 4). The solutions obtained represent a 4-dimensional family of locally maximally bipartite states for which we evaluated the set of local unitary invariants provided in Chapter 5. For this particular subset of the original family, we showed that the local unitary invariants presented are complete for entanglement classification (objective 4).

7.1 Future work

We propose several research ideas which could expand the work presented in this thesis. As mentioned, the $2d^2 - 3d + 1$ -dimensional family of maps we introduce generalises the set of mixed unitary maps. However, this family still fails to span all possible UCPT-extremal maps. It would be interesting to quantify the distance between the convex combinations of elements of the family and the set of mixed-unitary maps, as well as the distance between them and generic unital quantum maps. We could also study how these distances change as we increase the dimension of the quantum systems. In a different line of research, in this thesis, we derived a set of constants classifying the elements of the family of bipartite states presented in terms of their entanglement. We could express well-known entanglement measures using the derived constants. Some entanglement measures can be associated with various operational meanings. By finding the explicit relations between the LU-invariant constants and the different entanglement measures, we could explore the usefulness of the states of the family presented in other applications. Finally, we believe this work serves as an inspiration for other works further improving the characterisation of the state space for quantum systems of higher dimensions for which many questions are still unknown.

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