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Entanglement Witnessing based on Positive Maps

**Characterization of a Class of Bipartite
 $n \times n$ qubit Systems**

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To my mother,
For her unbounded love and patience.

به نام خداوند جان و خرد
خداوند نام و خداوند جای
خداوند کیوان و گردان سپهر
ز نام و نشان و گمان برترست
به بینندگان آفریننده را
نیابد بدو نیز اندیشه راه
سخن هر چه زین گوهران بگذرد
خرد گر سخن برگزیند همی
ستودن نداند کس او را چو هست
خرد را و جان را همی سنجد او
بدین آلت رای و جان و زبان
به هستیش باید که خستو شوی
پرستنده باشی و جوینده راه
توانا بود هر که دانا بود
از این پرده برتر سخن‌گاہ نیست

کزین برتر اندیشه برنگذرد
خداوند روزی ده رهنمای
فروزنده ماه و ناهید و مهر
نگارنده‌ی بر شده پیکرست
نبینی مرنجان دو بیننده را
که او برتر از نام و از جایگاه
نیابد بدو راه جان و خرد
همان را گزیند که بیند همی
میان بندگی را بیایدت بست
در اندیشه‌ی سخته کی گنجد او
ستود آفریننده را کی توان
ز گفتار بی‌کار یکسو شوی
به ژرفی به فرمانش کردن نگاه
ز دانش دل پیر برنا بود
ز هستی مر اندیشه را راه نیست

In the name of the Lord of both wisdom and mind,
To nothing sublimer can thought be applied,
The Lord of whatever is named or assigned
A place, the Sustainer of all and the Guide,
The Lord of Saturn and the turning sky,
Who causeth Venus, Sun, and Moon to shine,
Who is above conception, name, or sign,
The Artist of the heaven's jewellery!
Him thou canst see not though thy sight thou strain,
For thought itself will struggle to attain
To One above all name and place in vain,
Since mind and wisdom fail to penetrate
Beyond our elements, but operate
On matters that the senses render plain.
None then can praise God as He is. Observe
Thy duty: 'tis to gird thyself to serve.
He weigheth mind and wisdom; should He be
Encompassed by a thought that He hath weighed?
Can He be praised by such machinery
As this, with mind or soul or reason's aid?
Confess His being but affirm no more,
Adore Him and all other ways ignore,
Observing His commands. Thy source of might
Is knowledge: thus old hearts grow young again,
But things above the Veil surpass in height
All words: God's essence is beyond our ken.

From Shahname

By Hakim Abu'l-Qasim Ferdowsi Tusi (940-1020 CE)

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Declaration

I hereby declare that this thesis is my own work and effort and that it has not been submitted anywhere for any award. Where other sources of information have been used, they have been acknowledged.

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Chapter 1

Introduction

It is not exactly clear when the very first idea of a computer was born: It seems that the first idea of an automatic computing machine was proposed by Charles Babbage in 1822. In the middle of 1930, Alan Turing by introducing the universal Turing machine, made it clear what characteristics computing machines need to have, and how important programming is. Shortly after his paper, the first computer was built.

From 1947, onward transistors made the computer hardware develop very rapidly. So steadily the miniaturization pace that, in the middle of the sixties, Gordon Moore claimed that every two years the number of transistors used in a specific volume would double. This obviously had increased the speed of processing and the memory of the computers. This technology development went on until now, that we are not using the 30 tons computers anymore, but much smaller and lighter. However making computers and their hardware smaller, requires new considerations: when facing atomic scales, quantum effects play the major role instead of classical ones. Therefore if we want to have smaller computers, we might need to replace the classical computer technology by a quantum one.

In 1982, Richard Feynman, mentioned that simulating a quantum system by a classical computer is very difficult [26]. Instead he suggested to use a computer which is ruled by Quantum Mechanics. Three years later, in 1985, David Deutsch proposed a model of quantum Turing machine [22]. This was one of the first attempts to reveal the extreme power of quantum computing. The interesting point is that quantum technology not only permits the use of very small size microchips, but it also gives the possibility to tackle calculations by a new generation of algorithms based on Quantum Mechanics. It was Peter Shor, in 1994, who made one of the biggest steps in this field

and showed how powerful such a quantum algorithm can be in factorizing a given number into its prime factors [62].

In order to understand the main idea behind such an algorithm, let us mention some simple facts. From a physical point of view, a bit is a system which can be in two different states; these states can be yes or no, right or wrong, 0 or 1. A classical bit can be a mechanical on/off switch, or an electronic device capable of distinguishing a voltage difference. But if we choose an atom as a bit, in this case called qubit, then quantum mechanics tells us that the state of the atom can be a superposition the only two states available to a classical bit. Mathematically we write such a state as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1.$$

Now, consider a classical memory of three bits: at a given time, it can be in only one of the eight possible states 000, 001, 010, ..., 111. On the other hand, a quantum memory of three qubits, can instead be in all the eight states at the same time: $|\psi\rangle = a_1|000\rangle + a_2|001\rangle + \dots + a_8|111\rangle$. Therefore if we increase the number of qubits, the information stored in them increases exponentially: a memory of n qubits stores 2^n classical binary strings simultaneously, while its classical partner does store only one string. This gives the possibility of performing the computation on the superposition of all the possible states in one step. This is called parallelism: a quantum computer can do a certain computation on 2^n numbers using n qubits in one operation, while a classical computer has to do the same computation 2^n times with different entries, or it has to have 2^n processors operating at the same time. This means that quantum computers can in line of principle perform exponentially faster than the classical ones. Of course, after a quantum computation of sort, the solution of a given problem will be contained in just one of the classical strings appearing in the quantum superposition; indeed, the very core of quantum algorithmics is not only to write a sequence of quantum gates in order to solve the problem, but also to devise protocols able to read the superposition so that it gets projected onto the solution string with very high probability.

However this is not the only spectacular feature of the quantum computers. The other aspect which makes them very much different from their classical counterparts is the quantum effect called *entanglement*. In 1935, Einstein, Podolski and Rosen, tried to explain the odd characters of the *entangled quantum states*, using the hidden variables [25]. It was however, John Bell in the sixties, the one who deeply investigated, the borders between Classical

and Quantum Mechanics. His celebrated inequalities [10], that are to be satisfied by any local classical probabilistic theory, are violated by *entangled states*. That means that entanglement has no classically local counterpart.

Consider the following state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle), \quad (1.1)$$

where Alice has the first qubit and Bob owns the second one. Here the states $|0\rangle$ and $|1\rangle$ are the eigenstates of the spin along the Z axis, with eigenvalues $+1$ and -1 respectively. If Alice does no measurements on her qubit, she can only guess that Bob's qubit is in the state $|0\rangle$ with probability $\frac{1}{2}$ or, it is in the state $|1\rangle$ with the same probability. However if she does a measurement along the Z axis on her qubit, according to what she gets, she can say exactly in which state Bob's qubit is. For instance, if after measurement, she gets $+1$, then she can say that Bob's qubit is in state $|1\rangle$. While if she would have got -1 , then Bob's state would have been $|0\rangle$.

Now consider the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle. \quad (1.2)$$

In this case Alice can say that Bob's qubit is in the state $|0\rangle$ without doing any measurement on her qubit. Indeed Bob's qubit state, before and after the measurement on Alice's qubit does not change. While in the first case the state of Bob's qubit was modified by Alice's measurement, in the second case it did not.

This gives an idea that entangled states such as (1.1) are correlated in a way that the separable states as in (1.2) are not and that these correlations have no classical counterparts.

As we mentioned before entanglement plays a very important rule in quantum computation and quantum information. Quantum dense coding and quantum cryptography are examples of that. However the most astonishing application of entanglement is quantum teleportation, which concerns sending a qubit from one party to another one.

Suppose Alice wants to send the following state to Bob:

$$|\phi\rangle_C = \alpha|0\rangle + \beta|1\rangle.$$

All Alice knows about the coefficients α and β is that $|\alpha|^2 + |\beta|^2 = 1$; that is the state $|\phi\rangle_C$ is unknown to her. In order to send this state, they share one of the following maximally entangled states (later we will see that these states are called Bell states, and form an orthonormal basis in $\mathbb{C}^2 \otimes \mathbb{C}^2$):

$$\begin{aligned} |\Phi^\pm\rangle &= \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \\ |\Psi^\pm\rangle &= \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle). \end{aligned}$$

Let Alice and Bob share the state $|\Phi^+\rangle$. Then the overall state would be:

$$|\phi\rangle_C \otimes |\Phi\rangle_{AB} = \frac{1}{\sqrt{2}}(\alpha|000\rangle + \alpha|011\rangle + \beta|100\rangle + \beta|111\rangle)$$

This can be re-written as:

$$\begin{aligned} |\phi\rangle_C \otimes |\Phi\rangle_{AB} &= \frac{1}{2}(|\Phi^+\rangle_{AC} \otimes (\alpha|0\rangle + \beta|1\rangle)_B + |\Phi^-\rangle_{AC} \otimes (\alpha|0\rangle - \beta|1\rangle)_B \\ &+ |\Psi^+\rangle_{AC} \otimes (\alpha|1\rangle + \beta|0\rangle)_B + |\Psi^-\rangle_{AC} \otimes (\alpha|1\rangle - \beta|0\rangle)_B. \end{aligned}$$

Now if Alice does a measurement of the Bell basis on her first two qubits, according to whether she finds them in $|\Phi^\pm\rangle$, $|\Psi^\pm\rangle$ the state would collapse into one of the following states:

$$\begin{aligned} &|\Phi^+\rangle_{AC} \otimes (\alpha|0\rangle + \beta|1\rangle)_B \\ &|\Phi^-\rangle_{AC} \otimes (\alpha|0\rangle - \beta|1\rangle)_B \\ &|\Psi^+\rangle_{AC} \otimes (\alpha|1\rangle + \beta|0\rangle)_B \\ &|\Psi^-\rangle_{AC} \otimes (\alpha|1\rangle - \beta|0\rangle)_B. \end{aligned}$$

Therefore if she calls Bob through a classical channel (phone, e-mail, skype, etc.) and tell him what was the outcome of her measurement on Bell states basis, then Bob can do one of the following operations on his qubit in order to get it into the initial $|\phi\rangle_C$ state:

- If Alice gets $|\Phi^+\rangle$, Bob does nothing.
- If Alice gets $|\Phi^-\rangle$, Bob acts with σ_3 on his qubit.
- If Alice gets $|\Psi^+\rangle$, Bob acts with σ_1 on his qubit.
- If Alice gets $|\Psi^-\rangle$, Bob acts with $\sigma_3\sigma_1$ on his qubit.

Where σ_1 is the first Pauli matrix, and σ_3 is the third one. This way Alice has sent her unknown qubit to Bob. This process is called quantum teleportation: it amounts to sending one qubit of information using two classical bits and an entangled state as transmission channel.

Ever since, quantum entanglement has been one of the the main ingredients of quantum information theory, and the focus of many studies [37]. However very fundamental questions have still partial answers: when is it that a generic quantum state is entangled? How much entangled is it? Or, is its entanglement useful for quantum information processing or not? Indeed, just detecting entanglement in physical systems is one of the most challenging issues.

Interestingly, beside rejuvenating the whole of Quantum Mechanics, quantum information has also stimulated a more abstract interest in an old mathematical problem: the characterization of positive linear maps on (the states on) C^* algebras of operators [36].

From a physical point of view, all actually occurring processes must be described by completely positive (CP) maps whose structure was fully characterized by Stinespring in the 50ties and whose central role in Quantum Mechanics was clarified by Kraus in the 70ies [4]. Their importance is due to the fact that they are much more than positive: let the system on which they act (A) be coupled to an ancillary system (B) completely inert and extend the action of the map from A to A+B by composing it with the identity action on B. Then, CP maps preserve positivity when they act on the states of the bipartite system A+B. Instead, only positive maps do not because there surely exist entangled states of the compound system A+B whose spectrum does not remain positive under a positive, but not completely positive map composed with the identity.

Since one cannot physically exclude such statistical couplings, complete positivity is the only guarantee against the appearance of unphysical negative probabilities in the spectrum of a transformed entangled state in the case of couplings to ancillas. The most renown amongst positive, but not completely positive maps is matrix-transposition: as transposition, it preserves positivity, but fails to do so as partial-transposition, that is when acting on one party only of a bipartite compound system [36].

Thus, positive maps are not fully consistent as descriptions of actual physical processes; however, exactly because they do not preserve the positivity of all entangled states, they can then be used as entanglement witnesses. Transposition is such a witness, which is exhaustive only in lower dimension; that is for two qubits (2-dim. system), or one qubit and one qutrit (three-dim. system). Otherwise, for instance already for two pairs A and B of two qubits each, there are entangled states of A+B which remain positive under partial-transposition: they are called PPT entangled states, namely positive under partial transposition, but entangled nevertheless.

The physical interest of PPT entangled states is that their entanglement content cannot be augmented by any distillation protocol operating on great numbers of them: they are also called bound entangled states as their entanglement is somewhat locked in and cannot be extracted. The mathematical interest of these states is instead related to the notion of decomposable positive maps. It was introduced by Størmer and Choi in order to isolate a particular sub-class of positive maps and used by Woronowicz to characterize all positive maps in low dimension (this makes transposition an exhaustive witness in such cases) [36].

Only a sub-class of higher dimensional positive maps is decomposable, that is can be split into the sum of a CP map and a CP map composed with transposition and these cannot detect the entanglement of PPT states. Therefore, one is interested in constructing new families of non-decomposable positive maps able to witness certain bound-entangled states. This activity has been pursued in recent years, among others, by the Horodeccy [36], by Kossakowski and Chruściński [20, 21] in Poland.

In this thesis work we have studied of 16×16 density matrices of two pairs of qubits, equidistributed over particularly symmetric orthogonal one-dimensional projections $P_{\alpha\beta}, \alpha, \beta = 0, 1, 2, 4$, for which Benatti et al. have been able to classify all PPT states, but only a few entangled ones among them. As PPT states are related to specific discrete geometric structures associated to a 16 point lattice, the issue is to understand whether bound entanglement might be related to a further specification of such structures and, if so, to characterize all PPT entangled lattice states.

The organization of the thesis will be as follows:

Chapter 2: We present an essential introduction of Functional Analysis as the basic mathematical tools dealing with Quantum Mechanics: Hilbert spaces and operators acting on them with a couple of most important norms on them will be defined. In this work, we shall consider only finite dimensional Hilbert spaces, $\mathbb{H} = \mathbb{C}^d$; therefore the algebra of bounded linear operators defined on them will be isomorphic to the full matrix algebra $M_d(\mathbb{C})$.

Chapter 3: We explain how quantum systems can be described using the mathematical tools of Chapter 2. Density matrices will be introduced as quantum states, which are, in general, mixtures of pure states with corresponding weights. Pure states, that is projectors onto Hilbert space vectors, are a particular case when the physical state of a quantum system is completely known.

The von Neumann entropy as a counterpart of Shannon entropy will also be introduced; in compound systems, this quantity is used to compare the mixedness of density matrices of subsystems, called reduced density matrices, to the one of whole system. Throughout this work, we shall be interested in bipartite systems only. The definition of entangled and separable states in such systems will follow. We shall see, that as far as one is dealing with pure states, thanks to the Schmidt decomposition, distinguishing entangled and separable states is an easy task, which is not the case for mixed states. We will present Bell states and Werner states as examples of entangled states.

Chapter 4: We explain what are the requirements for a linear map which is to describe a physical transformation. We start by giving some mathematical definitions of positive maps and completely positive maps. Using the Kraus representation we will study the structure of CP maps. Then Choi matrix will be introduced, as it provides a technique based on its block positivity or positivity to decide whether the corresponding map is positive or completely positive. We shall see that, though positive maps are not suitable candidates for describing physical transformations, nevertheless they can be used as mathematical tools to detect the entanglement.

Many examples will be given throughout the chapter; particularly the Transposition Map, which will be used to define decomposable maps. We shall also see, how a generic positive map can be written in terms of the Trace Map and a suitable completely positive map.

Chapter 5: This chapter focuses on variety of entanglement detecting methods. Partial Transposition, which is exhaustive in low dimensions, and PPTness as a necessary condition for separability will be presented. Using the Hahn-Banach separation theorem, we introduce entanglement witnesses and how they can be connected to positive maps through the Jamiołkowski isomorphism. The Reduction Criterion, which is based on the Reduction Map, already introduced in chapter 4 as a decomposable map, will be presented. Further, we shall rapidly overview the Range Criterion, which was used to detect the first PPT entangled state in $\mathbb{C}^2 \otimes \mathbb{C}^4$, it will be followed by the notion of Unextendible Product Bases (UPB). We end this chapter by explaining the Realignment Method, which, unlike the other methods which manipulate only one subsystem, involves both subsystems to detect the entanglement. Many examples will be given throughout this chapter.

Chapter 6: The last chapter contains new results. They concern a class of states over two parties consisting of n qubits each. The states studied are

diagonal in the basis generated by the action of tensor products of the form $\mathbb{1}_{2^n} \otimes \sigma_{\vec{\mu}}$, $\sigma_{\vec{\mu}} = \otimes_{i=1}^n \sigma_{\mu_i}$, on the totally symmetric state $|\Psi_+^{2^n}\rangle \in \mathbb{C}^{2^n} \otimes \mathbb{C}^{2^n}$. We first characterize the structure of positive maps detecting the entangled ones among them; we will show that their possible entanglement will be witnessed using a subclass of positive maps, namely diagonal positive maps. Then, the result will be illustrated by examining some entanglement witnesses for the case $n = 2$. Further, we will show how, for pairs of two qubits, being separable, entangled and bound entangled are state properties related to the geometric patterns of subsets of a 16 point square lattice.

Chapter 2

Preliminaries

2.1 Banach and Hilbert spaces

In this chapter we focus on the essential background of functional analysis [57, 69, 44], and review the basic mathematical tools which are used in Quantum Mechanics as we are interested to describe it using the vector and operators over vector spaces, in particular Hilbert spaces.

Definition 1 *Banach Space*

A Banach space is a vector space with a norm defined on it, with respect to which, it is complete.

Definition 2 *Hilbert Space*

A Hilbert space \mathbb{H} is a Banach space with respect to a norm given by the scalar product $\langle \cdot | \cdot \rangle$. For every vector $\psi \in \mathbb{H}$, $\|\psi\| = \sqrt{\langle \psi | \psi \rangle}$ denotes its norm.

We shall consider Hilbert spaces with countable orthonormal bases $\{\psi_i\}_{i \in \mathbb{N}} \subset \mathbb{H}$, the corresponding projectors $P_i = |\psi_i\rangle\langle\psi_i|$ satisfying the completeness relation: $\sum_i P_i = \mathbb{1}$.

Definition 3 *Operator Norm*

The norm of an operator O on a Hilbert space \mathbb{H} is defined as:

$$\|O\| := \sup_{\|\psi\|=1} \|O|\psi\rangle\|. \quad (2.1)$$

It satisfies:

$$\|O^\dagger\| = \|O\|, \quad \|O^\dagger O\| = \|O\|^2. \quad (2.2)$$

O is said to be bounded if $\|O\| < \infty$. We denote the set of all bounded linear operators acting on \mathbb{H} by $B(\mathbb{H})$.

The linear combination and the product of two bounded operator is also bounded. Moreover all Cauchy type sequences with respect to the norm(3), converge to an element in $B(\mathbb{H})$ [3] which makes this space complete. That means that $B(\mathbb{H})$ is a C^* – algebra.

Definition 4 Spectrum

The spectrum of a bounded operator O denoted by $\sigma(O)$, is the set of all complex numbers λ such that $\lambda \text{id} - O$ has no inverse in $B(\mathbb{H})$, where id is the identity operator.

The projectors onto vectors of Hilbert spaces are the simplest examples of bounded operators on \mathbb{H} with the spectrum $\sigma(P_i) = \{0, 1\}$.

In Quantum Mechanics positive linear operators are highly important, they are bounded operators with non-negative spectrum, indeed they can be considered as observables whose measured outcomes are positive.

Definition 5 Positive Operator

An operator $O \in B(\mathbb{H})$ acting on \mathbb{H} , is positive if $\langle \psi | O \psi \rangle \geq 0$ for all $|\psi\rangle \in \mathbb{H}$.

$B^+(\mathbb{H})$ denotes the set of all bounded linear positive operators acting on a Hilbert space \mathbb{H} : $B^+(\mathbb{H}) \subset B(\mathbb{H})$.

A set is said to be a cone if it is invariant to non-negative scaling. For any positive operator $O \in B^+(\mathbb{H})$ it holds that $\alpha O \in B^+(\mathbb{H})$, where $\alpha \geq 0$, therefore the set $B^+(\mathbb{H})$ is a cone.

2.2 Operators on a Finite Dimensional Hilbert Space

Every finite Hilbert space \mathbb{H} of dimension d is isomorphic to vector space of d -dimensional complex vectors \mathbb{C}^d . Fixing the orthonormal basis set $\{|i\rangle\}$,

$$|i\rangle = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \text{ i-th,}$$

any vector $|\psi\rangle \in \mathbb{H}$ can be represented over the field of complex scalars:

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_d \end{pmatrix} \in \mathbb{C}^d,$$

and linear operators are represented by $d \times d$ matrices. Then the physical observables are Hermitian $d \times d$ matrices with complex entries, and their algebra is denoted by $M_d(\mathbb{C})$, the entries of $A \in M_d(\mathbb{C})$ being $A_{ij} = \langle i|A|j \rangle$.

Theorem 1 Spectral decomposition

Any normal operator A , $A^\dagger A = AA^\dagger$, on \mathbb{C}^d can be diagonalized with respect to the orthonormal basis of its eigenvectors:

$$A = \sum_i a_i |a_i\rangle \langle a_i|, \quad A|a_i\rangle = a_i |a_i\rangle.$$

Therefore, $A \in M_d(\mathbb{C})$ is positive semidefinite if all its eigenvalues are non-negative. Notice that matrix algebra $M_d(\mathbb{C})$ can be treated as a Hilbert space equipped with the Hilbert-Schmidt scalar product of two operators A and B in $M_d(\mathbb{C})$ which is defined to be :

$$\langle A|B \rangle = \text{Tr}(A^\dagger B), \quad (2.3)$$

where

$$\text{Tr}(A^\dagger B) = \sum_i \langle i|A^\dagger B|i \rangle$$

is the trace of $A^\dagger B$ which is defined with respect to any orthonormal basis set $\{|i\rangle\}$. The corresponding norm, called Hilbert-Schmidt norm:

$$\|A\|_2 = \sqrt{\text{Tr}(A^\dagger A)} = \sqrt{\sum_{i=1}^d a_i^2}, \quad (2.4)$$

can be expressed in terms of the eigenvalues a_i^2 of the positive operator $|A|^2 = A^\dagger A$. Another equivalent norm is the so called trace norm:

$$\|A\|_1 := \text{Tr}|A| = \sum_{i=1}^d |a_i|. \quad (2.5)$$

Example 1 Trace map [3]

Let $\mathbb{H} = M_d(\mathbb{C})$, where $\{F_i\}_{i=1}^{d^2}$ is a set of $d \times d$ matrices which are orthogonal with respect to the Hilbert-Schmidt scalar product, $\text{Tr}(F_l^\dagger F_k) = \delta_{lk}$. They form an orthonormal basis set, so that:

$$X = \sum_{i=1}^{d^2} \text{Tr}(X F_i^\dagger) F_i, \quad \forall X \in M_d(\mathbb{C}). \quad (2.6)$$

Now consider the Trace Map, $\text{Tr}_d : M_d(\mathbb{C}) \longrightarrow M_d(\mathbb{C})$ defined to be:

$$M_d(\mathbb{C}) \ni X \longmapsto \text{Tr}_d[X] := \text{Tr}(X)\mathbb{1}_d. \quad (2.7)$$

Given an orthonormal basis $\{|\alpha\rangle\}_{\alpha=1}^d$, one constructs the so called unit matrices $E_{\alpha\beta} := |\alpha\rangle\langle\beta|$ in $M_d(\mathbb{C})$, which form an orthonormal basis in $M_d(\mathbb{C})$ with respect to the Hilbert-Schmidt scalar product. Therefore, using this orthonormal set, the Trace Map reads:

$$\begin{aligned} \text{Tr}_d[X] = \text{Tr}(X)\mathbb{1}_d &= \sum_{\alpha=1}^d \langle\alpha|X|\alpha\rangle \sum_{\beta=1}^d |\beta\rangle\langle\beta| \\ &= \sum_{\alpha,\beta=1}^d |\beta\rangle\langle\alpha|X|\alpha\rangle\langle\beta| = \sum_{\alpha,\beta=1}^d E_{\alpha\beta}^\dagger X E_{\alpha\beta} \end{aligned}$$

since the two orthonormal basis $\{F_i\}_{i=1}^{d^2}$ and $\{E_{\alpha\beta}\}_{(\alpha,\beta=1)}^d$ can be transformed one into the other using a unitary matrix $U \in M_{d^2}(\mathbb{C})$: $E_{\alpha\beta} = \sum_{j=1}^{d^2} U_{\alpha\beta,j} F_j$. The Trace Map can thus be re-written as:

$$\begin{aligned} \text{Tr}_d[X] &= \sum_{\alpha,\beta=1}^d E_{\alpha\beta} X E_{\alpha\beta} \\ &= \sum_{i,j=1}^{d^2} \sum_{\substack{\alpha,\beta=1 \\ \gamma,\delta=1}}^d U_{j,\alpha\beta}^* U_{\gamma\delta,i} F_j^\dagger X F_i \\ &= \sum_{j=1}^{d^2} F_j^\dagger X F_j. \end{aligned} \quad (2.8)$$

Example 2 The simplest quantum systems are the 2-level systems, which are described by 2×2 matrices: $A \in M_2(\mathbb{C})$. Most distinguished among them are the self-adjoint Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.9)$$

with respect to the orthonormal basis $|0\rangle, |1\rangle$ of eigenvectors of σ_3 : $\sigma_3|0\rangle = |0\rangle$, $\sigma_3|1\rangle = -|1\rangle$, where $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. For the other matrices we have $\sigma_1|0\rangle = |1\rangle$, $\sigma_1|1\rangle = |0\rangle$, $\sigma_2|0\rangle = -i|1\rangle$ and $\sigma_2|1\rangle = i|0\rangle$.

The algebra of Pauli matrices is summarized by:

$$\sigma_j \sigma_k = \delta_{jk} \mathbb{1}_2 + i \varepsilon_{jkl} \sigma_l \quad (2.10)$$

where ε_{jkl} is the antisymmetric 3-tensor, $\mathbb{1}_2$ is the 2×2 identity matrix which we also denote by σ_0 . These four matrices are orthogonal in the sense of Hilbert-Schmidt scalar product, that is $\text{Tr}(\sigma_i \sigma_j) = \delta_{ij}$ if $i \neq j$, when normalized, $\tilde{\sigma}_i := \frac{\sigma_i}{\sqrt{2}}$ they form an orthonormal basis set in $M_2(\mathbb{C})$. Therefore any matrix $X \in M_2(\mathbb{C})$ can be written as:

$$X = \sum_{i=0}^3 (\text{Tr}(\tilde{\sigma}_i X)) \tilde{\sigma}_i.$$

Example 3 Trace map in $M_2(\mathbb{C})$ [4]

Using the Pauli matrices as an orthonormal basis set we can write the Trace Map defined in (2.7) as:

$$\text{Tr}[X] = \sum_{j=0}^3 \sigma_j X \sigma_j. \quad (2.11)$$

In this case Pauli matrices permit us to simplify this map even more. Let us define the map $S_\alpha : M_2(\mathbb{C}) \longrightarrow M_2(\mathbb{C})$ such that:

$$S_\alpha[\cdot] = \sigma_\alpha[\cdot]\sigma_\alpha. \quad (2.12)$$

The Trace Map is re-written as:

$$\text{Tr}_2[X] = \sum_{\alpha=0}^3 S_\alpha[X]. \quad (2.13)$$

We shall refer to this map in the next chapters.

Chapter 3

States and Operators

In this chapter, we present some mathematical aspects concerning quantum states of multipartite systems. The presence of many parties introduces the notion of quantum correlations and entanglement. For the rest of this work, we consider only finite complex Hilbert spaces $\mathbb{H} = \mathbb{C}^d$, where d denotes the dimension of the Hilbert space. States both in Classical and Quantum Mechanics are generic linear, positive, normalized functionals on the algebras of observables that fix their mean values. In Classical Mechanics one deals with probability distributions on phase-space; in Quantum Mechanics distributions are replaced by density matrices which extend the notion of quantum state beyond the single vectors in Hilbert spaces.

3.1 Density Matrices

Usually one is accustomed to states of quantum systems only as vectors in a suitable Hilbert space. However, more general ones need to be introduced. Consider an ensemble of projectors $P_i := |\psi_i\rangle\langle\psi_i| \in B(\mathbb{H})$ corresponding to the vector states $|\psi_i\rangle \in \mathbb{H}$, with weights p_i . If the only knowledge about the physical system is that it can be found in such states with weight p_i , one is effectively dealing with a statistical ensemble. Its mathematical description is by a density matrix, namely:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \in M_d(\mathbb{C}).$$

Definition 6 *Density Matrix*

Any positive operator $\rho \in M_d(\mathbb{C})$ with $\text{Tr}(\rho) = 1$ describes a mixed state; let $\rho = \sum_{j=1} r_j |r_j\rangle\langle r_j|$ be its spectral representation with $0 \leq r_j \leq 1$ and

$\sum_j r_j = 1$. Then ρ defines a positive, linear and normalized functional on $M_d(\mathbb{C})$ [3]:

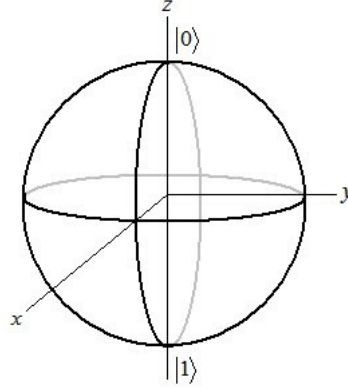
$$M_d(\mathbb{C}) \ni X \longmapsto \omega_\rho(X) := \text{Tr}(\rho X) = \sum_j r_j \langle \varphi_j | X | \varphi_j \rangle. \quad (3.1)$$

Remark 1 When the density matrix is a projector onto the corresponding state vector, which is its eigenvector with eigenvalue one, the state is said to be pure, hence the spectral representation of the density matrix reduces in to a one-dimensional projection.

The set of all the density matrices of a quantum system S , is denoted by $\mathbb{S}(S)$. Since any convex combination of two density matrices is a density matrix as well, therefore $\mathbb{S}(S)$ is a convex set. Its extreme points, which can not be written as a convex combination of other density matrices, correspond to pure states.

Example 4 Bloch Sphere

There is a very useful geometrical representation for density matrices $\rho \in M_2(\mathbb{C})$ of qubits: the Bloch sphere. Taking the two eigenvectors $|0\rangle$ and $|1\rangle$ of the Pauli matrix σ_3 as the axes of this sphere:



Then any normalized vector $|\psi\rangle$ in a two-level system can be represented in terms of these two vectors:

$$|\psi\rangle = \cos \theta |0\rangle + e^{i\phi} \sin \theta |1\rangle.$$

It corresponds to a point on the surface of this sphere, which can be also represented using polar coordination by a new vector $\vec{\alpha} \in \mathbb{R}^3$:

$$\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3) = (\sin 2\theta \cos \phi, \sin 2\theta \sin \phi, \cos 2\theta). \quad (3.2)$$

The vector $\vec{\alpha}$ is known as Bloch vector. In general a mixed density matrix $\rho \in M_2(\mathbb{C})$ can be represented in terms of Bloch vectors and Pauli matrices, called Bloch representation:

$$\rho = \frac{1}{2}(\mathbb{1}_2 + \sum_{i=0}^3 \alpha_i \sigma_i), \quad (3.3)$$

$$\text{where } \alpha_i = \text{Tr}(\rho \sigma_i).$$

The positivity of ρ is equivalent to asking that $\|\vec{\alpha}\|^2 = \sum_{i=1}^3 \alpha_i^2 \leq 1$. Note that pure qubit states correspond to Bloch vectors $\vec{\alpha}$ with norm one, i.e. to the points on the surface of the sphere. Mixed states are instead represented by points inside the sphere where $|\vec{\alpha}| < 1$. The maximally mixed state $\frac{\mathbb{1}_2}{2}$ corresponds to the center of the sphere, while orthogonal states, in the sense of the Hilbert-Schmidt product, are connected by diameters.

Therefore a density matrix is a Hermitian, unit-trace operator with non-negative eigenvalues. For pure states $\text{Tr}(\rho^2) = 1$, while for mixed states $\text{Tr}(\rho^2) < 1$. Given two density matrices, there are different methods to judge about their mixedness.

The mixedness measure on a Hilbert space with dimension d , is defined to be [54]:

$$M = \frac{d}{d-1}(1 - \text{Tr}(\rho^2)). \quad (3.4)$$

This quantity is known as linear entropy and is 0 for pure states and maximal for maximally mixed states, i.e. $\omega = \frac{1}{d}$.

However, the most reknown entropy is the von Neumann entropy [73].

Definition 7 von Neumann Entropy

Given a density matrix $\rho \in \mathbb{S}(S)$, the von Neumann entropy is defined:

$$S(\rho) = -\text{Tr}(\rho \log \rho) = -\sum_i^d \lambda_i \log \lambda_i \quad (3.5)$$

where λ_i are the eigenvalues of ρ and d is the dimension of the system.

Evidently this quantity is zero only for pure states, as the projectors have only eigenvalues equal to 0 or 1. For the maximally mixed states $\rho_0 = \frac{\mathbb{1}_d}{d}$, the von Neumann entropy is maximum:

$$S(\rho_0) = -\sum_i \frac{1}{d} \log \frac{1}{d} = \sum_i \frac{1}{d} \log d = \log d.$$

This shows that the von Neumann entropy can measure the mixedness of density matrices, and we have $0 \leq S(\rho) \leq \log d$.

3.2 Composite Systems

In Quantum Information, one very frequently deals with systems consisting of several subsystems, called multi-partite systems: $S = S_1 + S_2 + \dots + S_n$. The Hilbert space of S is the tensor product of the Hilbert spaces of its subsystems: $\mathbb{H}^{\otimes n} = \bigotimes_{i=1}^n \mathbb{H}_i$. On tensor product Hilbert spaces, operators act as tensor product of matrices.

Definition 8 *Matrix Tensor Product*

Consider a bipartite system described by the Hilbert space $\mathbb{C}^{d_1 d_2} = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$, together with the matrix algebra $M_{d_1}(\mathbb{C})$ for the first party and $M_{d_2}(\mathbb{C})$ for the second one. Thus the algebra of the whole system consists of the tensor product of the form [29, 15]:

$$A \otimes B = \begin{pmatrix} a_{1,1}B & a_{1,2}B & \cdots & a_{1,n}B \\ a_{2,1}B & a_{2,2}B & \cdots & a_{2,n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1}B & a_{m,2}B & \cdots & a_{m,n}B \end{pmatrix}, \quad A \in M_{d_1}(\mathbb{C}), B \in M_{d_2}(\mathbb{C}).$$

When $\mathbb{H}^{\otimes n} = \bigotimes_{i=1}^n \mathbb{C}^{d_i}$, the algebra of $\mathbb{H}^{\otimes n}$ is $M^{\otimes n}(\mathbb{C}) = \bigotimes_{i=1}^n M_{d_i}(\mathbb{C})$.

The opposite of combining the subsystems to get a bigger one, is partial tracing. By tracing over a subsystem S_j with respect to an orthonormal basis $|\psi_k^{(j)}\rangle \in \mathbb{C}^{d_j}$, one reduces a density matrix $\rho \in M^{\otimes n}(\mathbb{C})$ to another density matrix:

$$\rho_{\widehat{j}} := \text{Tr}_j \rho = \sum_k \langle \psi_k^{(j)} | \rho | \psi_k^{(j)} \rangle \in M_j^{\otimes(n-1)}(\mathbb{C}) = \bigotimes_{\substack{i=1 \\ i \neq j}}^n M_{d_i}(\mathbb{C}), \quad (3.6)$$

acting on $\mathbb{C}_j^{\otimes(n-1)} = \bigotimes_{\substack{i=1 \\ i \neq j}}^n \mathbb{C}^{d_i}$.

In the following, we will consider only finite-dimensional bipartite systems, i.e. $S = S_1 + S_2$, with $\mathbb{H}^{\otimes 2} = \mathbb{H}_1 \otimes \mathbb{H}_2$, $\mathbb{H}_1 = \mathbb{C}^{d_1}$ and $\mathbb{H}_2 = \mathbb{C}^{d_2}$. Therefore for the whole system we have $\mathbb{H} = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} = \mathbb{C}^{d_1 d_2}$. Density matrices are positive $\rho_{12} \in M_{d_1 d_2}(\mathbb{C})$ of trace 1. The partial trace yields:

$$M_{d_1}(\mathbb{C}) \ni \rho_1 = \text{Tr}_2(\rho_{12}) := \sum_{j=1}^{d_2} \langle f_j^2 | \rho_{12} | f_j^2 \rangle \quad (3.7)$$

$$M_{d_2}(\mathbb{C}) \ni \rho_2 = \text{Tr}_1(\rho_{12}) := \sum_{i=1}^{d_1} \langle e_i^1 | \rho_{12} | e_i^1 \rangle,$$

where ρ_1 (resp. ρ_2) is called reduced density matrix for the system S_1 (resp. for the system S_2), the sets $\{|e_i^1\rangle\}_{i=1}^{d_1}$ and $\{|f_j^2\rangle\}_{j=1}^{d_2}$ are orthonormal basis of \mathbb{C}^{d_1} and \mathbb{C}^{d_2} respectively.

The reduced density matrices describe the states that two parties locally possess. Their meaning is easy to understand in terms of local observables, of the first party, say: $A \otimes \text{id}$. The mean value of such a local observable, of the first party alone, with respect to the two party state ρ_{12} reads

$$\text{Tr}_{12}(\rho_{12}A \otimes \mathbb{1}) = \sum_{i=1}^{d_1} \langle e_i^1 | A \left(\sum_{j=1}^{d_2} \langle f_j^2 | \rho_{12} | f_j^2 \rangle \right) | e_i^1 \rangle = \text{Tr}_1(A \rho_1) ,$$

showing that it is completely specified by the reduced density matrix ρ_1 of the considered party.

For bipartite systems, we have the following lemma:

Lemma 1 *Schmidt decomposition*

Every vector $|\psi_{12}\rangle \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$, can be represented as [49]:

$$|\psi_{12}\rangle = \sum_{i=1}^M r_i^{(1)} |r_i^{(1)}\rangle \otimes |r_i^{(2)}\rangle \quad (3.8)$$

where $M \leq \min\{d_1, d_2\}$, and $\{|r_i^{(1)}\rangle\}_{i=1}^{d_1}$ and $\{|r_i^{(2)}\rangle\}_{i=1}^{d_2}$ are orthonormal sets of vectors in \mathbb{C}^{d_1} and \mathbb{C}^{d_2} respectively. The non-negative scalars $\{r_i\}$ are such that $\sum_{i=1}^M r_i^2 = 1$.

Proof: Without loss of generality let us assume $d_1 \leq d_2$. Given two ONB $\{|e_i\rangle\}_{i=1}^{d_1}$ and $\{|f_j\rangle\}_{j=1}^{d_2}$, any vector $\psi_{12} \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ can be written as:

$$|\psi_{12}\rangle = \sum_{i,j} c_{ij} |e_i^1\rangle \otimes |f_j^2\rangle, \quad c_{ij} \in \mathbb{C}. \quad (3.9)$$

Its corresponding density matrix is $\rho_{12} = |\psi_{12}\rangle\langle\psi_{12}|$. The reduced density matrix ρ_1 is obtained by partial tracing over the second subsystem, which in its spectral representation is:

$$\rho_1 = \text{Tr}_2(|\psi_{12}\rangle\langle\psi_{12}|) = \sum_{i=1}^{d_1} r_i^{(1)} |r_i^{(1)}\rangle\langle r_i^{(1)}|. \quad (3.10)$$

Choosing $\{|r_i^{(1)}\rangle\}_{i=1}^{d_1}$ as an ONB for \mathbb{C}^{d_1} , we can re-write (3.9) as:

$$\begin{aligned}
|\psi_{12}\rangle &= \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} c_{ij} |r_i^{(1)}\rangle \otimes |f_j\rangle \\
&= \sum_{i=1}^{d_1} |r_i^{(1)}\rangle \otimes |\phi_i^{(2)}\rangle,
\end{aligned} \tag{3.11}$$

where $|\phi_i^{(2)}\rangle = \sum_{j=1}^{d_2} c_{ij} |f_j\rangle$. Note that the vectors $|\phi_i^{(2)}\rangle$ are not in general orthonormal. Using this new ONB, partial tracing over the second subsystem of ρ_{12} , will be read as:

$$\rho_1 = \text{Tr}_2(|\psi_{12}\rangle\langle\psi_{12}|) = \sum_{i=1}^{d_1} |r_i^{(1)}\rangle\langle r_i^{(1)}| \langle\phi_i^{(2)}|\phi_j^{(2)}\rangle. \tag{3.12}$$

Comparing this with (3.10), we see that:

$$\langle\phi_i^{(2)}|\phi_j^{(2)}\rangle = \delta_{ij} r_i^{(1)}.$$

After normalization we have:

$$|\phi_i^{(2)}\rangle = \sqrt{r_i^{(1)}} |r_i^{(2)}\rangle \in \mathbb{C}^2.$$

Replacing this in to (3.11), we get:

$$|\psi_{12}\rangle = \sum_{i=1}^{d_1} \sqrt{r_i^{(1)}} |r_i^{(1)}\rangle \otimes |r_i^{(2)}\rangle. \tag{3.13}$$

Which ends the proof. \square

The coefficients r_i are called Schmidt coefficients, and their multiplicity is known as Schmidt rank. Note that using the Schmidt form of a given vector ψ_{12} , the reduced density matrices are:

$$\begin{aligned}
\rho_1 &= \text{Tr}_2(\rho_{12}) = \sum_{i=1}^M r_i^{(1)} |r_i^{(1)}\rangle\langle r_i^{(1)}|, \\
\rho_2 &= \text{Tr}_1(\rho_{12}) = \sum_{i=1}^M r_i^{(1)} |r_i^{(2)}\rangle\langle r_i^{(2)}|,
\end{aligned}$$

one sees that they have the same eigenvalues $r_i^{(1)}$, with the same multiplicity.

3.3 Separable and Entangled States

Consider a vector state $|\Psi\rangle \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$, which is a tensor product of two vector states: $|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$, where $|\psi_1\rangle \in \mathbb{C}^{d_1}$ and $|\psi_2\rangle \in \mathbb{C}^{d_2}$. The corresponding density matrix is of the form:

$$\rho_\Psi = |\Psi\rangle\langle\Psi| = |\psi_1\rangle\langle\psi_1| \otimes |\psi_2\rangle\langle\psi_2| = \rho_1 \otimes \rho_2,$$

where $\rho_{1,2}$ are pure states projections. As we see the density matrix corresponding to a product vector state is itself a tensor product. Using this fact we can give a definition for a separable state:

Definition 9 [30] *A bipartite pure state ρ is separable if and only if it is the tensor product of the density matrices of its subsystems:*

$$\rho = \rho_1 \otimes \rho_2. \quad (3.14)$$

Otherwise it is an entangled pure state.

For a pure separable state, tracing over one subsystem gives a projector over the other subsystem, i.e. pure states:

$$\rho_1 = \text{Tr}_2(\rho_{12}) = \text{Tr}_2(\rho_1 \otimes \rho_2).$$

Examples of entangled pure states are the Bell states which are maximally entangled.

Example 5 Bell States

The following four symmetric vectors in $\mathbb{C}^2 \otimes \mathbb{C}^2$ are known as Bell basis vectors [40]:

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \quad (3.15)$$

$$|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle). \quad (3.16)$$

For instance consider the density matrix corresponding to the ρ_{Φ^+} :

$$\begin{aligned} \rho_{\Phi^+} &= \frac{1}{2}(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|) + \\ &\quad \frac{1}{2}(|0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0|), \end{aligned}$$

reduced density matrices are:

$$\rho_1 = \text{Tr}_2(\rho_{\Phi^+}) = \rho_2 = \text{Tr}_1(\rho_{\Phi^+}) = \frac{\mathbb{1}_2}{2},$$

which are maximally mixed states.

The following theorem provides a necessary and sufficient condition of separability for bipartite pure states, based on their Schmidt decomposition:

Theorem 2 *The pure vector state $|\psi_{12}\rangle$ is separable if and only if only one Schmidt coefficient is different from zero.*

Therefore the pure states, whose Schmidt decomposition contains more than one Schmidt coefficient, or in other words, their Schmidt rank is greater than one, are entangled.

Example 6 *According to Schmidt decomposition the following state is separable:*

$$|\psi_{12}\rangle\langle\psi_{12}| = |\psi_1\rangle\langle\psi_1| \otimes |\psi_2\rangle\langle\psi_2|$$

One can easily see that the von Neumann entropy is zero for the density matrix ρ_{12} , as well as the reduced density matrices ρ_1 and ρ_2 :

$$S(\rho_{12}) = S(\rho_1) = S(\rho_2) = 0.$$

Example 7 *The Schmidt rank of Bell states in (3.15) is 2, and their Schmidt coefficients are $\frac{1}{\sqrt{2}}$.*

The symmetric states in (3.32) are another example of entangled states, which Schmidt rank d .

3.3.1 Shannon entropy and von Neumann entropy

Example 5 is a clear indication that entanglement embodies correlations that have no classical counterpart. Indeed, the von Neumann entropy is for quantum states what the Shannon entropy [19] is for classical states, that is for probability distributions of stochastic variables. Let $X = \{x_j\}_{j=1}^d$ be a d -valued stochastic variable whose outcomes x_i occur with probabilities p_i , then the Shannon entropy of X is defined by

$$H(X) = - \sum_{i=1}^d p_i \log p_i . \quad (3.17)$$

One thus sees that the von Neumann entropy of density matrix ρ is nothing else than the Shannon entropy of its spectrum. However, the Shannon entropy of a composite system, described say by two stochastic variables $X_1 = \{x_i^{(1)}\}_{i=1}^{d_1}$ and $X_2 = \{x_j^{(2)}\}_{j=1}^{d_2}$ is always larger than the Shannon entropy of each of its two parties, that is

$$H(X_1, X_2) \geq \max\{H(X_1), H(X_2)\} , \quad (3.18)$$

where $H(X_1, X_2)$ is the Shannon entropies of the joint probability distribution $\pi_{1,2} = \{p(x_i^{(1)}, x_j^{(2)})\}$ and $H(X_{1,2})$ are the Shannon entropy of the reduced probability distributions $\pi_1 = \{p(x_i^{(1)})\}_{i=1}^{d_1}$, $\pi_2 = \{p(x_j^{(2)})\}_{j=1}^{d_2}$ with

$$p(x_i^{(1)}) = \sum_{j=1}^{d_2} p(x_i^{(1)}, x_j^{(2)}) , \quad p(x_j^{(2)}) = \sum_{i=1}^{d_1} p(x_i^{(1)}, x_j^{(2)}) . \quad (3.19)$$

This can be seen as follows: let us introduce the *conditional probability*

$$p(x_i^{(1)}|x_j^{(2)}) = \frac{p(x_i^{(1)}, x_j^{(2)})}{p(x_j^{(2)})} \quad (3.20)$$

that the outcome for X_1 be $x_i^{(1)}$ given that the outcome $x_j^{(2)}$ has been obtained and the *conditional entropy* of X_1 given X_2 , namely the following convex combination of Shannon entropies

$$H(X_1|X_2) = - \sum_{j=1}^{d_2} p(x_j^{(2)}) \sum_{i=1}^{d_1} p(x_i^{(1)}|x_j^{(2)}) \log p(x_i^{(1)}|x_j^{(2)}) \quad (3.21)$$

$$= H(X_1, X_2) - H(X_2) . \quad (3.22)$$

Then, the result follows because $H(X_1|X_2)$ and $H(X_2|X_1)$ are ≥ 0 and

$$H(X_1, X_2) = H(X_2) + H(X_1|X_2) = H(X_1) + H(X_2|X_1) . \quad (3.23)$$

Remark 2 *Unlike the Shannon entropy, the von Neumann entropy of subsystems can be larger than that of the total system. This fact indeed signals entanglement but, as we shall see, is not always implied by entanglement.*

One could now guess that quantum states either carry entanglement or classical correlations. It is not so: there can be separable states which are not simply classical correlated.

In order to understand this fact one has to introduce the so-called Quantum Discord of a given state. One starts by recalling that, using the conditional entropy, one can define the mutual information:

$$\mathfrak{J}(X_1 : X_2) = H(X_1) - H(X_1|X_2) \quad (3.24)$$

which measures the amount of information that is common to both classical stochastic variables. It can also be rewritten as:

$$\mathfrak{J}(X_1 : X_2) = H(X_1) + H(X_2) - H(X_1, X_2). \quad (3.25)$$

One can extend the notion of mutual information to quantum systems [13, 14]; To do so, starting from (3.25), one can simply replace the probability distributions of individual systems by reduced density matrices of subsystems:

$$\mathfrak{I}_{A:B}(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \quad (3.26)$$

However this generalization, in the case of expression (3.24) for classical mutual information, is not trivial; in fact, the definition of conditional entropy of quantum systems involves quantum measurement processes. Expressing the state of system A , when the state of system B is known, is equivalent to having done a set of measurements on system B . Therefore the post-measurement state of system A , after performing measurement Π_i^B will be:

$$\rho_{A|\Pi_i^B} = \frac{1}{p_i}(\mathbb{1}_d \otimes \Pi_i^B \rho_{AB} \mathbb{1}_d \otimes \Pi_i^B), \quad p_i = \text{Tr}(\rho_B \Pi_i^B). \quad (3.27)$$

Given a complete set of orthogonal measurements $\Pi = \{\Pi_i, i = 1, \dots, d\}$, $\sum_i \Pi_i = \mathbb{1}_d$, $\Pi_i \Pi_j = \delta_{ij} \Pi_i$, on system B , the conditional entropy will be defined as [50]:

$$S(\rho_A|\Pi^B) := \sum_i p_i S(\rho_{A|\Pi_i^B}). \quad (3.28)$$

With this definition of quantum conditional entropy, \mathfrak{I} in (3.24) reads:

$$\mathfrak{I}_{A:B}(\rho_{AB}) := S(\rho_A) - S(\rho_A|\Pi^B). \quad (3.29)$$

Unlike in the classical case where the two expressions for mutual information, \mathfrak{I} and \mathfrak{J} , are equal, in quantum case, the two expressions are not in general the same [50, 28]. Their difference depends on the set of measurements performed on system B which can be removed by minimizing it over all possible sets $\{\Pi^B\}$, and define the minimum as the Quantum Discord of the given state ρ_{AB} :

$$\begin{aligned} D_{A:B}(\rho_{AB}) &= \min_{\{\Pi^B\}} [\mathfrak{I}_{A:B}(\rho - AB) - \mathfrak{I}_{A:B}(\rho_{AB})] \\ &= \min_{\{\Pi^B\}} [S(\rho_B) + S(\rho_A|\Pi^B) - S(\rho_{AB})]. \end{aligned} \quad (3.30)$$

The Quantum Discord measures the non-classical correlations which are present in a quantum state: it is 0 for separable states with only classical correlations, and maximal for entangled states which are extremely non-classical correlated. However, there exist separable, that is non-entangled, states with non-zero Quantum Discord.

3.3.2 Mixed entangled states

For mixed states the notion of separability extends as follows:

Definition 10 *A mixed state ρ is separable if and only if it cannot be written as a convex combination of product states:*

$$\rho = \sum_i p_i \rho_1^i \otimes \rho_2^i, \quad \sum_i p_i = 1, \quad p_i \geq 0. \quad (3.31)$$

Otherwise, it is an entangled mixed state.

Example 8 *Consider a bipartite system $S = S_1 + S_2$, where the Hilbert spaces of the subsystems are of the same dimension. Consider the symmetric states [4]:*

$$|\Psi_+^d\rangle = \frac{1}{d} \sum_{j=1}^d |j\rangle \otimes |j\rangle, \quad (3.32)$$

where $|j\rangle$, $j = 1, 2, \dots, d$ is any fixed orthonormal basis in \mathbb{C}^d . The corresponding projectors are:

$$P_+^d \equiv |\Psi_+^d\rangle\langle\Psi_+^d| = \sum_{i,j=1}^d |i\rangle\langle j| \otimes |i\rangle\langle j|. \quad (3.33)$$

Also in this case reduced density matrices are maximally mixed:

$$\rho_1 = \rho_2 = \frac{1}{2} \sum_{i=1}^d |i\rangle\langle i| = \frac{\mathbb{1}_d}{d}$$

which means that $|\Psi_+^d\rangle$ is entangled. We shall refer to this set of symmetric states in the future.

Example 9 Werner States

Werner states in $\mathbb{C}^2 \otimes \mathbb{C}^2$ are constructed as follows [56, 74]:

$$\rho_\alpha = \alpha |\Psi^-\rangle\langle\Psi^-| + \frac{1-\alpha}{4} \mathbb{1}_2 \otimes \mathbb{1}_2, \quad -\frac{1}{3} \leq \alpha \leq 1. \quad (3.34)$$

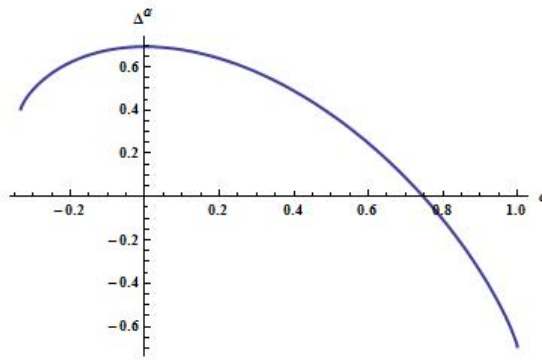
Where Ψ^- is one of the Bell states, introduced in (3.15). In the basis where σ_3 is diagonal, Werner states can be represented by the following matrix:

$$\rho_\alpha = \frac{1}{4} \begin{pmatrix} 1-\alpha & 0 & 0 & 0 \\ 0 & 1+\alpha & -2\alpha & 0 \\ 0 & -2\alpha & 1+\alpha & 0 \\ 0 & 0 & 0 & 1-\alpha \end{pmatrix}$$

The above range for α is to guarantee the positivity of ρ_α . Werner states are entangled for $\alpha \geq \frac{1}{3}$. The reduced density matrices are:

$$(\rho_\alpha)_1 = (\rho_\alpha)_2 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

As we see, also in this case the reduced density matrices are maximally mixed and therefore their von Neumann entropy is maximum. Indeed, by checking how the function $\Delta^\alpha = S(\rho_\alpha) - \log 2$ behaves:



one might then think that entangled Werner states are detected by checking whether their entropy is smaller than the entropy of one of the parties. We shall later see a counterexample to such a claim.

However the situation in case of pure states is completely clear thanks to Schmidt decomposition, deciding if a given mixed state is entangled or separable is still an open problem, even in case of bipartite systems. In the following chapters we will study how to partially answer this question.

Chapter 4

Positive and Completely Positive Maps

Physical transformations of Quantum systems are described by linear maps, either on the space of states or, dually, on the algebra of observables. If a linear map on the convex space of states describes a physical transformation (that, of course, transforms physical states into physical states), then it must transform density matrices into density matrices. It must thus be positivity preserving and trace preserving. However, though necessary, positivity is not sufficient to guarantee the physical consistency of a linear map. Via coupling the system affected by the transformation with a suitable unaffected ancilla, the existence of entanglement between the two subsystem requires the map to be also completely positive. In this section we will see how these constraints can take part in the challenge of detecting entangled states.

4.1 Positivity and Complete Positivity

Definition 11 *Positive Map* A linear map $\Lambda : M_m(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ is positive if and only if $M_n(\mathbb{C}) \ni \Lambda[X] \geq 0$ for all $X \in M_m(\mathbb{C})$ [31, 51]. The set of positive maps is denoted by \mathcal{P} .

Example 10 *Trace Map*

The Trace Map, introduced in (2.7), is a positive map, as it is the sum of the eigenvalues of an operator. Therefore if $M_d(\mathbb{C}) \ni X = \sum_i x_i |X_i\rangle\langle x_i|$, $x_i \geq 0$, then

$$\text{Tr} : X \longmapsto \text{Tr}(X)\mathbb{1}_d = \left(\sum_i x_i\right)\mathbb{1}_d \geq 0, \quad \forall X \in M_d(\mathbb{C}).$$

Example 11 Transposition Map

Transposition map is another example of positive maps:

$$T_d : M_d(\mathbb{C}) \ni X \longmapsto X^T \in M_d(\mathbb{C}) \quad (4.1)$$

with respect to a fixed orthonormal basis. Given a matrix $X = [X_{ij}]$, its transposed is $X^T = [X_{ji}]$. Since transposing an operator does not affect its spectrum, it preserves positivity, which means that it is a positive map.

Example 12 Transposition Map on $M_2(\mathbb{C})$

Using the Pauli matrices as an orthonormal basis set in $M_2(\mathbb{C})$, similarly to the Trace Map in Example 3, we can also write the Transposition Map as [4]:

$$M_2(\mathbb{C}) \ni X \longmapsto T_2[X] := \sum_{\alpha=0}^3 \varepsilon_\alpha \sigma_\alpha X \sigma_\alpha \quad (4.2)$$

where $\varepsilon_\alpha = 1$ when $\alpha \neq 2$, whereas $\varepsilon_2 = -1$. In terms of the map S_α as in (2.12), the Transposition Map is of the following form:

$$T[X] = \sum_{\alpha=0}^3 \varepsilon_\alpha S_\alpha[X]. \quad (4.3)$$

One can thus check that, in the standard representation, $T[\sigma_\alpha] = \sigma_\alpha$, $\alpha \neq 2$ and $T[\sigma_2] = -\sigma_2$, which is exactly what transposition does in the chosen representation.

Definition 12 K -positivity

A linear map $\Lambda : M_m(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ is k -positive if and only if $\text{id}_k \otimes \Lambda : M_k(\mathbb{C}) \otimes M_m(\mathbb{C}) \rightarrow M_k(\mathbb{C}) \otimes M_n(\mathbb{C})$ is a positive map, where $k \in \mathbb{N}$. \mathcal{P}_k denotes the set of k -positive maps [75, 63].

Definition 13 Complete Positivity

If a linear map Λ is k -positive for every $k \in \mathbb{N}$, it is called completely positive. The set of completely positive maps is denoted by \mathcal{CP} .

A linear map Λ is a CPU map if it is both CP and unital, that is $\Lambda[\mathbb{1}] = \mathbb{1}$.

The following theorem fully characterizes the completely positive maps:

Theorem 3 Kraus representation

A map $\Lambda : M_m(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ is completely positive if and only if there exists a set of operators $\{K_i\}$, such that [43, 17, 3]:

$$\Lambda[X] = \sum_i K_i^\dagger X K_i, \quad \forall X \in M_m(\mathbb{C}). \quad (4.4)$$

The operators $M_{n \times m}(\mathbb{C}) \ni K_i : \mathbb{C}^n \rightarrow \mathbb{C}^m$, are called Kraus operators. Furthermore, such a map is CPU if and only if $\sum_i K_i^\dagger K_i = \mathbb{1}$.

Theorem 3 concerns the action of maps on operators (Heisenberg representation); however, one is often interested in how states transform (Schrödinger representation). This fact can easily be derived by duality.

Definition 14 Dual map

For any map $\Lambda : M_m(\mathbb{C}) \rightarrow M_n(\mathbb{C})$, its dual map $\Lambda^T : M_n(\mathbb{C}) \rightarrow M_m(\mathbb{C})$ is defined as [4]:

$$\mathrm{Tr}(\Lambda[X]\rho) = \mathrm{Tr}(X\Lambda^T[\rho]) \quad (4.5)$$

for every $X \in M_m(\mathbb{C})$ and $\rho \in \mathbb{S}_n$.

The Kraus representation of the dual map $\Lambda^T : M_n(\mathbb{C}) \rightarrow M_m(\mathbb{C})$ will be:

$$\Lambda^T[\rho] = \sum_i K_i \rho K_i^\dagger. \quad (4.6)$$

Therefore, one can see that CPU maps and trace-preserving maps are dual:

$$\Lambda \text{ CPU} \iff \Lambda^T \text{ Trace-preserving.}$$

Consider a CP map $\Lambda : M_n(\mathbb{C}) \rightarrow M_n(\mathbb{C})$, with its Kraus representation as in (4.6). By choosing a Hilbert-Schmidt ONB set $\{F_j\}_{j=1}^{n^2} \in M_n(\mathbb{C})$, the Kraus operators K_i can be written as:

$$K_i = \sum_{j=1}^{n^2} c_{ij} F_j.$$

Therefore the Kraus representation of Λ will be:

$$\begin{aligned} \Lambda[X] &= \sum_i \sum_{j,k=1}^{n^2} c_{ij} \overline{c_{ik}} F_j X F_k^\dagger \\ &= \sum_{j,k=1}^{n^2} f_{jk} F_j X F_k^\dagger. \end{aligned} \quad (4.7)$$

Where $f_{jk} = \sum_i c_{ij} \overline{c_{ik}}$ are the entries of a positive matrix $F = [f_{jk}] \in M_{n^2}(\mathbb{C})$. The representation (4.7) of a CP map Λ is also known as Canonical Kraus Representation [7]. Indeed the Kraus form (4.6), is obtained by diagonalizing this general form.

One should also note that the set of Kraus operators $\{K_i\}$ is not unique, however, each two sets of Kraus operators corresponding to the same CP

map, can be related by a unitary matrix. Indeed, given a canonical Kraus form, of a CP map Λ :

$$\Lambda[X] = \sum_{j,k=1}^{n^2} g_{jk} F_j X F_k^\dagger, \quad 0 \leq G = [g_{jk}] \in M_{n^2}(\mathbb{C}). \quad (4.8)$$

Using the diagonal form of G in terms of its eigenvectors:

$$G = \sum_{l=1}^{n^2} g_l |g_l\rangle \langle g_l|, \quad g_l \geq 0,$$

the matrix elements g_{jk} are:

$$g_{jk} = \langle j|G|k\rangle = \sum_{l=1}^{n^2} g_l g_{lj} \overline{g_{lk}}.$$

Replacing this in (4.8), we get:

$$\begin{aligned} \Lambda[X] &= \sum_{j,k,l=1}^{n^2} g_l g_{lj} \overline{g_{lk}} F_j X F_k^\dagger \\ &= \sum_{l=1}^{n^2} \left(\sum_{j=1}^{n^2} \sqrt{g_l} g_{lj} F_j \right) X \left(\sum_{k=1}^{n^2} \sqrt{g_l} \overline{g_{lk}} F_k^\dagger \right) \\ &= \sum_{l=1}^{n^2} K_l X K_l^\dagger. \end{aligned}$$

Any hermiticity and trace-preserving linear map $\Lambda : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ can be written as [27]:

$$\Lambda[\rho] = \sum_{i,j=1}^d a_{ij} F_i^\dagger \rho F_j, \quad (4.9)$$

where $\sum_{i,j=1}^d a_{ij} F_i^\dagger F_j = \mathbb{1}_d$. This can be shown as follows: consider the d^2 elementary linear maps $X \rightarrow \mathcal{F}_{ij}[X] = F_i X F_j^\dagger$ and define on the linear space \mathcal{L} of maps $\Lambda : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ the scalar product

$$\langle\langle \Lambda_1 | \Lambda_2 \rangle\rangle = d^2 \text{Tr} \left(\text{id}_d \otimes \Lambda_1 [P_+^d]^\dagger \text{id}_d \otimes \Lambda_2 [P_+^d] \right), \quad (4.10)$$

where P_+^d is the completely symmetric projection (3.33). It turns out that $\langle\langle \mathcal{F}_{ij} | \mathcal{F}_{kl} \rangle\rangle = \delta_{ik} \delta_{jl}$; therefore, being orthogonal, the \mathcal{F}_{ij} constitute an

orthonormal basis in \mathcal{L} . As we shall soon see, the scalar product defined above is strictly related to the notion of Choi matrix.

When the map Λ is completely positive the matrix $A = [a_{ij}]$ is positive, while in case of positive maps, the matrix $A = [a_{ij}]$ is no longer positive, but with separating the positive and negative eigenvalues, one can write a positive map Λ as the difference of two completely positive maps:

$$\Lambda[\rho] = \sum_{a_l \geq 0} a_l K_l^\dagger \rho K_l - \sum_{a_l < 0} |a_l| K_l^\dagger \rho K_l. \quad (4.11)$$

Based on the complete characterization of the structure of CP maps, the following concept provides a simple test to determine if a given map is CP or not [52].

Definition 15 Choi-Jamiołkowski isomorphism

Given a linear map $\Lambda : M_n(\mathbb{C}) \mapsto M_m(\mathbb{C})$, its Choi matrix is the matrix on $\mathbb{C}^n \otimes \mathbb{C}^m$ defined by [18, 2, 55]

$$M_{n \times m}(\mathbb{C}) = M_n(\mathbb{C}) \otimes M_m(\mathbb{C}) \ni C_\Lambda = \text{id}_n \times \Lambda[P_+^{(n)}], \quad (4.12)$$

where $P_+^{(n)}$ projects onto the completely symmetric state

$$|\Psi^{(n)}\rangle = \frac{1}{n} \sum_{i=1}^n |e_i\rangle \otimes |e_i\rangle, \quad \{|e_i\rangle\}_{i=1}^n \text{ ONB in } \mathbb{C}^n.$$

It is useful to see how the Choi matrix of the map Λ looks like:

$$C_\Lambda = \begin{pmatrix} \Lambda[|1\rangle\langle 1|] & \Lambda[|1\rangle\langle 2|] & \cdots & \Lambda[|1\rangle\langle m|] \\ \Lambda[|2\rangle\langle 1|] & \Lambda[|2\rangle\langle 2|] & \cdots & \Lambda[|2\rangle\langle m|] \\ \vdots & \vdots & \ddots & \vdots \\ \Lambda[|m\rangle\langle 1|] & \Lambda[|m\rangle\langle 2|] & \cdots & \Lambda[|m\rangle\langle m|] \end{pmatrix}.$$

The Choi matrix, C_Λ , is uniquely defined by Λ since its entries $C_{\Lambda(ij,pq)}$ with respect to an orthonormal basis of the form $|e_i\rangle \otimes |f_j\rangle \in \mathbb{C}^n \otimes \mathbb{C}^m$ are

$$C_{\Lambda(ij,pq)} = \langle e_i \otimes f_j | C_\Lambda | e_p \otimes f_q \rangle = \frac{1}{n} \langle f_j | \Lambda[|e_i\rangle\langle e_p|] | f_q \rangle. \quad (4.13)$$

It turns out that the map $J : \Lambda \mapsto J[\Lambda] = C_\Lambda$ from the vector space $\mathcal{L}_{n,m}$ of linear maps onto the matrix algebra $M_{n \times m}(\mathbb{C})$ is invertible map and defines the so called Jamiołkowski isomorphism. In fact, any $\Lambda : M_n(\mathbb{C}) \mapsto M_m(\mathbb{C})$ is determined by its action on matrix units $|e_i\rangle\langle e_j|$ which is in turn completely characterized by the matrix elements in (4.13). Therefore, given

$C \in M_{n \times m}(\mathbb{C})$ this uniquely determines a linear map $\Lambda_C : M_n(\mathbb{C}) \mapsto M_m(\mathbb{C})$ such that

$$\langle f_j | \Lambda_C [|e_i\rangle\langle e_p|] f_q \rangle = C(ij, pq) .$$

Equipped with these tools one can readily prove the following

Theorem 4 *Every linear map $\Lambda : M_n(\mathbb{C}) \mapsto M_m(\mathbb{C})$ with positive semi-definite Choi matrix $C_\Lambda \geq 0$ is completely positive and vice versa [18, 32].*

Proof: By definition of complete positivity, $\text{id}_n \otimes \Lambda$ is positive if Λ is completely positive, and thus $C_\Lambda = \text{id}_n \otimes \Lambda[P^{(n)}] \geq 0$.

Vice versa, if $M_{n^2}(\mathbb{C}) \ni C_\Lambda \geq 0$, then it can be spectralized as

$$C_\Lambda = \sum_{j=1}^{n^2} c_j |c_j\rangle\langle c_j| , \quad c_j \geq 0 .$$

The eigenvectors $|c_j\rangle \in \mathbb{C}^n \otimes \mathbb{C}^n$ can be conveniently rewritten using the completely symmetric vector as follows:

$$|c_j\rangle = \sum_{p,q=1}^n c_j^{pq} |e_p\rangle \otimes |e_q\rangle = \frac{1}{n} \sum_{p=1}^n |e_p\rangle \otimes C_j |e_p\rangle = \mathbb{1}_n \otimes C_j |\Psi_+^{(n)}\rangle ,$$

with the matrix $C_j \in M_n(\mathbb{C})$ defined by

$$\langle e_q | C_j |e_p\rangle = n c_j^{pq} .$$

Therefore, one can rewrite

$$C_\Lambda = \sum_{j=1}^{n^2} \mathbb{1}_n \otimes K_j P_+^{(n)} \mathbb{1}_n \otimes K_j^\dagger , \quad K_j = \sqrt{L_j} \quad C_j \in M_n(\mathbb{C}) ,$$

Then, by the Jamiołkowski isomorphism, $\Lambda[X] = \sum_{j=1}^{n^2} K_j X K_j^\dagger$ can be written in the Kraus-Stinespring form and is thus completely positive. \square

Remark 3 *In general, positive maps $\Lambda : B(\mathbb{H}) \mapsto B(\mathbb{H})$ on bounded operators are completely positive if $\text{id}_d \otimes \Lambda$ for all $d \geq 2$. However, in the finite dimensional cases, when $B(\mathbb{H}) = M_n(\mathbb{C})$, the above result shows that one needs check the positivity of $\text{id}_n \otimes \Lambda$, only.*

Example 13 Consider the Trace Map $\Phi : M_d(\mathbb{C}) \mapsto M_d(\mathbb{C})$:

$$\Phi(X) = \frac{1}{d} \text{Tr}(X) \mathbb{1}_d. \quad (4.14)$$

It is easy to see that this map is CPU; indeed:

$$\Phi[\mathbb{1}_d] = \mathbb{1}_d.$$

It's Choi matrix is:

$$\begin{aligned} C_\Phi &= \frac{1}{d} \sum_{ij} |i\rangle\langle j| \otimes \text{Tr}(|i\rangle\langle j|) |i\rangle\langle j| \\ &= \frac{1}{d} \sum_{ij} |i\rangle\langle i| \otimes |i\rangle\langle i| = \frac{1}{d} \mathbb{1}_{d^2} \geq 0. \end{aligned}$$

The positivity of Choi matrix shows the Trace Map is completely positive.

Definition 16 Block Positive Operator

Given a matrix $A \in M_d^2(\mathbb{C})$, using any fixed orthonormal basis, we can write it as $A = \sum_{i,j} |i\rangle\langle j| \otimes A_{ij}$, where $A_{ij} \in M_d(\mathbb{C})$, for $\forall 1 \leq i, j \leq d$. Then matrix A is said to be block-positive if and only if for all $|\phi\rangle$ and $|\psi\rangle \in \mathbb{C}^d$, the following holds:

$$\begin{aligned} \langle \phi \otimes \psi | A | \phi \otimes \psi \rangle &= \langle \phi | \left(\sum_{i,j} \langle \psi | A_{ij} | \psi \rangle |i\rangle\langle j| \right) | \phi \rangle \\ &= \langle \phi | \begin{pmatrix} \langle \psi | A_{11} | \psi \rangle & \langle \psi | A_{12} | \psi \rangle & \cdots & \langle \psi | A_{1d} | \psi \rangle \\ \langle \psi | A_{21} | \psi \rangle & \langle \psi | A_{22} | \psi \rangle & \cdots & \langle \psi | A_{2d} | \psi \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \psi | A_{d1} | \psi \rangle & \langle \psi | A_{d2} | \psi \rangle & \cdots & \langle \psi | A_{dd} | \psi \rangle \end{pmatrix} | \phi \rangle \\ &\geq 0. \end{aligned}$$

In another word, block-positivity of A is equivalent to positivity of $\langle \psi | A_{ij} | \psi \rangle$ for $\forall |\psi\rangle \in \mathbb{C}^d$.

Theorem 5 A linear map $\Lambda : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ is positive if and only if its Choi matrix is block-positive [39, 42]:

$$\langle \psi \otimes \varphi | \mathbb{1}_d \otimes \Lambda[P_d^+] | \psi \otimes \varphi \rangle \geq 0$$

for every $|\psi\rangle$ and $|\varphi\rangle$ in \mathbb{C}^d .

Proof: Given a positive map $\Lambda : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$, by definition, it preserves positivity of matrices in $M_d(\mathbb{C})$:

$$\langle \phi \Lambda[|\psi\rangle\langle\psi|] \phi \rangle \geq 0 \quad \forall |\psi\rangle, |\phi\rangle \in \mathbb{C}^d. \quad (4.15)$$

Given an ONB $\{|i\rangle\}_{i=1}^d \in \mathbb{C}^d$, then any vector $|\psi\rangle$ is $|\psi\rangle = \sum_{i=1}^d \psi_i |i\rangle$, where $\psi_i = \langle i|\psi\rangle$. Using this (4.15) is

$$\begin{aligned} \langle \phi \Lambda[|\psi\rangle\langle\psi|] \phi \rangle &= \sum_{i,j=1}^d \psi_i \psi_j^* \langle \phi \Lambda[|i\rangle\langle j|] \phi \rangle \\ &= \langle \psi^* \otimes \phi | \sum_{i,j=1}^d |i\rangle\langle j| \otimes \Lambda[|i\rangle\langle j|] | \psi^* \otimes \phi \rangle \\ &= \langle \psi^* \otimes \phi | \mathbb{1}_d \otimes \Lambda[P_d^+] | \psi^* \otimes \phi \rangle \\ &= \langle \psi^* \otimes \phi | C_\Lambda | \psi^* \otimes \phi \rangle \\ &\geq 0. \end{aligned}$$

Which shows that the positivity of Λ is equivalent to the block positivity of its Choi matrix and vice versa. \square

Example 14 Consider the Transposition Map $T : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$, in (4.1). Its Choi matrix is:

$$C_T = \frac{1}{d} \sum_{i,j} |i\rangle\langle j| \otimes |j\rangle\langle i|.$$

Which coincides with the definition of the Flip operator:

$$V = \sum_{i,j=1}^d |i\rangle\langle j| \otimes |j\rangle\langle i| = d(\mathbb{1}_d \otimes T)P_d^+, \quad (4.16)$$

which is also that

$$V|\psi_1 \otimes \psi_2\rangle = |\psi_2 \otimes \psi_1\rangle.$$

Since $V^2 = \text{id}_d$, its eigenvalues are ± 1 .

For any vector $|\phi\rangle$ and $|\psi\rangle \in \mathbb{C}^d$, we have:

$$\begin{aligned} \langle \psi \otimes \phi | C_T | \psi \otimes \phi \rangle &= \langle \psi \otimes \phi | \left(\sum_{i,j} |i\rangle\langle j| \otimes |j\rangle\langle i| \right) | \psi \otimes \phi \rangle \\ &= \sum_{i,j} \langle \phi | i \rangle \langle j | \phi \rangle \langle \psi | j \rangle \langle i | \psi \rangle \\ &= \sum_i \langle \phi | i \rangle \langle i | \psi \rangle \sum_j \langle j | \phi \rangle \langle \psi | j \rangle \\ &= |\langle \psi | \phi \rangle|^2 \\ &\geq 0. \end{aligned}$$

Since C_T has negative eigenvalues, $C_T \not\geq 0$, Transposition Map is not completely positive.

Example 15 Reduction Map

In the next chapter we will introduce a number of positive maps, which are known to be able to detect some entangled states, one of them is called Reduction Map [32], which has the following form:

$$\Lambda_R = \text{Tr}_d - \text{id}_d \quad (4.17)$$

The Reduction map is positive: as the trace is the sum of the eigenvalues, which are non-negative as ρ is a density matrix, therefore $\text{Tr}_d[\rho] \geq 0$. Let $|\psi_i\rangle$ be eigenvectors of ρ with eigenvalues λ_i , then using the spectral decomposition of ρ , we have:

$$\begin{aligned} \Lambda_R[\rho] &= \left(\sum_i \lambda_i \right) \mathbb{1}_d - \sum_j \lambda_j |\psi_j\rangle\langle\psi_j| \\ &= \sum_j \left[\left(\sum_i \lambda_i \right) - \lambda_j \right] |\psi_j\rangle\langle\psi_j|. \end{aligned}$$

Since $\sum_i \lambda_i \geq \lambda_j$, $\Lambda_R[\rho]$ is a positive matrix. On the other hand, the Choi matrix of this map is:

$$\begin{aligned} C_{\Lambda_R} &= \text{id}_d \otimes \Lambda_R[P_d^+] = \mathbb{1}_{d^2} - dP_d^+ \\ \text{where } P_d^+ &= \frac{1}{d} \sum_{i,j=1}^d |i\rangle\langle j| \otimes |i\rangle\langle j|. \end{aligned}$$

Thus, C_{Λ_R} has one negative eigenvalue $1-d$ and is not positive semi-definite. Therefore, the Reduction Map is not completely positive.

In what follows, we shall explain the results given in [65], which is extensively used in the last chapter of this thesis.

Theorem 6 Let Tr be the Trace Map. Then, given any positive map $\phi : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ can be written as

$$\phi = \frac{1}{c} (\text{Tr} - \phi_{cp}), \quad (4.18)$$

where $c \geq 0$ is a positive constant and $\phi_{cp} : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ a completely positive map.

Proof:

Let ϕ be a self-adjoint map, that is $\phi[A^\dagger] = (\phi[A])^\dagger$, then its Choi matrix C_ϕ is self-adjoint as well. Therefore C_ϕ can be written as difference of two positive matrices, i.e. $C_\phi = C_\phi^+ - C_\phi^-$ where $C_\phi^+ C_\phi^- = 0$. Let $\mu \geq 0$ be the smallest positive number such that

$$\mu \mathbb{1} \geq C_\phi = C_\phi^+ - C_\phi^-.$$

The above inequality is satisfied by choosing $c = \|C_\phi^+\|$, which is the greatest eigenvalue of C_ϕ^+ .

Now consider the following positive matrix:

$$C_\phi^\mu = \mathbb{1} - \frac{1}{\mu} C_\phi \geq 0. \quad (4.19)$$

The completely positive map ϕ_{cp} of which C_ϕ^μ is the Choi matrix reads

$$\phi_{cp} = \text{Tr} - \frac{1}{\mu} \phi, \quad (4.20)$$

Now, re-arranging the (4.20), we have:

$$\phi = \frac{1}{c} (\text{Tr} - \phi_{cp}). \quad (4.21)$$

Note that the only assumption was to consider the map ϕ to be self-adjoint. Therefore any self-adjoint map can be written as in (4.21). Taking into account that the set of positive maps is a subset of self-adjoint maps completes the proof. \square

Example 16 We have seen in Example 3 that the transposition on $M_2(\mathbb{C})$ can be represented as

$$\begin{aligned} M_2(\mathbb{C}) \ni X \mapsto T[X] &= \frac{1}{2} \sum_{\alpha=0}^3 \varepsilon_\alpha S_\alpha[X], \\ S_\alpha[X] &= \sigma_\alpha X \sigma_\alpha, \quad \varepsilon_\alpha = (1, 1, -1, 1). \end{aligned} \quad (4.22)$$

Therefore, on $M_4(\mathbb{C})$,

$$\begin{aligned} M_4(\mathbb{C}) \ni X \mapsto T[X] &= \frac{1}{4} \sum_{\alpha, \beta=0}^3 \varepsilon_\alpha \varepsilon_\beta S_{\alpha\beta}[X], \\ S_{\alpha\beta}[X] &= \sigma_{\alpha\beta} X \sigma_{\alpha\beta}, \quad \sigma_{\alpha\beta} = \sigma_\alpha \otimes \sigma_\beta. \end{aligned} \quad (4.23)$$

Notice that the transposition is not written in the Kraus form (4.6) as the products $\varepsilon_\alpha \varepsilon_\beta = -1$ whenever $\alpha \neq \beta = 2$ or $\beta \neq \alpha = 2$.

On the other hand, the completely positive trace map Tr on $M_2(\mathbb{C})$ has the following Kraus representation:

$$\text{Tr}[X] = \frac{1}{2} \sum_{\alpha=0}^3 S_\alpha[X], \quad X \in M_2(\mathbb{C}), \quad (4.24)$$

Then, on $M_4(\mathbb{C})$, the trace map has the Kraus form (4.6):

$$M_4(\mathbb{C}) \ni X \mapsto \text{Tr}[X] = \frac{1}{4} \sum_{\alpha,\beta=0}^3 S_{\alpha\beta}[X]. \quad (4.25)$$

We would like to write the transposition map as in the form suggested by Theorem 6:

$$\Lambda = \mu(\text{Tr} - \Lambda^{CP}). \quad (4.26)$$

When Λ is the transposition map on $M_4(\mathbb{C})$, the CP maps ϕ_{CP} in (4.26) are easily found: the linear map

$$\text{Tr} - \frac{1}{\mu} \text{T} = \frac{1}{4} \sum_{\alpha,\beta=0}^3 \left(1 - \frac{\varepsilon_\alpha \varepsilon_\beta}{\mu} \right) S_{\alpha\beta},$$

is of the form (4.6), thus CP, if and only if $\mu \geq 1$. The smallest choice, $\mu = 1$, yields the completely positive map

$$\Lambda^{CP} = \frac{1}{2} \left(\sum_{\alpha \neq 2} S_{\alpha 2} + \sum_{\beta \neq 2} S_{2\beta} \right). \quad (4.27)$$

4.2 Entanglement and Positive Maps

As we have seen the structure of completely positive maps is wholly understood via the Kraus representation. Moreover Choi's theorem provides a technique to sort them out. Instead, as soon as one is dealing with positive maps, the situation becomes much less clear due to the lack of a complete structural representation of them. As we will see, only in low dimensions, when $d_1 \times d_2 \leq 6$, the structure of positive maps is under control [75, 63]. While in higher dimensions these maps are only partially understood [20, 21, 38, 70, 72, 48].

From a physical point of view, it turns out that a linear map which describes a physical transformation needs not to be only positive but completely positive [47]: since the eigenvalues of a system in statistical interpretation represent the probabilities, when a linear map describes a physical transformation, it has to preserve the positivity of the spectrum of the physical system, otherwise a negative eigenvalue representing a probability brings up a contradiction. As we have seen, by Definition 13 any extension of completely positive maps does this job. However this might not be true in general if the transformation is described by a positive, not CP, map. While the extension of positive maps preserves the positivity of separable states, it can fail when the subsystems are entangled. Consider a bipartite separable state which is a convex combination of tensor product of states its subsystems:

$$\rho = \sum_{i=1} p_i \rho_i^1 \otimes \rho_i^2 \quad p_i \geq 0, \quad \sum_i p_i = 1. \quad (4.28)$$

The action of $\text{id}_k \otimes \Lambda$ when Λ is a positive map gives:

$$\rho' = (\text{id}_k \otimes \Lambda)[\rho] = \sum_{i=1} p_i \text{id}_k[\rho_i^1] \otimes \Lambda[\rho_i^2].$$

The positivity of Λ guarantees that $\Lambda(\rho_i^2)$ and therefore ρ' , remains a positive state. But if the state ρ is not separable it cannot be written as (4.28), and consequently, for a generic ρ and k , $(\text{id}_k \otimes \Lambda)[\rho]$ is positive only if Λ is completely positive.

However, though positive maps cannot be used to describe physical transformations, they provide a new powerful theoretical approach to detect the entanglement. Indeed, if a given state ρ does not remain positive under the action of an extended positive maps, it must be entangled:

$$(\text{id}_k \otimes \Lambda)[\rho] \not\geq 0 \quad \Rightarrow \quad \rho \quad \text{entangled.}$$

The prototype of positive, but not completely positive map is transposition. In the following example we show that the extension of this map fails to be k -positive already when k is equal to 2, which means that it is not a complete positive map. In other words, though a positive matrix remains positive after being transposed, it might not be positive after being partially transposed.

Example 17 *Take one of the maximally entangled Bell states, introduced*

in (3.15), $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, its density matrix is:

$$\rho_{\Phi^+} = |\Phi^+\rangle\langle\Phi^+| = \frac{1}{2} \left(\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{array} \right)$$

The action of $\mathbb{1}_2 \otimes \mathbb{T}$ on this state is to transposing each block of the matrix, the result is the following matrix:

$$(\mathbb{1}_2 \otimes \mathbb{T})\rho_{\Phi^+} = \frac{1}{2} \left(\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right)$$

which has a negative eigenvalue $-\frac{1}{2}$.

According to Partial Transposition, the states can be divided into two classes: those which remain positive under this map, called PPT states, and those which turn out to have at least one negative eigenvalue after being partially transposed, known as NPT states.

The following class of positive maps has been used to classify these maps in low dimensional Hilbert spaces.

Definition 17 Decomposable Map

A positive map $\Lambda : M_d(\mathbb{C}) \longrightarrow M_d(\mathbb{C})$ is decomposable if and only if it can be written as [64]:

$$\Lambda = \Gamma_1 + \Gamma_2 \circ \mathbb{T}_d \tag{4.29}$$

where Γ_1 and Γ_2 are complete positive maps.

Theorem 7 All the positive maps $\Lambda : M_{d_1}(\mathbb{C}) \longrightarrow M_{d_2}(\mathbb{C})$ where $d_1 \times d_2 \leq 6$ are decomposable [75, 64].

Example 18 The reduction map $\Lambda_R : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ in (4.17) is decomposable [32].

The Choi matrix of this map reads:

$$C_{\Lambda_R} = \mathbb{1} \otimes \Lambda_R[P_d^+] = \mathbb{1}_{d^2} - dP_d^+$$

where $P_d^+ = \frac{1}{d} \sum_{i,j=1}^{d^2} |i\rangle\langle j| \otimes |i\rangle\langle j|.$

Its partial transposition with respect to the second subsystem yields:

$$\begin{aligned} C_{\Lambda_R}^{\mathbb{T}_2} &= (\mathbb{1}_d \otimes \mathbb{T}_d) \circ (\mathbb{1}_d \otimes \Lambda_R)[P_d^+] \\ &= (\mathbb{1}_d \otimes \mathbb{T} \circ \Lambda_R)[P_d^+] = \frac{1}{d}(\mathbb{1}_{d^2} - V). \end{aligned} \quad (4.30)$$

Since the flip operator V , introduced in (4.16), has eigenvalues ± 1 , it implies that $C_{\Lambda_R}^{\mathbb{T}_2}$ has no negative eigenvalue and therefore is a positive matrix, whence the corresponding map $\Lambda' = \mathbb{T}\Lambda_R$ is completely positive, according to Theorem 4. Furthermore, since $\Lambda_R = \mathbb{T}\Lambda'$ where Λ' is CP, results decomposable.

In the next chapters we will see how and under which conditions positive maps can detect the entanglement.

Chapter 5

Detecting Entanglement

In the previous chapter we have seen formal necessary and sufficient conditions for separability, practically, establishing whether a given state is separable or not is in general a very hard task. Indeed apart from PPT criterion in low dimensions, the available theorems do not provide constructive tools to detect entangled states in general. In the present chapter we will review some of the entanglement detecting methods. Though none of them is able to detect all entangled states, they nevertheless work for particular classes of states.

5.1 PPT Criterion

In the last chapter, we have introduced Transposition Map. Since this map is not CP, it can be used to detect entangled states. In fact, partial transposition provides one of the most easily applicable tools to detect entanglement. Unfortunately in higher dimensions, being PPT is no longer a sufficient condition for separability.

Theorem 8 *Horodecki Criterion*

A bipartite state $\rho \in \mathbb{S}_{d \times d}$ is separable if and only if for any positive map $\Lambda : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$, $(\text{id}_d \otimes \Lambda)\rho$ is positive [31].

As this must hold for any positive map Λ , so does it for Transposition Map:

Theorem 9 *Peres Criterion*

If a bipartite state $\rho \in \mathbb{S}_{d \times d}$ is separable, then $(\text{id}_d \otimes T)\rho \geq 0$ [53].

Obviously when $(\text{id}_d \otimes \Lambda)\rho \not\geq 0$, the state is NPT, and according to the above theorem, is entangled. As we have already mentioned, Transposition Map is an exhaustive entanglement witness in low dimensions:

Corollary 1 PPT Criterion *A state ρ acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$, $\mathbb{C}^2 \otimes \mathbb{C}^3$ or $\mathbb{C}^3 \otimes \mathbb{C}^2$ is separable if and only if its partial transposition is a positive matrix [31]*

Proof:

If ρ is separable, Theorem 8 tells us that its partial transposition ρ^{T_2} is also positive.

The sufficiency is proved as follows: In Theorem 7 we have seen that all positive maps $\Lambda : M_{d_1}(\mathbb{C}) \rightarrow M_{d_2}(\mathbb{C})$ when $d_1 \times d_2 \leq 6$ are decomposable and can be written as:

$$\Lambda = \Gamma_1 + \Gamma_2 \circ \text{T},$$

where $\Gamma_{1,2}$ are CP maps. The extension of this map acting on ρ gives:

$$(\text{id}_d \otimes \Lambda)[\rho] = (\text{id}_d \otimes \Gamma_1)[\rho] + (\text{id}_d \otimes \Gamma_2)[\rho^{\text{T}_2}].$$

The first term is positive because Γ_1 is a CP map and by definition $(\text{id}_d \otimes \Gamma_1)[\rho] \geq 0$. If ρ is PPT, then $\rho^{\text{T}_2} \geq 0$, then the second term remains positive as well, due to complete positivity of Γ_2 , which completes the proof. \square

Example 19 *All Bell states introduced in (3.15), have negative partial transposition and are NPT entangled.*

Example 20 *In (3.34), we have introduced the Werner States in $\mathbb{C}^2 \otimes \mathbb{C}^2$:*

$$(\mathbb{1}_2 \otimes \text{T}_2)\rho_\alpha = \rho_\alpha^{\text{T}_2} = \alpha|\Psi^-\rangle\langle\Psi^-| + \frac{1-\alpha}{4}\mathbb{1}_2 \otimes \mathbb{1}_2, \quad -\frac{1}{3} \leq \alpha \leq 1.$$

Their partially transposed density matrix is:

$$\rho_\alpha^{\text{T}_2} = \frac{1}{4} \begin{pmatrix} 1-\alpha & 0 & 0 & -2\alpha \\ 0 & 1+\alpha & 0 & 0 \\ 0 & 0 & 1+\alpha & 0 \\ -2\alpha & 0 & 0 & 1-\alpha \end{pmatrix}.$$

Its eigenvalues are:

$$\lambda_1 = \lambda_2 = \lambda_3 = \frac{1+\alpha}{4}, \lambda_4 = \frac{1-3\alpha}{4}.$$

As we see the first three eigenvalues are positive, while the fourth one when $\frac{1}{3} \leq \alpha \leq 1$ is negative. Therefore:

$$\frac{-1}{3} \leq \alpha < \frac{1}{3} \quad \Rightarrow \rho_\alpha \text{ is separable,}$$

$$\frac{1}{3} \leq \alpha \leq 1 \quad \Rightarrow \rho_\alpha \text{ is entangled.}$$

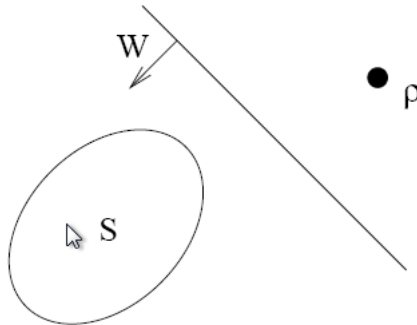
In Example 9, we have seen the behavior of $\Delta^\alpha = S(\rho_\alpha) - \log 2$, where we have mentioned, though it might look like that von Neumann entropy might be able to detect the entangled Werner states, however, it only detects entangled states for $0.75 < \alpha \leq 1$, but it fails to detect the entangled Werner states for $\frac{1}{3} \leq \alpha \leq 0.75$.

5.2 Entanglement Witness

The question of whether a given density matrix ρ of a higher system is separable or not is very difficult to answer due to the difficulties of reconstructing the whole density matrix in terms of tensor product of its subsystems, i.e. to write $\rho = \sum_i p_i |\psi_i^1\rangle\langle\psi_i^1| \otimes |\psi_i^2\rangle\langle\psi_i^2|$. However the fact that a set of such separable states is convex and closed, makes it possible to apply the Hahn-Banach separation theorem. This opens a new approach to detect entanglement, called entanglement witnessing.

Theorem 10 *Hahn-Banach Theorem*

Let X be a finite-dimensional Banach space and S a convex compact set in it. Let x_0 be a point in X such that $x_0 \notin S$. Then there exists a hyperplane which separates x_0 from S [15, 7].



Let the set \mathbb{S}_{sep} correspond to the set of separable states which by definition is convex, compact and closed. Therefore the Hahn Banach theorem 10 says that there must exist a hyperplane separating this set from an entangled state which lies outside. This separator is called Entanglement Witness, which is a Hermitian operator [31, 71].

Definition 18 Entanglement Witness

A Hermitian operator W acting on $\mathbb{H} = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ is called an entanglement witness if

1. $\exists \rho \in \mathbb{S}_{d_1 \times d_2}$ such that $\text{Tr}(\rho W) < 0$.
2. $\langle \varphi \otimes \psi | W | \varphi \otimes \psi \rangle \geq 0 \quad \forall |\varphi\rangle \in \mathbb{C}^{d_1}, |\psi\rangle \in \mathbb{C}^{d_2}$.
3. $\text{Tr}(W) = 1$

The second property shows the block-positivity of the non-positive operator W , while the last one asks only for normalization. There are immediate consequences:

Theorem 11 $\rho \in \mathbb{S}_{d \times d}$ is entangled if and only if there exists an entanglement witness such that $\text{Tr}(\rho W) < 0$ [31].

Theorem 12 $\sigma \in \mathbb{S}_{d \times d}$ is separable if and only if $\text{Tr}(\sigma W) \geq 0$ for all entanglement witnesses W [31].

Definition 19 Decomposable Entanglement Witness

Let P and Q be positive operators acting on $\mathbb{C}^d \otimes \mathbb{C}^d$, then W is a decomposable entanglement witness if and only if [76]

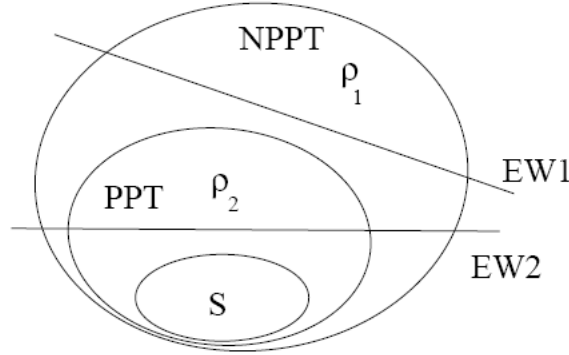
$$\exists a, b \geq 0 \quad \text{such that} \quad W = aP + bQ^{T_1}$$

where T_1 is Partial Transposition.

Theorem 13 An entanglement witness, EW , is non-decomposable if and only if it detects PPT entangled states [46].

Theorem 14 $\rho \in \mathbb{S}_{d \times d}$ is PPT entangled if and only if there exists a non-decomposable entanglement witness such that $\text{Tr}(\rho W) < 0$ [31, 76].

Given two entanglement witnesses W_1 and W_2 , the latter one is said to be finer [46] if all the entangled states detected by W_1 are also detected by W_2 . An EW, W_{opt} is optimal [46, 31] if there exists a separable state $\tilde{\rho}$ such that $\text{Tr}(\tilde{\rho}W_{opt}) = 0$. It means that the hyperplane corresponding to W_{opt} is tangent plane to \mathbb{S}_{sep} (for illustrations see Fig (5.2)). Since optimal entanglement witnesses detect more entangled states than those non-optimal ones, they are highly interesting. Indeed the set of separable states can be completely characterized by the set of optimal EW [11].



It has been shown [46] that a non-optimal EW can be optimized, but one should note that none of these entanglement witnesses can detect all the entangled states.

Both positive maps and entanglement witnesses provide necessary and sufficient conditions for separability. Indeed to some extent their behavior is quite similar toward entangled states; there exists a positive map and an EW for each entangled state. This brings up the conjecture that these connections can be explained through an isomorphism.

Definition 20 Jamiolkowski Isomorphism

Jamiolkowski isomorphism says that there is a one-to-one relation between an EW as an operator and a positive map $\Lambda : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ [39]:

$$\Lambda_W \longleftrightarrow W_\Lambda \in M_{d^2}(\mathbb{C})$$

Given an operator W_Λ acting on $M_{d^2}(\mathbb{C})$ and choosing an orthonormal product basis set $\{|e_i \otimes f_i\rangle\}$ in $\mathbb{H} = \mathbb{C}^d \otimes \mathbb{C}^d$, the corresponding linear map $\Lambda_W : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ is defined [15]:

$$\Lambda_W[\rho] = \text{Tr}_2[W\rho^{\text{T}2}].$$

Conversely from a given map Λ , the operator W_Λ is obtained:

$$W_\Lambda = (\mathbb{1}_d \otimes \Lambda)|\psi_d^+\rangle\langle\psi_d^+|$$

where $|\psi_d^+\rangle$ is defined in (3.32).

The following properties hold [31, 39, 76]

- $W \geq 0$ if and only if Λ_W is completely positive.
- W is EW, if and only if Λ_W is positive.
- W is decomposable if and only if Λ_W is decomposable.
- W is non-decomposable if and only if Λ_W is non-decomposable.

5.3 Reduction Map

In the previous chapter, we have introduced a positive (not CP) map $\Lambda_R : M_d(\mathbb{C}) \longrightarrow M_d(\mathbb{C})$, called Reduction map:

$$\Lambda_R[\rho] = \text{Tr}_d[\rho] - \rho. \quad (5.1)$$

Below we will see how this map can be used to detect the entanglement:

Theorem 15 *Reduction Criterion*

A bipartite state ρ_{12} acting on $\mathbb{H} = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ with $d_1 \times d_2 \leq 6$, is separable if and only if [32]

$$\text{id}_d \otimes \rho_2 - \rho_{12} \geq 0.$$

For states acting on higher dimensional Hilbert spaces, the criterion is only necessary for separability.

This map however can not detect PPT entangled states, as we have shown in the last chapter, that this map is decomposable.

5.4 Range Criterion

The range criterion is another approach to detect entanglement. This method is based on finding the product vectors in the range of the states. The range of ρ is the set of all the vectors $|\psi\rangle$ for which there is another vector $|\phi\rangle$ such that:

$$|\psi\rangle = \rho|\phi\rangle.$$

Definition 21 Product Vector

Let $\mathbb{H} = \bigotimes_{i=1}^m \mathbb{C}^{d_i}$ be an m -partite Hilbert space. A vector $|\psi\rangle \in \mathbb{H}$ is called product vector if and only if it has the form $|\psi\rangle = \bigotimes_{i=1}^m |\phi_i\rangle$ where $|\phi_i\rangle \in \mathbb{C}^{d_i}$.

Note that a product vector is not necessarily separable with respect to all the partitions of Hilbert space. For example consider the vector $|\psi\rangle = \frac{1}{\sqrt{2}}(|001\rangle + |111\rangle)$. This is a product vector when we look at it a bipartite state, i.e. in $\mathbb{C}^4 \otimes \mathbb{C}^2$ it can be written as $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \otimes |1\rangle$. However in three-partite system in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ the vector $|\psi\rangle$ is no longer a product vector.

Theorem 16 Range Criterion

If a bipartite density matrix ρ_{12} acting on Hilbert space $\mathbb{H} = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$, is separable then there exists a set of product vectors $\{|e_i \otimes f_i\rangle\}$ where $|e_i\rangle \in \mathbb{C}^{d_1}$, $|f_i\rangle \in \mathbb{C}^{d_2}$, where $|f_i^*\rangle$ is complex conjugate, such that $\{|e_i \otimes f_i\rangle\}$ spans the range of ρ_{12} and $\{|e_i \otimes f_i^*\rangle\}$ spans the range of $\rho_{12}^{\text{T}_2}$ [34].

Example 21 The following PPT state in $\mathbb{C}^3 \otimes \mathbb{C}^3$ has been shown [34] to be entangled:

$$\rho_a = \frac{1}{8a+1} \begin{bmatrix} a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+a}{2} & 0 & \frac{\sqrt{1-a^2}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 \\ a & 0 & 0 & 0 & a & 0 & \frac{\sqrt{1-a^2}}{2} & 0 & \frac{1+a}{2} \end{bmatrix}$$

where $0 < a < 1$.

Note that the range criterion is neither stronger nor weaker than PPT criterion, as it can detect PPT entangled states, while there are NPT states which do not violate this criterion either.

There are some states which extremely violate this criterion, such states are called Edge states [45, 35].

Definition 22 Edge state

An edge state δ is a PPT entangled state such that, for all product vectors $|e \otimes f\rangle$ ($|e\rangle \in \mathbb{C}^{d_1}$ and $|f\rangle \in \mathbb{C}^{d_2}$) and $\epsilon > 0$, $\delta - \epsilon|e \otimes f\rangle\langle e \otimes f|$ is not positive or does not have a positive partial transposition [34, 35, 46].

Obviously the edge states lie between PPT entangled states and NPT states.

Example 22 *Indeed the first PPT entangled state in $\mathbb{C}^2 \otimes \mathbb{C}^4$ found in [34] is an example of an edge state:*

$$\sigma_b = \frac{1}{7b+1} \begin{bmatrix} b & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1+b}{2} & 0 & 0 & \frac{\sqrt{1-b^2}}{2} \\ b & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & b & 0 & \frac{\sqrt{1-b^2}}{2} & 0 & 0 & \frac{1+b}{2} \end{bmatrix}$$

where $0 \leq b \leq 1$.

Using an edge state δ , one can construct a non-decomposable entanglement witness as follows [46]:

Let us denote the range and kernel of δ by $R(\delta)$ and $K(\delta)$ respectively. Let P and Q denote the projector onto $K(\delta)$ and $K(\delta^{T_2})$ respectively and define

$$W_\delta = a(P + Q^{T_2}) \quad (5.2)$$

where $a = \frac{1}{\text{Tr}(P + Q)}$.

Define also

$$\epsilon \equiv \inf_{|e \otimes f\rangle} \langle e \otimes f | W_\delta | e \otimes f \rangle. \quad (5.3)$$

Theorem 17 [46] *Given an edge PPT entangled state δ , then $W \propto W_\delta - \epsilon \mathbb{1}$ is a non-decomposable entanglement witness, where ϵ and W_δ are defined in (5.2) and (5.3).*

Proof:

To show that W is an entanglement witness, we have to show that it satisfies the requirements in (18). The block positivity of W requires that for any $|\psi\rangle \in \mathbb{C}^{d_1}$ and $|\phi\rangle \in \mathbb{C}^{d_2}$ we have:

$$\begin{aligned} \langle \psi \otimes \phi | W | \psi \otimes \phi \rangle &\geq \langle \psi \otimes \phi | W_\delta | \psi \otimes \phi \rangle - \epsilon \langle \psi \otimes \phi | \mathbb{1} | \psi \otimes \phi \rangle \\ &= a(\langle \psi \otimes \phi | P | \psi \otimes \phi \rangle + \langle \psi \otimes \phi | Q^{T_2} | \psi \otimes \phi \rangle) - \epsilon. \end{aligned}$$

The first two terms cannot vanish simultaneously, as δ is an edge state: If $\langle \psi \otimes \phi | P | \psi \otimes \phi \rangle = 0$ then $|\psi \otimes \phi\rangle \in R(\delta)$, then by definition of an edge state, $|\psi \otimes \phi^*\rangle \notin R(\delta^{\text{T}_2})$, which implies that $|\psi \otimes \phi^*\rangle \in K(\delta^{\text{T}_2})$ and therefore $\langle \psi \otimes \phi^* | Q | \psi \otimes \phi^* \rangle = 1$, and vice versa. Therefore $\langle \psi \otimes \phi | W_\delta | \psi \otimes \phi \rangle \geq 0$ for all $|\psi\rangle$ and $|\phi\rangle$.

On the other hand W detects δ :

$$\begin{aligned} \text{Tr}(W\delta) &= a(\text{Tr}(P\delta) + \text{Tr}(Q_2^{\text{T}}\delta)) - \epsilon \text{Tr}(\mathbb{1}\delta) \\ &= -\epsilon. \end{aligned}$$

The first two terms are zero due to fact that $P\delta = Q\delta^{\text{T}_2} = 0$. Since W detects a PPT entangled states, by (13) it is a non-decomposable entanglement witness. \square

5.5 Unextendible Product Basis

Searching for the product states in the range of a density matrix was leading into a new method called Unextendible product basis, mentioned for the first time in [9].

Definition 23 *Unextendible Product Basis*

Consider a multipartite quantum system $\mathbb{H} = \bigotimes_{i=1}^m \mathbb{C}^{d_i}$ with m parties. An orthogonal product basis (PB) is a set S of pure orthogonal product states spanning a subspace \mathbb{H}_s of \mathbb{H} . An uncompletable product basis (UCPB) is a PB whose complementary subspace \mathbb{H}^\perp i.e. the subspace in \mathbb{H} spanned by vectors that are orthogonal to all the vectors in \mathbb{H}_s , contains fewer mutually orthogonal product states than its dimension. An unextendible product basis (UPB) is an uncompletable product basis for which \mathbb{H}_s contains no product state.

As an example of product basis which does not span the whole space, one can take $|0\rangle \otimes |0\rangle$ and $|0\rangle \otimes |1\rangle$. As we see these two orthogonal vectors form a PB which spans a two dimensional subspace in $\mathbb{C}^2 \otimes \mathbb{C}^2$.

Example 23 Consider the following example of UPB given in [23], known as Tiles. It is a set of five product vectors in $\mathbb{C}^3 \otimes \mathbb{C}^3$, spanning a 5-dimensional

subspace:

$$\begin{aligned}
|\psi_0\rangle &= |0\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \\
|\psi_1\rangle &= |2\rangle \otimes \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \\
|\psi_2\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \otimes |2\rangle \\
|\psi_3\rangle &= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \otimes |0\rangle \\
|\psi_4\rangle &= \frac{1}{3}(|0\rangle + |1\rangle + |2\rangle) \otimes (|0\rangle + |1\rangle + |2\rangle).
\end{aligned} \tag{5.4}$$

One sees that as all of these vectors are mutually orthogonal and each three of them span a full 3-dimensional Hilbert space, therefore it is not possible to find another product vector which would be orthogonal to all of them.

For the bipartite Hilbert space $\mathbb{H} = \mathbb{C}^d \otimes \mathbb{C}^d$, when d is even, one can construct UPB as follows [24]; Let's denote the set of d orthonormal vectors by $|0\rangle, \dots, |d-1\rangle$, then the set of vertical tiles are constructed as follows:

$$\begin{aligned}
|\psi_{mn}\rangle &= |n\rangle \otimes |\omega_{m,n+1}\rangle = |n\rangle \otimes \sum_{j=0}^{d/2-1} \omega^{jm} |j+n+1 \pmod{d}\rangle, \tag{5.5} \\
m &= 1, \dots, \frac{d}{2} - 1 \quad \text{and} \quad n = 0, \dots, d-1,
\end{aligned}$$

where $\omega = e^{i4\pi/d}$. Similarly, the horizontal tiles are defined to be:

$$\begin{aligned}
|\phi_{mn}\rangle &= |\omega_{m,n}\rangle \otimes |n\rangle = \sum_{j=0}^{d/2-1} \omega^{jm} |j+n \pmod{d}\rangle \otimes |n\rangle, \tag{5.6} \\
m &= 1, \dots, \frac{d}{2} - 1 \quad \text{and} \quad n = 0, \dots, d-1.
\end{aligned}$$

The following theorem illustrates the role of the UPB in the challenge of detecting entanglement.

Theorem 18 *The state that corresponds to the uniform mixture on the space complementary of a UPB $\{\psi_i : i = 1, \dots, n\}$ in a Hilbert space of total dimension d*

$$\bar{\rho} = \frac{1}{d-n} (\mathbb{1} - \sum_{j=1}^n |\psi_j\rangle\langle\psi_j|) \tag{5.7}$$

is a PPT entangled state [9].

Proof:

Partial Transposition maps a set of UPB into another set of UPB, while leaving the identity unchanged, this shows that the state in (5.7) is indeed a PPT state. On the other hand, $\bar{\rho}$ by construction contains no product state which means that it is entangled, all together it is a PPT entangled state. \square

5.6 Realignment

We first introduce some new notions which will be used in the following.

Definition 24 *Reshaping*

Consider an $m \times n$ matrix $A = [a_{ij}]$ where a_{ij} are its entries. By putting the elements of each column one after another, one obtains a vector, which can be associated to this matrix. Conversely, a vector of length mn can be turned into an $m \times n$ matrix [16].

$$A_{m,n} = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{pmatrix} \longleftrightarrow \vec{a} = (a_{11}, \cdots, a_{m1}, \cdots, a_{mn})^T \quad (5.8)$$

Let X be an $mn \times mn$ block matrix and $\vec{a}_{kl} = (a_{11}, \cdots, a_{n1}, \cdots, a_{nn})^T$ the vector corresponding to the block kl of size n . The realigned matrix X^R of size $m^2 \times n^2$, is defined by:

$$X^R = \begin{pmatrix} a_{11}^T \\ \vdots \\ a_{1m}^T \\ \vdots \\ a_{mm}^T \end{pmatrix}$$

Example 24 As an example let us take $m = n = 2$:

$$X = \left(\begin{array}{cc|cc} x_{1,1} & x_{1,2} & x_{1,3} & x_{1,4} \\ x_{2,1} & x_{2,2} & x_{2,3} & x_{2,4} \\ \hline x_{3,1} & x_{3,2} & x_{3,3} & x_{3,4} \\ x_{4,1} & x_{4,2} & x_{4,3} & x_{4,4} \end{array} \right) \quad (5.9)$$

The vector corresponding to the first block is $\vec{a}_{11} = (x_{11}, x_{21}, x_{12}, x_{22})^T$ and the realigned matrix is:

$$X^R = \begin{pmatrix} x_{1,1} & x_{2,1} & x_{1,2} & x_{2,2} \\ x_{3,1} & x_{4,1} & x_{3,2} & x_{4,2} \\ x_{1,3} & x_{2,3} & x_{1,4} & x_{2,4} \\ x_{3,3} & x_{4,3} & x_{3,4} & x_{4,4} \end{pmatrix}$$

In [7], reshaping a matrix is performed by aligning its rows one by one in a vector, instead of its columns:

$$A_{m,n} = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{pmatrix} \longleftrightarrow \vec{a}' = (a_{11}, a_{12}, \dots, a_{1n}, \dots, a_{mn})^T$$

Now any $mn \times mn$ square matrix can be reshuffled by reshaping each row into a square matrix and putting them block after block into a new matrix. The new reshuffled matrix, $X^{R'}$ obtained from matrix X in (5.9) is:

$$X^{R'} = \left(\begin{array}{cc|cc} x_{1,1} & x_{1,2} & x_{2,1} & x_{2,2} \\ x_{1,3} & x_{1,4} & x_{2,3} & x_{2,4} \\ \hline x_{3,1} & x_{3,2} & x_{4,1} & x_{4,2} \\ x_{3,3} & x_{3,4} & x_{4,3} & x_{4,4} \end{array} \right)$$

In general, given a matrix $X \in M_d(\mathbb{C}) \otimes M_d(\mathbb{C}) = M_{d^2}(\mathbb{C})$, let us consider the orthonormal basis consisting of tensor products $|e_m \otimes f_\mu\rangle \in \mathbb{C}^{d^2}$, where $\{|e_m\rangle\}_{m=1}^d$ and $\{|f_\mu\rangle\}_{\mu=1}^d$ are orthonormal bases in \mathbb{C}^d . Further, let us denote as in [7] by

$$X_{\nu\mu}^{m\mu} = \langle e_m \otimes f_\mu | X | e_n \otimes f_\nu \rangle. \quad (5.10)$$

Then, the matrix elements of reshuffled matrix $X^{R'}$ are given by

$$X_{\nu\mu}^{R'} = X_{nm}^{\nu\mu}. \quad (5.11)$$

Remark 4 Note that the result of both methods are equivalent up to a permutation. In both cases after reshaping a matrix into a vector, the Hilbert-Schmidt product [7] will be read as scalar product between two vectors:

$$\langle A | B \rangle = \text{Tr} A^\dagger B = \langle a' | b' \rangle.$$

Reshuffling the tensor product of two matrices turns to be very simple. Consider two matrices $X \in M_p(\mathbb{C})$ and $Y \in M_q(\mathbb{C})$. We denote the vectors

assigned to each matrix by $\text{vec}(X)$ and $\text{vec}(Y)$. Now consider their tensor product:

$$\begin{aligned}
X \otimes Y &= \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{p1} & x_{p2} & \cdots & x_{pp} \end{pmatrix} \otimes \begin{pmatrix} y_{11} & y_{12} & \cdots & y_{1q} \\ y_{21} & y_{22} & \cdots & y_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ y_{q1} & y_{q2} & \cdots & y_{qq} \end{pmatrix} \\
&= \left(\begin{array}{ccc|ccc} x_{11}y_{11} & \cdots & x_{11}y_{1q} & & & \\ x_{11}y_{21} & \cdots & x_{11}y_{2q} & x_{12}Y & \cdots & x_{1p}Y \\ \vdots & \ddots & \vdots & & & \\ \hline x_{11}y_{q1} & \cdots & x_{11}y_{qq} & & & \\ \hline & & & x_{21}Y & \cdots & x_{2p}Y \\ & & & \vdots & \ddots & \vdots \\ & & & x_{p1}Y & \cdots & x_{pp}Y \end{array} \right). \quad (5.12)
\end{aligned}$$

By the above method the vector corresponding to the first block is:

$$\vec{a}_1 = (x_{11}y_{11}, \dots, x_{11}y_{1q}, \dots, x_{11}y_{q1}, \dots, x_{11}y_{qq})^T = x_{11} \vec{Y},$$

where \vec{Y} is the vector corresponding to the matrix Y (see (5.8)). Putting all these vectors as rows of a new matrix, we have the reshuffled matrix of this tensor product:

$$(X \otimes Y)^R = \begin{pmatrix} x_{11}(\vec{Y})^T \\ \vdots \\ x_{1p}(\vec{Y})^T \\ \vdots \\ x_{pp}(\vec{Y})^T \end{pmatrix} = \vec{X}(\vec{Y})^T$$

We now show that reshuffling a density matrix can be useful to detect its entanglement.

Theorem 19 Reshuffling Criterion *If a bipartite density matrix ρ_{12} is separable, then the trace norm of its reshuffled matrix will not be increased [16, 59], i.e.:*

$$\|\rho_{12}^R\|_{\text{Tr}} \leq \|\rho_{12}\|_{\text{Tr}} = 1.$$

Proof:

If ρ_{12} is separable, then it can be written as $\rho_{12} = \sum_i p_i \rho_i^1 \otimes \rho_i^2$ where $\sum_i p_i = 1$. Consider the pure separable state: $\rho_{12} = \rho^1 \otimes \rho^2$. As we have

seen in the last remark, by reshuffling this state we have: $\rho_{12}^R = \vec{\rho}^1[\vec{\rho}^2]^T$. But in this case, ρ^1 and ρ^2 are projectors and therefore their norm is equal to the norm of the corresponding vectors. We have:

$$\|\rho_{12}^R\| \leq \|\vec{\rho}^1[\vec{\rho}^2]^T\| \leq \|\vec{\rho}^1\| \|\vec{\rho}^2\| = \|\rho_1\| \|\rho_2\| = 1 .$$

By properties of the norm, we can see that:

$$\|\rho_{12}^R\| \leq \sum_i p_i \|(\rho_i^1 \otimes \rho_i^2)^R\| \leq \sum_i p_i \leq 1.$$

□

This theorem provides a necessary condition for separability, therefore if one finds that for a given density matrix ρ , after reshuffling $\|\rho^R\| > 1$, this means that the state is entangled. Note that ρ^R is not Hermitian. It was proved [60, 61] that realignment is independent of Partial Transposition, therefore none of them is neither stronger nor weaker than the other one.

Example 25 *As an example one can consider the density matrix constructed as in theorem (5.7), using the UPB given in example (5.4), called tiles:*

$$\rho = \frac{1}{4}(\mathbb{1} - \sum_{i=0}^4 |\psi_i\rangle\langle\psi_i|).$$

However we know that this state is entangled but we can also see it by direct calculation of the norm of $\|\rho^R\| = 1.32$. Since $\|\rho\| < \|\rho^R\|$ it reveals the entanglement of this state using the reshuffling method.

Chapter 6

σ -diagonal States

In the following chapter, we consider bipartite states that are diagonal in the basis generated by the action of tensor products of the form $\mathbb{1}_{2^n} \otimes \sigma_{\vec{\mu}}$, $\sigma_{\vec{\mu}} = \otimes_{i=1}^n \sigma_{\mu_i}$, on the totally symmetric state $|\Psi_+^{2^n}\rangle \in \mathbb{C}^{2^n} \otimes \mathbb{C}^{2^n}$. We first characterize the structure of positive maps detecting the entangled ones among them; then, the result will be illustrated by examining some entanglement witnesses for the case $n = 2$. Further, we will show how, for pairs of two qubits, being separable, entangled and bound entangled are state properties related to the geometric patterns of subsets of a 16 point square lattice.

6.1 σ -diagonal and lattice states

In the following we shall freely call *entanglement witness* both positive maps Λ such that $\text{id}_d \otimes \Lambda[\rho_{ent}] \not\geq 0$ and their Choi matrices M_Λ .

We shall consider a bipartite system consisting of two parties in turn comprising n qubits; the corresponding matrix algebra $M_{2^{2n}}(\mathbb{C})$ is linearly spanned by 4^n tensor products of the form $\sigma_{\vec{\mu}} := \otimes_{i=1}^n \sigma_{\mu_i} = \sigma_{\mu_1} \otimes \sigma_{\mu_2} \otimes \cdots \otimes \sigma_{\mu_n}$.

Given the totally symmetric state, already introduced in (3.32):

$$|\Psi_+^d\rangle = \frac{1}{d} \sum_{j=1}^d |j\rangle \otimes |j\rangle$$

with $d = 2^n$, the vectors

$$|\Psi_{\vec{\mu}}\rangle := \mathbb{1}_{2^n} \otimes \sigma_{\vec{\mu}} |\Psi_+^{2^n}\rangle \in \mathbb{C}^{2^n} \otimes \mathbb{C}^{2^n}, \quad (6.1)$$

form orthogonal projectors

$$P_{\vec{\mu}} := |\Psi_{\vec{\mu}}\rangle \langle \Psi_{\vec{\mu}}| = (\mathbb{1}_{2^n} \otimes \sigma_{\vec{\mu}}) |\Psi_+^{2^n}\rangle \langle \Psi_+^{2^n}| (\mathbb{1}_{2^n} \otimes \sigma_{\vec{\mu}}). \quad (6.2)$$

Orthonormality follows since

$$\langle \Psi_{\vec{\nu}} | \Psi_{\vec{\mu}} \rangle = \langle \Psi_+^{2^n} | \mathbb{1}_{2^n} \otimes \sigma_{\vec{\mu}} \sigma_{\vec{\mu}} | \Psi_+^{2^n} \rangle = \frac{1}{2^n} \text{Tr}(\sigma_{\vec{\nu}} \sigma_{\vec{\mu}}) = \frac{1}{2^n} \prod_{i=1}^n \text{Tr}(\sigma_{\nu_i} \sigma_{\mu_i}) = \prod_{i=1}^n \delta_{\nu_i \mu_i} .$$

Definition 25 *The class of bipartite states we shall study will consist of states of the form*

$$\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}} , \quad 0 \leq r_{\vec{\mu}} \leq 1 , \quad \sum_{\vec{\mu}} r_{\vec{\mu}} = 1 , \quad (6.3)$$

that is diagonal with respect to the chosen orthonormal basis in $\mathbb{C}^{2^n} \otimes \mathbb{C}^{2^n}$: we shall call them σ -diagonal states.

A particular sub-class of states of two pairs of two qubits, $n = 2$ and $\sigma_{\vec{\mu}} = \sigma_{\alpha} \otimes \sigma_{\beta} = \sigma_{\alpha\beta} \in M_4(\mathbb{C})$, are considered in [4, 5, 6] and called lattice states. In this case the orthonormal basis vectors and their corresponding projectors are the following:

$$\begin{aligned} |\Psi_{\alpha\beta}\rangle &= \mathbb{1}_4 \otimes \sigma_{\alpha\beta} |\Psi^+\rangle \in \mathbb{C}^{16}, \\ P_{\alpha\beta} &\equiv |\Psi_{\alpha\beta}\rangle \langle \Psi_{\alpha\beta}| = (\mathbb{1}_4 \otimes \sigma_{\alpha\beta}) P_4^+ (\mathbb{1}_4 \otimes \sigma_{\alpha\beta}), \end{aligned}$$

where P_+^4 is defined in (3.33).

For them partial results concerning their entanglement properties have been obtained. We shall tackle them again in the following: the class of lattice-states is defined as follows.

Definition 26 Lattice States

Taking a subset $I \subseteq L_{16}$ of cardinality N_I , then the corresponding lattice state ρ_I is defined by:

$$\rho_I = \frac{1}{N_I} \sum_{\alpha, \beta \in I} P_{\alpha\beta} . \quad (6.4)$$

Let L_{16} denote the set of pairs (α, β) , where α and β run from 0 to 3: it corresponds to a 4×4 square lattice, whereas the subsets

$$\begin{aligned} C_{\alpha} &:= \{(\alpha, \beta) \in L_{16} : \beta = 0, 1, 2, 3\} \\ R_{\beta} &:= \{(\alpha, \beta) \in L_{16} : \alpha = 0, 1, 2, 3\} \end{aligned} \quad (6.5)$$

correspond to the columns and rows of the lattice, respectively.

If compared with those in (6.3), the lattice states are uniformly distributed over, and thus completely characterized by chosen subsets of L_{16} .

Example 26 *As an example consider the lattice states associated with the following subsets:*

$$\rho_8 = \frac{1}{8}(P_{00} + P_{02} + P_{11} + P_{13} + P_{20} + P_{21} + P_{23} + P_{32})$$

$$N_I = 8 : \begin{array}{c|c|c|c|c} 3 & & \times & \times & \\ \hline 2 & \times & & & \times \\ \hline 1 & & \times & \times & \\ \hline 0 & \times & & \times & \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad (6.6)$$

$$\rho_4 = \frac{1}{4}(P_{00} + P_{11} + P_{22} + P_{33})$$

$$N_I = 4 : \begin{array}{c|c|c|c} 3 & & & \times \\ \hline 2 & & & \times \\ \hline 1 & & \times & \\ \hline 0 & \times & & \\ \hline & 0 & 1 & 2 & 3 \end{array} . \quad (6.7)$$

In the following, we shall be interested in investigating the entanglement properties of such states. As an appetizer, we consider whether the von Neumann entropy of any ρ_I can be smaller than that of its reduced density matrices. Indeed, we have seen that, if so, ρ_I would be entangled. By tracing over the first or the second party we get as reduced density matrices

$$\rho_I^{(1),(2)} = \text{Tr}_{2,1}\rho_I = \frac{\mathbb{1}_4}{4}$$

with maximal von Neumann entropy $S(\rho_I^{(1),(2)}) = 2 \log 2$. On the other, end each lattice state is already spectralized with equal non-zero eigenvalues $1/N_I$; therefore, $S(\rho_I) = \log N_I \geq 2 \log 2$ whenever $N_I \geq 4$.

Furthermore, if we consider the Reshuffling Criterion in Theorem 19, using the relations (5.10) and (5.11), we obtain as reshuffled lattice states

$$(\rho_I^{R'})_{n\nu}^{m\mu} = (\rho_I^{R'})_{nm}^{\nu\mu} = \frac{1}{4N_I} \sum_{(\alpha,\beta) \in I} \langle \mu | \sigma_{\alpha\beta} | \nu \rangle \langle n | \sigma_{\alpha\beta} | m \rangle ,$$

whence

$$\rho_I^{R'} = \frac{1}{4N_I} \sum_{(\alpha,\beta) \in I} \sigma_{\alpha\beta}^T \otimes \sigma_{\alpha\beta} ,$$

where we chose the ortonormal basis vectors in (5.10) to be the ones used in writing the Lattice States, namely $|e_i\rangle = |f_i\rangle = |i\rangle$. Thus, using the

properties of the trace norm, one gets

$$\|\rho_I^{R'}\|_{\text{Tr}} \leq \frac{1}{4N_I} \sum_{(\alpha,\beta) \in I} \|\sigma_{\alpha\beta}\|_{\text{Tr}}^2 = \frac{4}{N_I},$$

whence for $N_I \geq 4$ no entangled lattice state can be detected by the chosen criterion.

We now proceed to examine the lattice states from the point of view of partial transposition. Positivity under partial transposition (PPT-ness) of lattice states ρ_I is completely characterized by the geometry of I [4].

Proposition 1 *A necessary and sufficient condition for a lattice state ρ_I to be PPT is that for every $(\alpha, \beta) \in L_{16}$ the number of points on C_α and R_β belonging to I and different from (α, β) be not greater than $N_I/2$. In terms of the characteristic functions $\chi_I(\alpha, \beta) = 1$ if $(\alpha, \beta) \in I$, $= 0$ otherwise, a lattice state ρ_I is PPT if and only if for all $(\alpha, \beta) \in L_{16}$:*

$$\sum_{0=\delta \neq \beta}^3 \chi_I(\alpha, \delta) + \sum_{0=\delta \neq \alpha}^3 \chi_I(\delta, \beta) \leq \frac{N_I}{2}.$$

Example 27 *Consider the following lattice states:*

$$N_I = 5 : \begin{array}{c|c|c|c|c} 3 & & & \times & \\ \hline 2 & \times & & & \times \\ \hline 1 & & & \times & \\ \hline 0 & & & & \times \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad (6.8)$$

$$N_I = 4 : \begin{array}{c|c|c|c|c} 3 & & & \times & \\ \hline 2 & & \times & & \\ \hline 1 & & & \times & \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad (6.9)$$

These states do not remain positive under partial transposition and are therefore entangled: in the first state ρ_5 , the row and column passing through the point $(2, 2) \notin I$ contains $4 > 5/2$ points in I , while in the second one $3 > 4/2 = 2$ points.

Example 28 *By the same criterion, the following two states are instead PPT,*

$$\begin{array}{c}
 N_I = 6 : \\
 \begin{array}{c|c|c|c|c}
 3 & & & \times & \times \\
 \hline
 2 & \times & & & \times \\
 \hline
 1 & & \times & & \times \\
 \hline
 0 & & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \end{array}
 \quad
 \begin{array}{c}
 N_I = 8 : \\
 \begin{array}{c|c|c|c|c}
 3 & & \times & \times & \times \\
 \hline
 2 & \times & & \times & \times \\
 \hline
 1 & & & \times & \times \\
 \hline
 0 & & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \end{array}
 \quad (6.10)$$

They need not be separable as in lower dimension; indeed, a sufficient criterion devised in [3] show them to be entangled.

Proposition 2 *A sufficient condition for a PPT lattice state ρ_I to be entangled is that there exists at least a pair $(\alpha, \beta) \in L_{16}$ not belonging to I such that only one point on C_α and R_β belongs to I . Equivalently, ρ_I is entangled if there exists a pair $(\alpha, \beta) \in L_{16}$, $(\alpha, \beta) \notin I$, such that*

$$\sum_{0=\delta \neq \beta}^3 \chi_I(\alpha, \delta) + \sum_{0=\delta \neq \alpha} \chi_I(\delta, \beta) = 1 \quad .$$

In both patterns of the states in Example (28), it is the point $(0, 0) \notin I$ which satisfies the sufficient criterion.

Example 29 *Unfortunately, this criterion fails in the case of the PPT lattice state characterized by the following subset*

$$\begin{array}{c}
 N_I = 10 : \\
 \begin{array}{c|c|c|c|c}
 3 & \times & & & \times \\
 \hline
 2 & & \times & \times & \\
 \hline
 1 & \times & \times & & \times \\
 \hline
 0 & \times & \times & & \times \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \end{array}
 \quad . \quad (6.11)$$

Indeed, the only candidate point to fulfill the criterion in Proposition (2) is $(2, 2)$; however, it belongs to I .

Luckily, a refined criterion [6] based on [12] shows it to be entangled.

Proposition 3 *A PPT lattice state ρ_I is entangled if the quantity*

$$k_I^{\mu\nu} = \sum_{\alpha \neq \nu \oplus 2} \chi_I(\alpha, \nu \oplus 2) + \sum_{\beta \neq \mu \oplus 2} \chi_I(\mu \oplus 2, \beta) ,$$

where \oplus denotes summation modulo 4, is such that $k_I^{\mu\nu} = 1$ for a column $C_{\mu \oplus 2}$ and a row $R_{\nu \oplus 2}$, independently of whether $(\mu \oplus 2, \nu \oplus 2)$ belongs to I or not.

Example 30 Thus, the state in (29) fulfills the sufficient condition $k_I^{00} = 1$.

Another example of a lattice state detected by the last proposition is the following:

$$N_I = 11 : \quad \begin{array}{c|c|c|c|c} 3 & \times & \times & \times & \\ \hline 2 & \times & \times & \times & \times \\ \hline 1 & \times & \times & \times & \\ \hline 0 & & & & \times \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

As it is apparent from these examples the various criteria for entanglement are closely related to the structure of the subsets that define the lattice states; in the following we will try to clarify this correspondence.

6.2 Entanglement detection for σ -diagonal states

In this section, we will show that positive maps that be entanglement witnesses for states of the form (6.3) can be sought in a particular subclass of them.

Any linear map on $\Lambda : M_d(\mathbb{C}) \mapsto M_d(\mathbb{C})$ can be written as [3]:

$$M_d(\mathbb{C}) \ni X \mapsto \Lambda[X] = \sum_{i,j=0}^{d^2-1} \lambda_{ij} G_i X G_j^\dagger ,$$

where the matrices $G_i \in M_d(\mathbb{C})$ form an orthonormal basis with respect to Hilbert-Schmidt scalar product, namely $\text{Tr}(G_i^\dagger G_j) = \delta_{ij}$ and the coefficients λ_{ij} are complex numbers.

In the present case, the normalized tensor products $\frac{\sigma_{\vec{\mu}}}{\sqrt{2^n}}$ constitute such a basis in $M_{2^n}(\mathbb{C})$, whence linear maps $\Lambda : M_{2^n}(\mathbb{C}) \mapsto M_{2^n}(\mathbb{C})$ can be expressed as

$$M_{2^n}(\mathbb{C}) \ni X \mapsto \Lambda[X] = \sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} S_{\vec{\mu}\vec{\nu}}[X] , \quad S_{\vec{\mu}\vec{\nu}}[X] = \sigma_{\vec{\mu}} X \sigma_{\vec{\nu}} . \quad (6.12)$$

The next one is a simple observation based on (6.1) and (6.2).

Lemma 2 A σ -diagonal state $\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}}$ is entangled if and only if there exists a positive map Λ as in (6.12) such that $\sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} r_{\vec{\mu}} < 0$.

Proof: According to Horodecki Criterion in (8), the state $\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}}$ is entangled if and only if

$$\text{Tr} (\text{id}_{2^n} \otimes \Lambda[P_+^{2^n}] \rho) < 0 ,$$

for some positive map $\Lambda : M_{2^n}(\mathbb{C}) \mapsto M_{2^n}(\mathbb{C})$.

Using the orthogonality of the vectors $|\Psi_{\vec{\mu}}\rangle$ in (6.1), ρ is entangled if and only if there is a positive map Λ such that:

$$\text{Tr}(\text{id}_{2^n} \otimes \Lambda[P_+^{2^n}]\rho) = \sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} \langle \Psi_{\vec{\nu}} | \rho | \Psi_{\vec{\mu}} \rangle = \sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} r_{\vec{\mu}} < 0 .$$

□

The lemma indicates that the class of diagonal positive maps of the form $\Lambda = \sum_{\vec{\mu}} \lambda_{\vec{\mu}} S_{\vec{\mu}\vec{\mu}}$ might suffice to witness the entanglement of states of the form $\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}}$. What is needed to show that it is indeed so is the following result.

Lemma 3 *Given a positive map of the form $\Lambda = \sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} S_{\vec{\mu}\vec{\nu}}$, the diagonal map $\Lambda_{\text{diag}} = \sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} S_{\vec{\mu}\vec{\mu}}$ is also positive.*

Proof: From Choi's theorem (5), we know that a given map is positive if and only if its Choi matrix is block positive. Considering the map $\Lambda = \sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} S_{\vec{\mu}\vec{\nu}}$, the positivity assumption is equivalent to

$$\sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} \langle \varphi | \sigma_{\vec{\mu}} | \psi \rangle \langle \psi | \sigma_{\vec{\nu}} | \varphi \rangle \geq 0 \quad \forall |\psi\rangle, |\varphi\rangle \in \mathbb{C}^{2^n} . \quad (6.13)$$

Given a pair $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^{2^n}$, consider another pair $|\psi_{\delta_i}\rangle = \sigma_{\delta_i} |\psi\rangle$, $|\varphi_{\delta_i}\rangle = \sigma_{\delta_i} |\varphi\rangle$, where σ_{δ_i} denotes the tensor product $\sigma_{\vec{\mu}}$ where $\mu_j = 0$ for $j \neq i$ and $\mu_i = \delta_i \neq 0$. Inserting the new pair into (6.13), we get

$$\begin{aligned} \sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} \langle \varphi | \bigotimes_{j=1}^{i-1} \sigma_{\mu_j} \otimes \left(\sigma_{\delta_i} \sigma_{\mu_i} \sigma_{\delta_i} \right) \bigotimes_{j=i+1}^n \sigma_{\mu_j} | \psi \rangle \times \\ \times \langle \psi | \bigotimes_{j=1}^{i-1} \sigma_{\nu_j} \otimes \left(\sigma_{\delta_i} \sigma_{\nu_i} \sigma_{\delta_i} \right) \bigotimes_{j=i+1}^n \sigma_{\nu_j} | \varphi \rangle \geq 0 . \end{aligned} \quad (6.14)$$

Consider $\mu_i \neq \nu_i$; because of the Pauli algebraic relations, one can always choose σ_{δ_i} in such a way that

$$\sigma_{\delta_i} \sigma_{\mu_i} \sigma_{\delta_i} = \sigma_{\mu_i} \quad \text{and} \quad \sigma_{\delta_i} \sigma_{\nu_i} \sigma_{\delta_i} = -\sigma_{\nu_i} ,$$

whence all the terms in (6.14) corresponding to the chosen pair of indices (μ_i, ν_i) contribute with

$$- \lambda_{\vec{\mu}\vec{\nu}} \langle \varphi | \bigotimes_{j=1}^{i-1} \sigma_{\mu_j} \otimes \sigma_{\mu_i} \bigotimes_{j=i+1}^n \sigma_{\mu_j} | \psi \rangle \langle \psi | \bigotimes_{j=1}^{i-1} \sigma_{\nu_j} \otimes \sigma_{\nu_i} \bigotimes_{j=i+1}^n \sigma_{\nu_j} | \varphi \rangle .$$

Then, adding inequalities (6.13) and (6.14) yields

$$\sum_{\vec{\mu}, \vec{\nu}; \mu_i = \nu_i} \lambda_{\vec{\mu}\vec{\nu}} \langle \varphi | \sigma_{\vec{\mu}} | \psi \rangle \langle \psi | \sigma_{\vec{\nu}} | \varphi \rangle \geq 0 \quad .$$

By applying the very same argument for pairs (μ_i, ν_i) with varying index i , one cancels all contributions from $\mu_i \neq \nu_i$ and remains with

$$\sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} \langle \varphi | \sigma_{\vec{\mu}} | \psi \rangle \langle \psi | \sigma_{\vec{\mu}} | \varphi \rangle \geq 0 \quad \forall |\psi\rangle, |\varphi\rangle \in \mathbb{C}^{2^n} \quad . \quad (6.15)$$

This, by Choi's theorem (5) amounts to the positivity of the diagonalized map $\Lambda_{diag} = \sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} S_{\vec{\mu}\vec{\mu}}$. \square

The previous result allows us to conclude with

Proposition 4 *Entangled $\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}}$ can be witnessed by diagonal positive maps $\Lambda = \sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} S_{\vec{\mu}\vec{\mu}}$.*

Proof: By the previous lemma, diagonalizing a positive map

$$\Lambda = \sum_{\vec{\mu}, \vec{\nu}} \lambda_{\vec{\mu}\vec{\nu}} S_{\vec{\mu}\vec{\nu}}$$

always yields a positive map $\Lambda_{diag} = \sum_{\vec{\mu}} \lambda_{\vec{\mu}\vec{\mu}} S_{\vec{\mu}\vec{\mu}}$. Then, from Lemma (2) it follows that either the entanglement of ρ is witnessed by an already diagonal map or, if by a non-diagonal one, also by the map obtained by diagonalizing the latter. \square

Remark 5 *From the above Proposition we only get that entangled states of the form (6.3) can be witnessed by diagonal maps $\Lambda_{diag} = \sum_{\vec{\mu}} \lambda_{\vec{\mu}} S_{\vec{\mu}\vec{\mu}}$; the main problem is of course to characterize the coefficients $\lambda_{\vec{\mu}}$ in such a way that (6.15) be satisfied and thus Λ_{diag} be positive.*

Expression (4.25) for Trace map in $M_4(\mathbb{C})$ can be extended to the trace operation on $M_{2^n}(\mathbb{C})$,

$$\text{Tr} = \frac{1}{2^n} \sum_{\vec{\mu}} S_{\vec{\mu}\vec{\mu}} \quad .$$

In the second part of chapter 4, we have seen that positive maps can be related to the complete positive maps. This relation was given in Theorem (4.26), which allows us to write a positive map as:

$$\Lambda = \mu(\text{T} - \Lambda_{cp}).$$

Therefore diagonal positive maps Λ_{diag} are also related to completely positive diagonal maps

$$\Lambda_{diag}^{CP} = \sum_{\vec{\mu}} \lambda_{\vec{\mu}} S_{\vec{\mu}\vec{\mu}} , \quad \lambda_{\vec{\mu}} \geq 0 ,$$

by setting

$$\Lambda_{diag} = \mu \sum_{\vec{\mu}} \left(\frac{1}{2^n} - \lambda_{\vec{\mu}} \right) S_{\vec{\mu}\vec{\mu}} , \quad \mu > 0 , \quad (6.16)$$

and asking for block positivity of its Choi matrix, which is

$$\begin{aligned} \langle \varphi | \Lambda_{diag} [|\psi\rangle\langle\psi|] | \varphi \rangle &\geq 0, \quad \forall |\varphi\rangle, |\psi\rangle \in \mathbb{C}^{2^n}, \\ \langle \varphi | \left(\text{Tr} - \Lambda_{diag}^{CP} \right) [|\psi\rangle\langle\psi|] | \varphi \rangle &= 1 - \sum_{\vec{\mu}} \lambda_{\vec{\mu}} |\langle \varphi | \sigma_{\vec{\mu}} | \psi \rangle|^2 \geq 0 \quad \forall |\varphi\rangle, |\psi\rangle \in \mathbb{C}^{2^n} . \end{aligned} \quad (6.17)$$

Using these observations, we get necessary and sufficient conditions for the separability of σ -diagonal states.

Proposition 5 *A σ -diagonal state $\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}}$ is separable if and only if for all sets of 4^n positive real numbers $\lambda_{\vec{\mu}} \geq 0$, such that*

$$\sum_{\vec{\mu}} \lambda_{\vec{\mu}} |\langle \varphi | \sigma_{\vec{\mu}} | \psi \rangle|^2 \leq 1 \quad \forall |\psi\rangle, |\varphi\rangle \in \mathbb{C}^{2^n} , \quad (6.18)$$

it holds that

$$\sum_{\vec{\mu}} \lambda_{\vec{\mu}} r_{\vec{\mu}} \leq \frac{1}{2^n} . \quad (6.19)$$

Otherwise, if a set of 4^n positive real numbers $\lambda_{\vec{\mu}} \geq 0$ can be found that satisfy (6.18) and such that

$$\sum_{\vec{\mu}} \lambda_{\vec{\mu}} r_{\vec{\mu}} > \frac{1}{2^n} , \quad (6.20)$$

then the σ -diagonal state $\rho = \sum_{\vec{\mu}} r_{\vec{\mu}} P_{\vec{\mu}}$ is entangled.

Before tackling the case of lattice states, that is of σ -diagonal states with $n = 2$, as a simple application, we consider the case of only two qubits, $n = 1$, for which we know PPT-ness to coincide with separability.

Example 31 *In the case $n = 2$, σ -diagonal states have the form*

$$\rho = \sum_{\mu=0}^3 r_{\mu} P_{\mu} , \quad r_{\mu} \geq 0 , \quad \sum_{\mu=0}^3 r_{\mu} = 1$$

and the P_μ 's project onto the Bell states, already introduced in (3.15):

$$\begin{aligned} |\Psi_0\rangle &= |\Psi_+^2\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, & |\Psi_1\rangle &= \frac{|01\rangle + |10\rangle}{\sqrt{2}} \\ |\Psi_2\rangle &= \frac{|00\rangle - |11\rangle}{\sqrt{2}}, & |\Psi_3\rangle &= \frac{|01\rangle - |10\rangle}{\sqrt{2}}. \end{aligned} \quad (6.21)$$

Under transposition $T[\sigma_\mu] = \varepsilon_\mu \sigma_\mu$, $\varepsilon_\mu = (1, 1, -1, 1)$ and under partial transposition the projection P_0 goes into the flip operator $V|\psi \otimes \varphi\rangle = |\varphi \otimes \psi\rangle$:

$$\text{id} \otimes T[P_0] = \frac{1}{2} V = \frac{1}{2} \sum_{\mu=0}^3 v_\mu P_\mu, \quad v_\mu = (1, 1, 1, -1).$$

Therefore, the action of partial transposition on a σ -diagonal state yields

$$\begin{aligned} \text{id} \otimes T[\rho] &= \frac{1}{2} \sum_{\mu=0}^3 r_\mu \mathbb{1} \otimes \sigma_\mu V \mathbb{1} \otimes \sigma_\mu \\ &= \frac{1}{2} \sum_{\mu,\nu=0}^3 r_\mu v_\nu \mathbb{1} \otimes \sigma_\mu \sigma_\nu P_0 \mathbb{1} \otimes \sigma_\nu \sigma_\mu \\ &= \frac{1}{2} \sum_{\mu,\nu=0}^3 v_\nu r_\mu P_{[\mu,\nu]} \\ &= \frac{1}{2} \sum_{\alpha=0}^3 \left(\sum_{\nu=0}^3 v_\nu r_{[\alpha,\nu]} \right) P_\alpha \\ &= \frac{1}{2} \sum_{\alpha=0}^3 \left(r_{[\alpha,0]} + r_{[\alpha,1]} + r_{[\alpha,2]} - r_{[\alpha,3]} \right) P_\alpha \\ &= \frac{1}{2} \sum_{\alpha=0}^3 \left(1 - 2 r_{[\alpha,3]} \right) P_\alpha. \end{aligned} \quad (6.22)$$

Definition 27 In the above expression, the following construction has been employed: given (α, μ) , $\alpha, \mu = 0, 1, 2, 3$, $[\alpha, \mu]$ is the unique index from 0 to 3 such that $\sigma_\alpha \sigma_\mu = \eta_{\alpha\mu}^{[\alpha,\mu]} \sigma_{[\alpha,\mu]}$, where $\eta_{\alpha\mu}^{[\alpha,\mu]}$ is a phase ± 1 or $\pm i$, they can be

considered as non-zero elements of the following matrices:

$$\eta^1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}, \quad \eta^2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -i \\ 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}$$

$$\eta^3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \eta^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Because of the Pauli algebraic relations, the symbol $[\cdot, \cdot]$ enjoys the following properties that can be used to derive (6.22):

$$[\alpha, \mu] = [\mu, \alpha], \quad [\alpha, \mu] = \gamma \Rightarrow [\alpha, \gamma] = \mu \Rightarrow [\mu, \gamma] = \alpha.$$

Thus, $[\alpha, \cdot]$ is a one to one map from the set $(0, 1, 2, 3)$ onto itself.

Since positivity under partial transposition identifies all separable states of two qubits, a σ -diagonal state is separable if and only if $r_\mu \leq \frac{1}{2}$ for all $\mu = 0, 1, 2, 3$.

On the other hand we have seen that all positive maps acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$ are decomposable, therefore using (4.26), (4.22) and (4.24), we can write any diagonal positive map $\Lambda_{diag} : M_2(\mathbb{C}) \mapsto M_2(\mathbb{C})$ as

$$\begin{aligned} \Lambda_{diag} &= \sum_{\alpha=0}^3 \lambda_\alpha^{(1)} S_\alpha + \sum_{\alpha=0}^3 \lambda_\alpha^{(2)} S_\alpha \circ T \\ &= \sum_{\alpha=0}^3 \lambda_\alpha^{(1)} S_\alpha + \frac{1}{2} \sum_{\alpha, \beta=0}^3 \varepsilon_\beta \lambda_\alpha^{(2)} S_\alpha \circ S_\beta \\ &= \sum_{\gamma=0}^3 \left(\lambda_\gamma^{(1)} + \frac{1}{2} \sum_{\beta=0}^3 \varepsilon_\beta \lambda_{[\beta, \gamma]}^{(2)} \right) S_\gamma \\ &= \mu \sum_{\gamma=0}^3 \left(\frac{1}{2} - \lambda_\gamma \right) S_\gamma, \end{aligned}$$

where $\lambda_\alpha^{(1,2)}$ are, according to Theorem (4.4), positive numbers. Then, the coefficients

$$\lambda_\gamma = \frac{1}{2} - \frac{1}{\mu} \left(\lambda_\gamma^{(1)} + \frac{1}{2} \sum_{\beta=0}^3 \varepsilon_\beta \lambda_{[\beta, \gamma]}^{(2)} \right)$$

can always be made positive and thus $\Lambda = \sum_{\alpha=0}^3 \lambda_{\alpha} S_{\alpha}$ completely positive, by choosing μ large enough. Then, they fulfill the condition (6.18) that corresponds to Λ_{diag} being positive. We can thus consider when and whether inequality (6.19) which reads

$$\frac{1}{2} - \sum_{\gamma=0}^3 \lambda_{\gamma} r_{\gamma} = \frac{1}{\mu} \sum_{\gamma=0}^3 r_{\gamma} \left(\lambda_{\gamma}^{(1)} + \frac{1}{2} \sum_{\beta=0}^3 \varepsilon_{\beta} \lambda_{[\beta,\gamma]}^{(2)} \right) \geq 0 ,$$

is satisfied. By choosing $\lambda_{\gamma}^{(1)} = 0$ for all γ and $\lambda_{\gamma}^{(2)} = \delta_{\gamma\alpha}$, one gets

$$\sum_{\beta=0}^3 r_{[\alpha,\beta]} \varepsilon_{\beta} = r_{[\alpha,0]} + r_{[\alpha,1]} - r_{[\alpha,2]} + r_{[\alpha,3]} = 1 - 2r_{[\alpha,2]} \geq 0$$

and thus, by varying α , $r_{\mu} \leq \frac{1}{2}$ for all $\mu = 0, 1, 2, 3$. Vice versa, if $r_{\mu} \leq \frac{1}{2}$ for all $\mu = 0, 1, 2, 3$, one obtains

$$\begin{aligned} \sum_{\gamma=0}^3 r_{\gamma} \sum_{\beta=0}^3 \varepsilon_{\beta} \lambda_{[\beta,\gamma]}^{(2)} &= \sum_{\alpha=0}^3 \lambda_{\alpha}^{(2)} \sum_{\beta=0}^3 \varepsilon_{\beta} r_{[\alpha,\beta]} \\ &= \sum_{\alpha=0}^3 \lambda_{\alpha}^{(2)} \left(r_{[\alpha,0]} + r_{[\alpha,1]} - r_{[\alpha,2]} + r_{[\alpha,3]} \right) \\ &= \sum_{\alpha=0}^3 \lambda_{\alpha}^{(2)} \left(1 - 2r_{[\alpha,2]} \right) \geq 0 . \end{aligned}$$

6.3 Lattice states

In this section we shall restrict ourselves to the lattice states $\rho_I \in M_{16}(\mathbb{C})$ in (6.4), namely to uniformly distributed σ -diagonal states with $n = 2$. Proposition (5) now reads

Corollary 2 *A lattice state ρ_I is separable if and only if*

$$\sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} \leq \frac{N_I}{4} \quad (6.23)$$

for all choices of 16 coefficients $\lambda_{\alpha\beta} \geq 0$ such that

$$\sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 \leq 1 \quad \forall |\varphi\rangle, |\psi\rangle \in \mathbb{C}^4 . \quad (6.24)$$

Otherwise, if a choice of positive coefficients exists that satisfy (6.24) and for which

$$\sum_{(\alpha,\beta)\in I} \lambda_{\alpha\beta} > \frac{N_I}{4}, \quad (6.25)$$

then a lattice-state ρ_I is entangled.

Before drawing concrete conclusions from this result, we examine the entanglement criteria in Propositions (2) and (3) in the light of the diagonal structure of witnessing maps which is the main result of the previous section.

Example 32 *The states considered in Example (28) were found to be entangled by showing that they do not remain positive under the action of $\text{id} \otimes \Gamma_t$ where*

$$\Gamma^t = g_{00}(t) S_{00} + \sum_{i=1}^3 \left(g_{0i}(t) S_{0i} + g_{i0}(t) S_{i0} \right), \quad (6.26)$$

with

$$\begin{aligned} g_{00}(t) &= \frac{1 + 3e^{-4t}}{4} \frac{3 + e^{-4t}}{4}, \\ g_{0i}(t) &= \varepsilon_i \frac{1 + 3e^{-4t}}{4} \frac{1 - e^{-4t}}{4}, \\ g_{i0}(t) &= \frac{1 - e^{-4t}}{4} \frac{3 + e^{-4t}}{4}, \end{aligned}$$

was proved to be a positive map from $M_4(\mathbb{C})$ into itself. This map, expressed by means of the notation of the last Example in chapter 4 (4.25), is already in diagonal form; the diagonal completely positive maps associated to it by Størmer Theorem (4.26) have the form

$$\begin{aligned} \Lambda^{cp}(t) &= \text{Tr} - \frac{\Gamma^t}{\mu} \\ &= \left(\frac{1}{4} - \frac{g_{00}(t)}{\mu} \right) S_{00} \\ &+ \sum_{i=1}^3 \left[\left(\frac{1}{4} - \frac{g_{0i}(t)}{\mu} \right) S_{0i} + \left(\frac{1}{4} - \frac{g_{i0}(t)}{\mu} \right) S_{i0} \right] + \frac{1}{4} \sum_{\alpha,\beta \neq 0} S_{\alpha\beta}, \end{aligned} \quad (6.27)$$

with μ which has to be adjusted taking into account that

$$g_{0i}(t) \leq \frac{1}{16}, \quad g_{i0}(t) \leq \frac{1}{16}, \quad g_{00}(t) \leq 1.$$

Then, complete positivity of the map Λ^{cp} is guaranteed by $\mu \geq \frac{1}{4}$ which yields

$$\begin{aligned}\lambda_{00}(t) &= \frac{1}{4} - \frac{g_{00}(t)}{\mu} \geq 0 \\ \lambda_{0i}(t) &= \frac{1}{4} - \frac{g_{0i}(t)}{\mu} \geq 0, \\ \lambda_{i0}(t) &= \frac{1}{4} - \frac{g_{i0}(t)}{\mu} \geq 0 \\ \lambda_{ij} &= \frac{1}{4} .\end{aligned}$$

These coefficients surely satisfy condition (6.24) as the latter just reflects the positivity of the originating map Γ^t ; they also satisfy condition (6.25). Indeed,

$$\begin{aligned}\sum_{\alpha, \beta \in I} \lambda_{\alpha\beta}(t) &= \frac{N_I}{4} \tag{6.28} \\ &- \frac{1}{\mu} \sum_{\alpha, \beta \in I} \left[g_{00}(t) \delta_{\alpha,0} \delta_{\beta,0} + g_{0\beta}(t) \delta_{\alpha,0} + g_{\alpha 0}(t) \delta_{\beta,0} \right] \\ &\stackrel{t \rightarrow 0}{\simeq} \frac{N_I}{4} - \frac{1}{\mu} \sum_{\alpha, \beta \in I} \left[(1 - 4t) \delta_{\alpha,0} \delta_{\beta,0} + t(\delta_{\alpha,0} \varepsilon_\beta + \delta_{\beta,0}) \right] \tag{6.29}\end{aligned}$$

For both subsets in (28), the second term in (6.29) is negative due to $\varepsilon_2 = -1$. Thus, $\sum_{\alpha, \beta \in I} \lambda_{\alpha\beta}(t) > \frac{N_I}{4}$ for small times.

Example 33 Let us now consider the lattice state in Example (29):

$$N_I = 10 : \begin{array}{c|c|c|c|c} 3 & \times & & & \times \\ 2 & & \times & \times & \\ \hline 1 & \times & \times & & \times \\ 0 & \times & \times & & \times \\ \hline 0 & 1 & 2 & 3 & \end{array} . \tag{6.30}$$

In [6], it has been shown to be entangled by using the following positive map

$$M_4(\mathbb{C}) \ni X \mapsto \Phi_V[X] = \text{Tr}[X] - \left(\text{T}[X] + \mathcal{V}[X] \right), \quad \mathcal{V}[X] = V^\dagger X V, \tag{6.31}$$

consisting of the trace map to which one subtracts the transposition map and a completely positive map \mathcal{V} constructed with a 4×4 matrix V such that, in the standard representation,

$$V = \sum_{\alpha \neq 2} v_{\alpha 2} \sigma_{\alpha 2} + \sum_{\beta \neq 2} v_{2\beta} \sigma_{2\beta} = -V^T, \quad \sum_{\alpha \neq 2} (|v_{\alpha 2}|^2 + |v_{2\alpha}|^2) = 1. \tag{6.32}$$

In this way,

$$\Phi_V[|\psi\rangle\langle\psi|] = 1 - |\psi^*\rangle\langle\psi^*| - V^\dagger |\psi\rangle\langle\psi| V = 1 - P - Q ,$$

where P and Q are orthogonal one-dimensional projections and thus ensure the positivity of the map.

Because of \mathcal{V} , the map Φ_V is non-diagonal in the maps $S_{\alpha\beta}$: in order to illustrate the content of Proposition (5) we diagonalize it. Using

$$M_4(\mathbb{C}) \ni X \mapsto T[X] = \frac{1}{4} \sum_{\alpha,\beta=0}^3 \varepsilon_\alpha \varepsilon_\beta S_{\alpha\beta}[X] , \quad S_{\alpha\beta}[X] = \sigma_{\alpha\beta} X \sigma_{\alpha\beta} . \quad (6.33)$$

one gets

$$\Phi_V^{diag} = \sum_{\alpha \neq 2} \left(\left(\frac{1}{2} - |v_{\alpha 2}|^2 \right) S_{\alpha 2} + \left(\frac{1}{2} - |v_{2\beta}|^2 \right) S_{2\beta} \right) .$$

The mean value of the Choi matrix of Φ_V^{diag} with respect to the lattice state in (6.30) reads

$$\text{Tr} \left(\rho_I \text{id} \otimes \Phi_V^{diag}[P_+^4] \right) = \frac{1}{N_I} \left(\frac{1}{2} - |v_{12}|^2 \right)$$

and becomes negative choosing $|v_{12}|^2 > 1/2$ hence revealing the entanglement of ρ_I .

Proposition associates to Φ_V^{diag} completely positive maps of the form

$$\begin{aligned} \Lambda^{CP} &= \text{Tr} - \frac{\Phi_V^{diag}}{\mu} = \sum_{\alpha \neq 2} \left(\frac{1}{4} - \frac{1}{2\mu} \frac{|v_{\alpha 2}|^2}{\mu} \right) S_{\alpha 2} \\ &+ \sum_{\beta \neq 2} \left(\frac{1}{4} - \frac{1}{2\mu} + \frac{|v_{2\beta}|^2}{\mu} \right) S_{2\beta} + \frac{1}{4} \left(S_{22} + \sum_{\alpha \neq 2, \beta \neq 2} S_{\alpha\beta} \right) , \end{aligned}$$

whose coefficients can always be made positive by choosing $\mu \geq 2$. The sum of the coefficients corresponding to the subset I of the lattice state in (6.30) yields

$$\sum_{\alpha, \beta \in I} \lambda_{\alpha\beta} = \frac{N_I}{4} - \frac{1}{\mu} \left(\frac{1}{2} - |v_{12}|^2 \right) > \frac{N_I}{4}$$

for the choice of v_{12} which exposes the entanglement of ρ_I , in agreement with (6.25).

6.4 Separable Lattice States

In absence of a positive map that witness the entanglement of a lattice state ρ_I , one can check its separability by trying to express it as a convex combination by other lattice states that are known to be separable. For some ρ_I this is feasible as shown in [6]; for instance, consider the lattice state

$$\rho_I = \frac{1}{8} \left(P_{11} + P_{12} + P_{13} + P_{21} + P_{23} + P_{31} + P_{32} + P_{33} \right).$$

According to Proposition (1), it is PPT and is also separable; indeed, the defining subset I splits as follows

$$\begin{array}{c} \begin{array}{c|ccc} 3 & & \times & \times & \times \\ \hline 2 & & \times & & \times \\ \hline 1 & & \times & \times & \times \\ \hline 0 & & & & \\ \hline \hline & 0 & 1 & 2 & 3 \\ \hline \end{array} \\ \underbrace{\hspace{10em}} \\ I \end{array} = \begin{array}{c} \begin{array}{c|ccc} 3 & & \times & \times & \\ \hline 2 & & & & \\ \hline 1 & & \times & \times & \\ \hline 0 & & & & \\ \hline \hline & 0 & 1 & 2 & 3 \\ \hline \end{array} \\ \underbrace{\hspace{10em}} \\ I_1 \end{array} + \begin{array}{c} \begin{array}{c|ccc} 3 & & & & \\ \hline 2 & & \times & & \times \\ \hline 1 & & \times & & \times \\ \hline 0 & & & & \\ \hline \hline & 0 & 1 & 2 & 3 \\ \hline \end{array} \\ \underbrace{\hspace{10em}} \\ I_2 \end{array} \\ + \begin{array}{c} \begin{array}{c|ccc} 3 & & & \times & \times \\ \hline 2 & & & & \\ \hline 1 & & & \times & \times \\ \hline 0 & & & & \\ \hline \hline & 0 & 1 & 2 & 3 \\ \hline \end{array} \\ \underbrace{\hspace{10em}} \\ I_3 \end{array} + \begin{array}{c} \begin{array}{c|ccc} 3 & & \times & & \times \\ \hline 2 & & \times & & \times \\ \hline 1 & & & & \\ \hline 0 & & & & \\ \hline \hline & 0 & 1 & 2 & 3 \\ \hline \end{array} \\ \underbrace{\hspace{10em}} \\ I_4 \end{array} . \end{array}$$

The 4-point subsets I_i are not disjoint, but all points contribute exactly twice to I , thence one rewrites

$$\rho_I = \frac{1}{4} \sum_{i=1}^4 \rho_{I_i},$$

in terms of rank-4 lattice states corresponding to the subsets I_i . The result follows since the criterion of Proposition (1) ensures that they are all PPT [35].

6.4.1 Special Quadruples

A more general sufficient condition for the separability of lattice states can be derived by introducing the notion of *special quadruples*.

Definition 28 *Special Quadruples*

A special quadruple Q is any subset of the square lattice L_{16} consisting of 4 points (α, β) such that there exist $|\varphi\rangle, |\psi\rangle \in \mathbb{C}^4$ for which

$$\frac{1}{4} \sum_{(\alpha, \beta) \in Q} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 = 1. \quad (6.34)$$

Given a lattice point $(\alpha, \beta) \in L_{16}$, we will denote by $Q_{\alpha\beta} \in \mathcal{Q}$ any special quadruple containing (α, β) , by $\mathcal{Q}_{\alpha\beta}$ the set of such quadruples and by $n_{\alpha\beta}$ its cardinality.

Example 34 Consider the lattice state:

$$\rho_4 = \frac{1}{4}(P_{02} + P_{03} + P_{12} + P_{13})$$

$$N_I = 4 : \begin{array}{c|c|c|c|} 3 & \times & \times & & \\ \hline 2 & \times & \times & & \\ \hline 1 & & & & \\ \hline 0 & & & & \\ \hline & 0 & 1 & 2 & 3 \end{array}.$$

By choosing $|\varphi\rangle = |+-\rangle$ and $|\psi\rangle = |++\rangle$, where $\sigma_2|\pm\rangle = \mp i|\mp\rangle$ and $\sigma_3|\pm\rangle = |\mp\rangle$, we see that the set $\{\sigma_{02}, \sigma_{03}, \sigma_{12}, \sigma_{13}\}$ satisfies (6.34).

Example 35 Some more examples of special quadruples are the following lattice states:

$$\begin{array}{c|c|c|c|} 3 & & & & \times \\ \hline 2 & & & \times & \\ \hline 1 & & \times & & \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array}, \quad \begin{array}{c|c|c|c|} 3 & \times & & & \\ \hline 2 & & \times & & \\ \hline 1 & & & \times & \\ \hline 0 & & & & \times \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

$$\begin{array}{c|c|c|c|} 3 & & & \times & \\ \hline 2 & & & & \times \\ \hline 1 & & \times & & \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array}, \quad \begin{array}{c|c|c|c|} 3 & & \times & & \\ \hline 2 & & & \times & \\ \hline 1 & & & & \times \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

Since $|\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 = 1$ if and only if $\sigma_{\alpha\beta} | \psi \rangle = \eta | \phi \rangle$ with η a pure phase, a set of 4 points $\{(\alpha_j, \beta_j)\}_{j=0}^3 \subset I$ is a special quadruple if and only there exist $|\psi\rangle, |\phi\rangle \in \mathbb{C}^4$ such that

$$\sigma_{\alpha_j \beta_j} | \psi \rangle = e^{i\chi_j} | \phi \rangle \quad \forall j = 0, 1, 2, 3. \quad (6.35)$$

Let us focus upon \mathcal{Q}_{00} , the set of all special quadruples $\{(0, 0), (\alpha_1, \beta_1), (\alpha_2, \beta_2), (\alpha_3, \beta_3)\}$ containing the point $(0, 0)$. Each of them is obtained from the fact that, using (6.35) with $(\alpha_0, \beta_0) = (00)$,

$$|\varphi\rangle = |\psi\rangle \Rightarrow \sigma_{\alpha_j \beta_j} |\psi\rangle = e^{i\chi_j} |\psi\rangle, \quad j = 1, 2, 3.$$

Therefore, the $\sigma_{\alpha\beta}$ of a special quadruple must commute. Indeed,

$$\begin{aligned} [\sigma_{\alpha\beta}, \sigma_{\gamma\delta}] &= \sigma_\alpha \sigma_\gamma \otimes \sigma_\beta \sigma_\delta - \sigma_\gamma \sigma_\alpha \otimes \sigma_\delta \sigma_\beta \\ &= (1 - \epsilon_{\alpha\gamma} \epsilon_{\beta\delta}) \sigma_\alpha \sigma_\gamma \otimes \sigma_\beta \sigma_\delta \end{aligned} \quad (6.36)$$

$$= (1 - \epsilon_{\alpha\gamma} \epsilon_{\beta\delta}) \eta_{\alpha\gamma}^\mu \eta_{\beta\delta}^\nu \sigma_{\mu\nu}, \quad (6.37)$$

where $\eta_{\alpha\beta}^\mu$ are the coefficients ± 1 and $\pm i$, introduced in Definition (27), such that $\sigma_\alpha \sigma_\beta = \eta_{\alpha\beta}^\mu \sigma_\mu$ and the 16 coefficients $\epsilon_{\alpha\gamma} = \pm 1$ are given by the Pauli matrix commutation relations, which can be considered as the elements of the following matrix:

$$\epsilon = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \quad (6.38)$$

It thus follows that $[\sigma_{\alpha\beta}, \sigma_{\gamma\delta}] |\psi\rangle = 0$ if and only if $\epsilon_{\alpha\gamma} \epsilon_{\beta\delta} = 1$, whence \mathcal{Q}_{00} consists of the following 15 special quadruples (omitting the point $(0, 0)$ common to all of them)

$$\begin{aligned} &\{(0, 1); (1, 0); (1, 1)\} \quad \{(0, 2); (2, 0); (2, 2)\} \quad \{(0, 3); (3, 0); (3, 3)\} \\ &\{(0, 1); (2, 1); (2, 0)\} \quad \{(0, 2); (1, 2); (1, 0)\} \quad \{(0, 3); (1, 3); (1, 0)\} \\ &\{(0, 1); (3, 1); (3, 0)\} \quad \{(0, 2); (3, 2); (3, 0)\} \quad \{(0, 3); (2, 3); (2, 0)\} \\ &\{(1, 1); (2, 2); (3, 3)\} \quad \{(1, 2); (2, 3); (3, 1)\} \\ &\{(1, 1); (2, 3); (3, 2)\} \quad \{(1, 3); (2, 2); (3, 1)\} \\ &\{(1, 2); (2, 1); (3, 3)\} \quad \{(1, 3); (2, 1); (3, 2)\}. \end{aligned} \quad (6.39)$$

Knowledge of \mathcal{Q}_{00} is sufficient to derive the form of all $\mathcal{Q}_{\alpha\beta}$; in order to prove this fact, let us introduce the following family of maps indexed by lattice points $(\alpha, \beta) \in L_{16}$:

$$\tau_{\alpha\beta} : L_{16} \mapsto L_{16}, \quad \tau_{\alpha\beta}[(\gamma, \delta)] = ([\alpha, \gamma], [\beta, \delta]), \quad (6.40)$$

where the map $(\alpha, \gamma) \mapsto [\alpha, \gamma]$ has been introduced in Definition (27). It follows that the maps $\tau_{\alpha\beta}$ are invertible: $\tau_{\alpha\beta} \circ \tau_{\alpha\beta}[(\gamma, \delta)] = (\gamma, \delta)$. Given a subset $I = \{(\alpha_i, \beta_i)\} \subseteq L_{16}$, $\tau_{\alpha\beta}[I]$ will denote the subset $\{\tau_{\alpha\beta}[(\alpha_i, \beta_i)]\}$.

Lemma 4 *The map $\mathcal{Q}_{\alpha\beta} \ni Q \mapsto \tau_{\alpha\beta}[Q] \in \mathcal{Q}_{00}$ is one-to-one.*

Proof: If $Q = \{(\alpha_j, \beta_j)\}_{j=0}^3$ is a special quadruple for $(\alpha, \beta) = (\alpha_0, \beta_0)$, then $\sigma_{\alpha_j\beta_j}|\psi\rangle = e^{i\chi_j}|\phi\rangle$ for some $|\psi\rangle, |\phi\rangle \in \mathbb{C}^4$. Right multiplication by $\sigma_{\alpha\beta}$ yields:

$$\begin{aligned} \sigma_{\alpha\beta}\sigma_{\alpha_j\beta_j}|\psi\rangle &= \sigma_{\alpha}\sigma_{\alpha_j} \otimes \sigma_{\beta}\sigma_{\beta_j}|\psi\rangle \\ &= \sigma_{[\alpha, \alpha_j], [\beta, \beta_j]}|\psi\rangle \\ &= e^{i\chi'_j}\sigma_{\alpha\beta}|\phi\rangle. \end{aligned}$$

Then, $\{([\alpha, \alpha_j], [\beta, \beta_j])\}_{j=0}^3 = \tau_{\alpha\beta}[Q]$ is a special quadruple for $(0, 0)$ exposed by the vectors $|\psi\rangle$ and $\sigma_{\alpha\beta}|\phi\rangle$. The one-to-one correspondence follows from the invertibility of the maps $\tau_{\alpha\beta}$. \square

It is easy to check that all $Q \in \mathcal{Q}_{00}$ in (6.40) give rise to lattice states ρ_Q that satisfy the criterion in Proposition (1) for being PPT; this is also true for lattice states corresponding to $Q \in \mathcal{Q}_{\alpha\beta}$: indeed, they are obtained from the previous ones by the local action $\sigma_{\alpha\beta} \otimes \mathbb{1}\rho_Q\sigma_{\alpha\beta} \otimes \mathbb{1}$.

Lemma 5 *Properties of the special quadruples \mathcal{Q}_{00}*

1. *Given two commuting $\sigma_{\alpha\beta}$ and $\sigma_{\gamma\delta}$ there is a unique $\sigma_{\mu\nu}$ commuting with both of them.*
2. *Two quadruples cannot have more than one pair (α, β) in common; otherwise they would coincide.*
3. *Each $\sigma_{\alpha\beta}$ commutes with 6 $\sigma_{\gamma\delta}$ different from itself and from σ_{00}*
4. *Each $\sigma_{\alpha\beta}$ belongs to three different quadruples.*
5. *The pairs $(\gamma, \delta) \neq (\alpha, \beta)$ belonging to the 3 quadruples with (α, β) in common correspond to anti-commuting σ 's.*

Proof: The first and second property follow directly from (6.37), they implies the third and fourth ones, while the last one is a consequence of the fourth property. \square

The following Lemma shows that they are indeed separable as dictated by the general result in [35].

Lemma 6 *Let $I \subset L_{16}$; all positive coefficients $\lambda_{\alpha\beta}$ satisfying inequality (6.23) are such that $\sum_{(\alpha,\beta) \in Q} \lambda_{\alpha\beta} \leq 1$ for all special quadruples $Q \subseteq I$.*

Proof: Recall the trace map (4.25):

$$M_4(\mathbb{C}) \ni X \mapsto \text{Tr}[X] = \frac{1}{4} \sum_{\alpha,\beta=0}^3 S_{\alpha\beta}[X] .$$

It follows that

$$1 = \langle \phi | \text{Tr}[\psi \langle \psi | | \phi \rangle] = \frac{1}{4} \sum_{(\alpha,\beta) \in L_{16}} |\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 .$$

Consider a given special quadruple $Q \in L_{16}$, then we can split (6.4.1) into two terms:

$$\begin{aligned} 1 &= \langle \phi | \text{Tr}[\psi \langle \psi | | \phi \rangle] \\ &= \frac{1}{4} \sum_{(\alpha,\beta) \in L_{16}} |\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 \\ &= \frac{1}{4} \sum_{(\alpha,\beta) \in Q} |\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 + \frac{1}{4} \sum_{(\alpha,\beta) \in L_{16} \setminus Q} |\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 . \end{aligned}$$

Therefore, if $|\psi\rangle$ and $|\phi\rangle$ satisfy (6.34) for a given special quadruple Q , then $\langle \phi | \sigma_{\alpha\beta} | \psi \rangle = 0$ for all (α, β) not belonging to Q , i.e. the last term in the above equality vanishes, on the other hand $|\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 = 1$ for all $(\alpha, \beta) \in Q$.

Consider now a set of positive coefficients $\lambda_{\alpha\beta}$ satisfying

$$\sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} |\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 \leq 1 \quad \forall |\psi\rangle, |\phi\rangle \in \mathbb{C}^4 .$$

If $Q \subset I$ is a special quadruple and $|\psi\rangle, |\phi\rangle$ satisfy (6.34), then

$$1 \geq \sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} |\langle \phi | \sigma_{\alpha\beta} | \psi \rangle|^2 = \sum_{(\alpha,\beta) \in Q} \lambda_{\alpha\beta} .$$

□

Corollary 3 *Each rank 4 lattice state ρ_I with $I \in \mathcal{Q}$ is separable.*

Proof: Given any four positive coefficients $\{\lambda_{\alpha\beta}\}_{(\alpha,\beta) \in I}$ satisfying (6.24), from the assumption and the previous Lemma it follows that:

$$\sum_{(\alpha,\beta) \in I = Q_{\alpha_0\beta_0}} \lambda_{\alpha\beta} \leq 1 ,$$

since I is a special quadruple for each of its points (α_0, β_0) . Summing over all $(\alpha_0, \beta_0) \in I$, each point is counted four times, thus

$$\begin{aligned} 4 \sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} &= \sum_{(\alpha_0,\beta_0) \in I} \sum_{(\alpha,\beta) \in Q_{\alpha_0\beta_0}} \lambda_{\alpha\beta} \leq 4 \\ &\implies \sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} \leq 1 = \frac{N_I}{4} , \end{aligned}$$

whence the criterion (6.24) for separability is satisfied. \square

6.4.2 Separability and Quadruples

The main tool in the previous proof is the fact that all points in I belongs to a same number, 1, of special quadruples, I itself; that is each point in I belongs to a special quadruple contained in I .

Because of its importance in what follows, we now study this occurrence in more detail considering a higher rank lattice state corresponding to the subset

$$I = \{(0, 0), (1, 1), (1, 2), (1, 3), (2, 1), (2, 2), (2, 3), (3, 1), (3, 2), (3, 3)\}$$

$$\begin{array}{c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & & \times & \times & \times \\ \hline 1 & & \times & \times & \times \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} . \quad (6.41)$$

For $(0, 0)$, of the set (6.40) the following quadruples are contained in I :

$$\begin{array}{c}
 \begin{array}{|c|c|c|c|} \hline 3 & & & \times \\ \hline 2 & & & \times \\ \hline 1 & & \times & \\ \hline 0 & \times & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}
 \quad , \quad
 \begin{array}{|c|c|c|c|} \hline 3 & & & \times \\ \hline 2 & & & \times \\ \hline 1 & & \times & \\ \hline 0 & \times & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array} \\
 \\
 \begin{array}{c}
 \begin{array}{|c|c|c|c|} \hline 3 & & \times & \\ \hline 2 & & & \times \\ \hline 1 & & & \times \\ \hline 0 & \times & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}
 \quad , \quad
 \begin{array}{|c|c|c|c|} \hline 3 & & & \times \\ \hline 2 & & \times & \\ \hline 1 & & & \times \\ \hline 0 & \times & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array} \\
 \\
 \begin{array}{c}
 \begin{array}{|c|c|c|c|} \hline 3 & & \times & \\ \hline 2 & & & \times \\ \hline 1 & & & \times \\ \hline 0 & \times & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}
 \quad , \quad
 \begin{array}{|c|c|c|c|} \hline 3 & & & \times \\ \hline 2 & & \times & \\ \hline 1 & & & \times \\ \hline 0 & \times & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}
 \end{array}
 \tag{6.42}$$

Given another point $I \ni (\alpha, \beta) \neq (0, 0)$, consider the lattice state $\rho_{I_{\alpha\beta}} = \sigma_{\alpha\beta} \otimes \mathbb{1} \rho_I \sigma_{\alpha\beta} \otimes \mathbb{1}$, where $I_{\alpha\beta} \subseteq L_{16}$ is the set I transformed into $\tau_{\alpha\beta}[I]$ by the map $\tau_{\alpha\beta}$ introduced in Lemma (6.40). The point $(\alpha, \beta) \in I$ is mapped into $(0, 0) \in I_{\alpha\beta}$ and, by Lemma (4), it belongs to 5 special quadruples contained in $I_{\alpha\beta}$ that are images under $\tau_{\alpha\beta}$ of the 5 special quadruples relative to $(0, 0) \in I$. Therefore, each point $(\alpha, \beta) \in I$ belongs to 5 special quadruples contained in I .

Example 36 *As a concrete example, consider the following quadruples*

$$\underbrace{\begin{array}{|c|c|c|c|} \hline 3 & & & \times & \times \\ \hline 2 & & & & \\ \hline 1 & & & \times & \times \\ \hline 0 & & & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}}_{Q_1}
 \quad , \quad
 \underbrace{\begin{array}{|c|c|c|c|} \hline 3 & & & & \\ \hline 2 & & \times & & \times \\ \hline 1 & & \times & & \times \\ \hline 0 & & & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}}_{Q_2}
 \quad , \quad
 \underbrace{\begin{array}{|c|c|c|c|} \hline 3 & & \times & \times & \\ \hline 2 & & \times & \times & \\ \hline 1 & & & & \\ \hline 0 & & & & \\ \hline 0 & 1 & 2 & 3 \\ \hline \end{array}}_{Q_3}
 \tag{6.43}$$

They are contained in I but do not belong to \mathcal{Q}_{00} ; consider the point $(3, 3) \in$

Q_1 , it is mapped into $(0,0)$ by τ_{33} which sends I and Q_1 into

$$\begin{array}{l}
 I_{33} = \tau_{33}[I] = \begin{array}{c|c|c|c}
 3 & & & \times \\
 \hline
 2 & \times & \times & \times \\
 \hline
 1 & \times & \times & \times \\
 \hline
 0 & \times & \times & \times \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array} \\
 \\
 \tau_{33}[Q_1] = \begin{array}{c|c|c|c}
 3 & & & \\
 \hline
 2 & \times & & \times \\
 \hline
 1 & & & \\
 \hline
 0 & \times & & \times \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array} \in \mathcal{Q}_{00} .
 \end{array}$$

One thus checks that $\tau_{33}[Q_1]$ is a special quadruple contained in the transformed subset I_{33} . Analogously, τ_{32} , respectively τ_{12} , map $(3,2)$, respectively $(1,2)$, into $(0,0)$ and I , Q_2 , respectively Q_3 , into

$$\begin{array}{l}
 I_{32} = \tau_{32}[I] = \begin{array}{c|c|c|c}
 3 & \times & \times & \times & \times \\
 \hline
 2 & & & & \times \\
 \hline
 1 & & \times & \times & \\
 \hline
 0 & \times & \times & \times & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array} \\
 \\
 \tau_{32}[Q_2] = \begin{array}{c|c|c|c}
 3 & \times & & \times & \\
 \hline
 2 & & & & \\
 \hline
 1 & & & & \\
 \hline
 0 & \times & & \times & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array} \in \mathcal{Q}_{00} \\
 \\
 I_{12} = \tau_{12}[I] = \begin{array}{c|c|c|c}
 3 & \times & & \times & \times \\
 \hline
 2 & & \times & & \\
 \hline
 1 & & & \times & \times \\
 \hline
 0 & \times & \times & \times & \times \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array} \\
 \\
 \tau_{12}[Q_3] = \begin{array}{c|c|c|c}
 3 & & & & \\
 \hline
 2 & & & & \\
 \hline
 1 & \times & & & \times \\
 \hline
 0 & \times & & & \times \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array} \in \mathcal{Q}_{00} .
 \end{array}$$

Definition 29 Given a subset $I \subseteq L_{16}$ we shall term a covering of I any collection \mathcal{Q}_I of special quadruples (not necessarily disjoint) contained in I and denote by $N_{\mathcal{Q}_I}$ its cardinality. Further, we shall denote by $M_{\alpha\beta}^{\mathcal{Q}_I}$ the number of special quadruples in \mathcal{Q}_I that contains the point $(\alpha, \beta) \in I$ and refer to them as to the multiplicities of \mathcal{Q}_I . Finally, we shall call uniform any covering \mathcal{Q}_I of I of constant multiplicity: $M_{\alpha\beta}^{\mathcal{Q}_I} = M_{\mathcal{Q}_I}$, for all $(\alpha, \beta) \in I$.

The usefulness of uniform coverings can be seen as follows: summations over $(\alpha, \beta) \in I$ can be split into sums of contributions from the special quadruples of any covering by taking into account to how many special quadruples $M_{\alpha\beta}^{\mathcal{Q}_I}$ a point (α, β) does belong:

$$\sum_{(\alpha, \beta) \in I} M_{\alpha\beta}^{\mathcal{Q}_I} \lambda_{\alpha\beta} = \sum_{Q \in \mathcal{Q}_I} \sum_{(\alpha, \beta) \in Q} \lambda_{\alpha\beta} ,$$

whence, if the covering is uniform with multiplicity $M_{\mathcal{Q}_I}$,

$$\sum_{(\alpha, \beta) \in I} \lambda_{\alpha\beta} = \frac{1}{M_{\mathcal{Q}_I}} \sum_{Q \in \mathcal{Q}_I} \sum_{(\alpha, \beta) \in Q} \lambda_{\alpha\beta} .$$

Lemma 7 Let $I \subseteq L_{16}$ contain N_I points and \mathcal{Q}_I be a uniform covering of I of cardinality $N_{\mathcal{Q}_I}$ and multiplicity $M_{\mathcal{Q}_I}$; then,

$$N_{\mathcal{Q}_I} = \frac{M_{\mathcal{Q}_I} N_I}{4} . \quad (6.44)$$

Proof: Each of the N_I points in I belongs to n_I special quadruples each containing 4 points of I . \square

In the case of (6.41), the special quadruples in (6.42) form a covering of I , but not a uniform one as its multiplicities are

$$\begin{aligned} n_{00}^{\mathcal{Q}_I} &= 5 , \\ n_{11}^{\mathcal{Q}_I} &= n_{22}^{\mathcal{Q}_I} = n_{23}^{\mathcal{Q}_I} = n_{32}^{\mathcal{Q}_I} = n_{13}^{\mathcal{Q}_I} = n_{31}^{\mathcal{Q}_I} = 2 , \\ n_{33}^{\mathcal{Q}_I} &= n_{21}^{\mathcal{Q}_I} = n_{12}^{\mathcal{Q}_I} = 1 . \end{aligned}$$

A uniform covering I is provided by 2 special quadruples in (6.42) and the

3 in (6.43):

$$\begin{array}{c}
\begin{array}{c|c|c|c|c}
3 & & \times & \times & \times \\
\hline
2 & & \times & \times & \times \\
\hline
1 & & \times & \times & \times \\
\hline
0 & \times & & & \\
\hline
0 & 1 & 2 & 3 & \\
\hline
\end{array} & = & \begin{array}{c|c|c|c|c}
3 & & & & \times \\
\hline
2 & & & \times & \\
\hline
1 & & \times & & \\
\hline
0 & \times & & & \\
\hline
0 & 1 & 2 & 3 & \\
\hline
\end{array} & + & \begin{array}{c|c|c|c|c}
3 & & \times & & \\
\hline
2 & & & & \times \\
\hline
1 & & & \times & \\
\hline
0 & \times & & & \\
\hline
0 & 1 & 2 & 3 & \\
\hline
\end{array} \\
+ & & \begin{array}{c|c|c|c|c}
3 & & & \times & \times \\
\hline
2 & & & & \\
\hline
1 & & & \times & \times \\
\hline
0 & & & & \\
\hline
0 & 1 & 2 & 3 & \\
\hline
\end{array} & + & \begin{array}{c|c|c|c|c}
3 & & & & \\
\hline
2 & & \times & & \times \\
\hline
1 & & \times & & \times \\
\hline
0 & & & & \\
\hline
0 & 1 & 2 & 3 & \\
\hline
\end{array} \\
+ & & \begin{array}{c|c|c|c|c}
3 & & \times & \times & \\
\hline
2 & & \times & \times & \\
\hline
1 & & & & \\
\hline
0 & & & & \\
\hline
0 & 1 & 2 & 3 & \\
\hline
\end{array} . & & (6.45)
\end{array}$$

Since all points of I belongs to exactly 2 special quadruples contained in I , this uniform covering has multiplicity $n_I^{\mathcal{Q}} = 2$:

$$4 \times N_{\mathcal{Q}_I} = 20 = n_I N_I = 2 \times 10 .$$

This is also a minimal covering among the uniform ones; indeed, by (6.44), as $N_{\mathcal{Q}_I}$ is an integer, $4N_{\mathcal{Q}} = 10 \times n_I$ can only be satisfied by $n_I = 2m$, $\mathbb{N} \ni m \geq 1$.

It thus follows that the lattice state corresponding to the subset (6.41) is separable as it can be decomposed into a convex combination of PPT separable rank-4 lattice states:

$$\rho_I = \frac{1}{10} \left(P_{00} + P_{11} + P_{12} + P_{13} + P_{21} + P_{22} + P_{23} + P_{31} + P_{32} + P_{33} \right) = \frac{1}{5} \sum_{j=1}^5 \rho_{\mathcal{Q}_j} ,$$

where $\{\mathcal{Q}_j\}_{j=1}^5$ are the special quadruples of the minimal covering (6.45).

The previous argument proves the separability of the lattice state (6.41), an issue which left unsettled in [6]; it can be generalized as follows.

Proposition 6 *Suppose $I \subseteq L_{16}$ is a subset with minimal covering \mathcal{Q}_I of cardinality $N_{\mathcal{Q}_I}$ and multiplicity $M_{\mathcal{Q}_I}$, then ρ_I can be convexly decomposed as*

$$\rho_I = \frac{1}{N_{\mathcal{Q}_I}} \sum_{j=1}^{N_{\mathcal{Q}_I}} \rho_{\mathcal{Q}_j} , \quad (6.46)$$

where $\mathcal{Q}_j \subseteq I$ are the special quadruples in \mathcal{Q} , and is thus separable.

Proof: Let Q_j , $1 \leq j \leq N_{\mathcal{Q}_I}$, be the elements of the minimal covering \mathcal{Q}_I . From Lemma (6) it follows that

$$\begin{aligned} N_{\mathcal{Q}_I} &\geq \sum_{j=1}^{N_{\mathcal{Q}_I}} \sum_{(\alpha,\beta) \in Q_j} \lambda_{\alpha\beta} = M_{\mathcal{Q}_I} \sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} \\ \implies \sum_{(\alpha,\beta) \in I} \lambda_{\alpha\beta} &\leq \frac{N_{\mathcal{Q}_I}}{M_{\mathcal{Q}_I}} = \frac{N_I}{4} \end{aligned}$$

so that Corollary (2) ensures separability. Furthermore, using (6.44),

$$\begin{aligned} \rho_I &= \frac{1}{N_I} \sum_{(\alpha,\beta) \in I} P_{\alpha\beta} \\ &= \frac{4}{M_{\mathcal{Q}_I} N_{\mathcal{Q}_I}} \sum_{j=1}^{N_{\mathcal{Q}_I}} \frac{1}{4} \sum_{(\alpha,\beta) \in Q_j} P_{\alpha\beta} \\ &= \frac{1}{N_{\mathcal{Q}_I}} \sum_{j=1}^{Q_I} \rho_{Q_j}. \end{aligned}$$

□

Example 37 *The following lattice states mentioned in [6] were also unknown to be separable:*

$$\rho_8 = \frac{1}{8}(P_{00} + P_{11} + P_{12} + P_{13} + P_{23} + P_{31} + P_{32} + P_{33}),$$

$$\begin{array}{c|c|c|c|c} 3 & & \times & \times & \times \\ 2 & & \times & & \times \\ 1 & & \times & & \times \\ 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} = \begin{array}{c|c|c|c|c} 3 & & & \times & \\ 2 & & & & \times \\ 1 & & \times & & \\ 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} + \begin{array}{c|c|c|c|c} 3 & & & \times & \\ 2 & & \times & & \\ 1 & & & & \times \\ 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} \\ + \begin{array}{c|c|c|c|c} 3 & & \times & & \times \\ 2 & & & & \\ 1 & & \times & & \times \\ 0 & & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} + \begin{array}{c|c|c|c|c} 3 & & \times & & \times \\ 2 & & \times & & \times \\ 1 & & & & \\ 0 & & & & \\ \hline & 0 & 1 & 2 & 3 \end{array}.$$

The next state is:

$$\rho_9 = \frac{1}{9}(P_{00} + P_{11} + P_{12} + P_{13} + P_{21} + P_{23} + P_{31} + P_{32} + P_{33}),$$

$$\begin{array}{c}
 \begin{array}{c|c|c|c}
 3 & & \times & \times \\
 \hline
 2 & & \times & \times \\
 \hline
 1 & & \times & \times \\
 \hline
 0 & \times & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 & = &
 \begin{array}{c|c|c|c}
 3 & & & \times \\
 \hline
 2 & & \times & \times \\
 \hline
 1 & & \times & \\
 \hline
 0 & \times & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 & + &
 \begin{array}{c|c|c|c}
 3 & & \times & \\
 \hline
 2 & & & \times \\
 \hline
 1 & & & \times \\
 \hline
 0 & \times & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \\
 \\
 + & &
 \begin{array}{c|c|c|c}
 3 & & & \times \\
 \hline
 2 & & \times & \\
 \hline
 1 & & & \times \\
 \hline
 0 & \times & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 & + &
 \begin{array}{c|c|c|c}
 3 & & \times & \\
 \hline
 2 & & \times & \\
 \hline
 1 & & & \times \\
 \hline
 0 & \times & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \\
 \\
 + & &
 \begin{array}{c|c|c|c}
 3 & & \times & \times \\
 \hline
 2 & & & \\
 \hline
 1 & & \times & \times \\
 \hline
 0 & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 & + &
 \begin{array}{c|c|c|c}
 3 & & & \times \\
 \hline
 2 & & & \times \\
 \hline
 1 & & & \times \\
 \hline
 0 & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \\
 \\
 + & &
 \begin{array}{c|c|c|c}
 3 & & \times & \times \\
 \hline
 2 & & & \\
 \hline
 1 & & \times & \times \\
 \hline
 0 & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 & + &
 \begin{array}{c|c|c|c}
 3 & & & \\
 \hline
 2 & & \times & \times \\
 \hline
 1 & & \times & \times \\
 \hline
 0 & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 \\
 \\
 + & &
 \begin{array}{c|c|c|c}
 3 & & \times & \times \\
 \hline
 2 & & \times & \times \\
 \hline
 1 & & & \\
 \hline
 0 & & & \\
 \hline
 & 0 & 1 & 2 & 3
 \end{array}
 .
 \end{array}$$

From Proposition (6) one draws the following conclusions:

Corollary 4 *All the lattice states with $N_I \geq 14$ are separable.*

Proof:

1. $N_I=16$: is trivial.
2. $N_I=15$: As we have seen in (section III of this chapter), every point (α, β) can take part in 15 quadruples. Therefore in L_{16} we have:

$$N_Q = \frac{16 \times 15}{4}.$$

By dropping out one point from the lattice, we decrease the number of quadruples by three for each point and therefore each point has 12

quadruples contained in I:

$$N_Q = \frac{15 \times 12}{4}.$$

3. $N_I = 14$: Here there are two points missing from L_{16} , note that every two given points can share three quadruples. This is easy to verify it; by sending one of the two into the origin $(0, 0)$, one sees that the other one appears in exactly three Q's (section III). Therefore, there are six pairs $(\alpha, \beta) \in I$, where the two points (α_1, β_1) and (α_2, β_2) , remove only five quadruples, leaving 10 special quadruples contained in I. While for the other eight pairs $(\alpha, \beta) \in I$, they remove six quadruples. Therefore any $\rho_1 4$ would look like:

3			×	×
2	×	×	×	×
1	×	×	×	×
0	×	×	×	×
	0	1	2	3

Then one can divide it into two subsets: I_1 : the six elements with 10 special quadruples contained in I, and I_2 : the eight elements with 9 special quadruples contained in I:

$$I_1 = \begin{array}{c|ccc|} 3 & & & \\ \hline 2 & \times & \times & \\ \hline 1 & \times & \times & \\ \hline 0 & \times & \times & \\ \hline & 0 & 1 & 2 & 3 \end{array}, \quad I_2 = \begin{array}{c|ccc|} 3 & & & \times & \times \\ \hline 2 & & & \times & \times \\ \hline 1 & & & \times & \times \\ \hline 0 & & & \times & \times \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

In order to show that all $\rho_1 4$ are separable, we need to show that they satisfy (6.23):

$$\sum_{\alpha, \beta \in I} \lambda_{\alpha\beta} \leq \frac{14}{4}$$

for all choices of the coefficients $\lambda_{\alpha\beta}$ introduced in Corollary 2. But since we can divide $\rho_1 4$ into two subsets, we have:

$$\begin{aligned} \sum_{\alpha, \beta \in I} \lambda_{\alpha\beta} &= \sum_{\alpha, \beta \in I_1} \lambda_{\alpha\beta} + \sum_{\alpha, \beta \in I_2} \lambda_{\alpha\beta} \\ &\leq \frac{N_{I_1}}{4} + \frac{N_{I_2}}{4} \\ &\leq \frac{N_{I_1} + N_{I_2}}{4} = \frac{14}{4}. \end{aligned}$$

Where we have used the separability of the two states ρ_{I_1} and ρ_{I_2} . Indeed in case of $N_I = 14$ the minimum number of special quadruples for every point to be included in I , is equal to $n^* = 2$, which is much less than what happens.

□

6.5 Entanglement and lattice geometry

In this section we single out a family \mathcal{I}_{spec} of geometric patterns such that, if $I \in \mathcal{I}_{spec}$, then ρ_I is surely entangled. Given a sub-set $I \subseteq L_{16}$, choose $\lambda_{\alpha\beta}$ such that for a certain $(\alpha_0, \beta_0) \in I$

$$\lambda_{\alpha_0\beta_0} = \frac{1 + \delta}{4}, \quad \lambda_{\alpha\beta} = \frac{1}{4} \quad \forall (\alpha, \beta) \neq (\alpha_0, \beta_0), \quad (6.47)$$

where $\delta > 0$ is a suitable parameter. Then, $\sum_{(\alpha\beta) \in I} \lambda_{\alpha\beta} = \frac{N_I + \delta}{4} > \frac{N_I}{4}$ and inequality (6.25) in Corollary 2 is satisfied. According to the same corollary, given such a subset I , the corresponding lattice state ρ_I is entangled, if also inequality (6.24) is fulfilled, namely if

$$\exists \delta > 0 \text{ such that } \frac{\delta}{4} |\langle \varphi | \sigma_{\alpha_0\beta_0} | \psi \rangle|^2 + \frac{1}{4} \sum_{(\alpha,\beta) \in I} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 \leq 1, \quad \forall |\varphi\rangle, |\psi\rangle \in \mathbb{C}^4. \quad (6.48)$$

Remark 6 *Suppose that inequality (6.48) can be satisfied by $\delta > 0$ uniformly in the vectors $|\psi\rangle$ and $|\varphi\rangle$. Then, using (4.25) and (4.26), the choice of coefficients in (6.47) corresponds to a witness of the form*

$$\Lambda = \text{Tr} - \Lambda_{cp} = \frac{1}{4} \sum_{(\alpha,\beta) \notin I} S_{\alpha\beta} - \frac{\delta}{4} S_{\alpha_0\beta_0}. \quad (6.49)$$

By comparison with the expression of the transposition in (4.23), one sees that, unlike the 6 negative contribution of the latter, Λ presents only one negative contribution. Yet, for the special subset \mathcal{I}_{spec} , it proves to be more flexible as an entanglement witness.

Clearly, if (α_0, β_0) belongs to a special quadruple contained in I , such a $\delta > 0$ cannot exist; indeed, if $|\psi\rangle$ and $|\varphi\rangle$ satisfy (6.34), then $|\langle\varphi|\sigma_{\alpha_0\beta_0}|\psi\rangle| > 0$ and $\frac{1}{4} \sum_{(\alpha,\beta) \in I} |\langle\varphi|\sigma_{\alpha\beta}|\psi\rangle|^2 = 1$, together with inequality (6.48) yield $\delta = 0$.

We now show that lattice state ρ_I for which not all points of I belong to special quadruples contained in I , such a $\delta > 0$ can indeed be found and thus that they are entangled.

Theorem 20 *Given a lattice state ρ_I , if there exists a point $(\alpha_0, \beta_0) \in I$ such that $Q_{\alpha_0\beta_0} \not\subseteq I$ for all $Q_{\alpha_0\beta_0} \in \mathcal{Q}$, then ρ_I is entangled. We shall call any such I a special sub-set and denote by \mathcal{I}_{spec} their family.*

It is very constructive to present some examples before going through the proof.

Example 38 *According to the last theorem the following state is entangled, as non of the special quadruples of $(0, 0)$ are included in I :*

$$N_I = 8 \quad \begin{array}{c|c|c|c|c} 3 & & & \times & \times \\ \hline 2 & & \times & \times & \\ \hline 1 & & & & \times \\ \hline 0 & \times & & \times & \times \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad (6.50)$$

Another example of such entangled lattice states is the following:

$$N_I = 10 \quad \begin{array}{c|c|c|c|c} 3 & \times & \times & \times & \times \\ \hline 2 & \times & & \times & \\ \hline 1 & & & & \times \\ \hline 0 & \times & \times & \times & \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad (6.51)$$

As we observe the point $(3, 3)$ has no special quadruple contained in I , it can be easily verified when this point is sent to $(0, 0)$, the resulting state is:

$$N_I = 10 \quad \begin{array}{c|c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & \times & & & \\ \hline 1 & & \times & & \times \\ \hline 0 & \times & \times & \times & \times \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

As the last example consider the following state:

$$N_I = 11 \quad \begin{array}{c|c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & \times & & & \\ \hline 1 & & \times & \times & \times \\ \hline 0 & \times & \times & \times & \times \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad (6.52)$$

Also in this case $(0, 0)$ has no special quadruple contained in I .

Proof of Theorem 20:

According to Lemma 4, the point (α_0, β_0) can be transformed into $(0, 0)$ and I into a new set, that we shall denote again by I for sake of simplicity, without altering the entanglement or separability of the transformed ρ_I with respect to the initial one. Then, the assumption of the theorem translates into the fact that no special quadruple in the list (6.40) is contained in I . Having set $(\alpha_0, \beta_0) = (00)$, inequality (6.48) now reads

$$\Delta_{I,\delta}^{\psi,\varphi} = \frac{\delta}{4} |\langle \varphi | \psi \rangle|^2 + \Delta_I^{\psi,\varphi}, \quad \text{where} \quad \Delta_I^{\psi,\varphi} = \frac{1}{4} \sum_{(\alpha,\beta) \in I} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2. \quad (6.53)$$

It proves convenient to introduce the following ψ -dependent 4×4 matrices

$$\widehat{\Delta}_{I,\delta}^{\psi} = \frac{\delta}{4} |\psi\rangle\langle\psi| + \widehat{\Delta}_I^{\psi}, \quad \widehat{\Delta}_I^{\psi} = \frac{1}{4} \sum_{(\alpha,\beta) \in I} \sigma_{\alpha\beta} |\psi\rangle\langle\psi| \sigma_{\alpha\beta}, \quad (6.54)$$

so that one has to prove that

$$\exists \delta > 0 \quad \text{such that} \quad \Delta_{I,\delta}^{\psi,\varphi} = \langle \varphi | \widehat{\Delta}_{I,\delta}^{\psi} | \varphi \rangle \leq 1 \quad \forall |\psi\rangle, |\varphi\rangle \in \mathbb{C}^4. \quad (6.55)$$

Further, from (4.25)

$$\widehat{\Delta}_I^{\psi} + \widehat{\Delta}_{I^c}^{\psi} = \mathbb{1} \implies 0 \leq \widehat{\Delta}_I^{\psi} \leq \mathbb{1}. \quad (6.56)$$

Clearly, the major obstruction to $\Delta_{I,\delta}^{\psi,\varphi} \leq 1$ with $\delta > 0$ arises when $\widehat{\Delta}_I^{\psi}$ has eigenvalue 1. Then, because of (6.56), the corresponding eigenvectors, $\widehat{\Delta}_I^{\psi} |\varphi\rangle = |\varphi\rangle$, satisfy

$$\langle \varphi | \widehat{\Delta}_{I^c}^{\psi} | \varphi \rangle = \frac{1}{4} \sum_{(\alpha,\beta) \in I^c} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 = 0 \iff |\varphi\rangle \perp \sigma_{\alpha\beta} | \psi \rangle \quad \forall (\alpha, \beta) \in I^c. \quad (6.57)$$

Let the eigenvalues of $\widehat{\Delta}_I^\psi$ be decreasingly ordered and consider the spectral decomposition

$$\widehat{\Delta}_I^\psi = P_I^\psi(1) + R_I^\psi, \quad R_I^\psi = \sum_{j>1} d_I^\psi(j) P_I^\psi(j), \quad (6.58)$$

where $P_I^\psi(1)$ projects onto the eigenspace relative to the eigenvalue 1 and $P_I^\psi(j)$ are the other orthogonal spectral projections relative to the eigenvalues $0 \leq d_I^\psi(j) < 1$. Then, if $P_I^\psi(1) \neq 0$, $\delta > 0$ in (6.55) is only possible with $P_I^\psi(1)|\psi\rangle = 0$. These preliminary considerations allow us to prove (6.48) through a series of lemmas and corollaries. \square

Lemma 8 *With the notation of (6.58), if $P_I^\psi(1)|\psi\rangle = 0$ for all $|\psi\rangle \in \mathbb{C}^4$, then (6.55) is satisfied.*

Proof: If $M_I = \sup_{|\psi\rangle \in \mathbb{C}^4} \|R_I^\psi\| = 1$, then, by compactness, there exists a converging sequence $\psi_n \rightarrow \psi^*$ of vectors in \mathbb{C}^4 such that $R_I^{\psi_n} \perp P_I^{\psi_n}(1)$ and $\|R_I^{\psi_n}\| \rightarrow 1$. Then, $\widehat{\Delta}_I^{\psi_n}$ converges in norm to $\widehat{\Delta}_I^{\psi^*}$ with $\|R_I^{\psi^*}\| = 1$ and $R_I^{\psi^*} \perp P_I^{\psi^*}(1)$ which is a contradiction. Therefore, $M_I < 1$; hence, choosing $0 < \delta \leq 4(1 - M_I)$, from $P_I^\psi(1)|\psi\rangle = 0$ and $P_I^\psi(1)R_I^\psi = 0$, one gets

$$\|\widehat{\Delta}_{I,\delta}^\psi\| = \max \left\{ 1, \left\| \frac{\delta}{4} |\psi\rangle\langle\psi| + R_I^\psi \right\| \right\} \leq \max \left\{ 1, \frac{\delta}{4} + M_I \right\} \leq 1.$$

\square

Corollary 5 *Given a lattice state ρ_I and $|\psi\rangle \in \mathbb{C}^4$, let V_{I^c} be the subspace spanned by the vectors $\sigma_{\alpha\beta}|\psi\rangle$ with $(\alpha, \beta) \in I^c$, where I^c is the complement of I . If $V_{I^c}^\psi = \mathbb{C}^4$ for all $|\psi\rangle \in \mathbb{C}^4$, then ρ_I is entangled.*

Proof: From (6.57) it follows that $P_I^\psi(1) = 0$ for all $|\psi\rangle \in \mathbb{C}^4$; thus Lemma 8 applies. \square

Based on the previous two results, we now focus upon when $P_I^\psi(1) \neq 0$ and show that it projects onto a subspace orthogonal to $|\psi\rangle$.

Lemma 9 *If $\sigma_{\mu\nu}|\psi\rangle = \pm|\psi\rangle$ for some $(\mu, \nu) \in L_{16}$, then, with the notation of (6.58), $P_I^\psi(1)|\psi\rangle = 0$.*

Proof: If $(\mu, \nu) \in I^c$ and $\langle \varphi | \widehat{\Delta}_I^\psi | \varphi \rangle = 1$, then, from (6.57), $|\varphi\rangle \perp \sigma_{\alpha\beta}|\psi\rangle$ for all $(\alpha, \beta) \in I^c$, hence to $\pm|\psi\rangle = \sigma_{\mu\nu}|\psi\rangle$. Suppose then that $(\mu, \nu) \in I$ and rewrite inequality (6.55) as

$$\frac{\delta}{4} |\langle \varphi | \psi \rangle|^2 + \frac{1}{4} \sum_{(\alpha, \beta) \in I_1} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 + \frac{1}{4} \sum_{(\alpha, \beta) \in I_2} |\langle \varphi | \sigma_{\alpha\beta} | \psi \rangle|^2 \leq 1,$$

where the index set I has been split into

$$I_1 = \{(\alpha, \beta) \in I : [\sigma_{\alpha\beta}, \sigma_{\mu\nu}] = 0\} \quad \text{and} \quad I_2 = \{(\alpha, \beta) \in I : \{\sigma_{\alpha\beta}, \sigma_{\mu\nu}\} = 0\}.$$

The vectors $\sigma_{\alpha\beta}|\psi\rangle$ from these two subsets are orthogonal; indeed, $[\sigma_{\gamma\delta}, \sigma_{\mu\nu}] = 0$ and $\{\sigma_{\alpha\beta}, \sigma_{\mu\nu}\} = 0$ yield

$$\langle \psi | \sigma_{\alpha\beta} \sigma_{\gamma\delta} | \psi \rangle = \langle \psi | \sigma_{\mu\nu} \sigma_{\alpha\beta} \sigma_{\gamma\delta} \sigma_{\mu\nu} | \psi \rangle = -\langle \psi | \sigma_{\alpha\beta} \sigma_{\gamma\delta} | \psi \rangle = 0.$$

Therefore, the following two are orthogonal matrices:

$$\widehat{\Delta}_{I_1}^\psi = \frac{1}{2} |\psi\rangle \langle \psi| + \frac{1}{4} \sum_{I_1 \ni (\alpha, \beta) \neq (00), (\mu, \nu)} \sigma_{\alpha\beta} |\psi\rangle \langle \psi| \sigma_{\alpha\beta} \quad (6.59)$$

$$\widehat{\Delta}_{I_2}^\psi = \frac{1}{4} \sum_{(\alpha, \beta) \in I_2} \sigma_{\alpha\beta} |\psi\rangle \langle \psi| \sigma_{\alpha\beta}. \quad (6.60)$$

Then, $\widehat{\Delta}_I^\psi |\phi\rangle = |\phi\rangle$ can only be due to $\widehat{\Delta}_{I_2}^\psi |\varphi\rangle = |\varphi\rangle$, in which case $|\varphi\rangle \perp |\psi\rangle$. Indeed, $\|\widehat{\Delta}_{I_1}^\psi\| \leq 1$.

This can be seen as follows: at most three $\sigma_{\alpha\beta}$ may contribute to the sum in $\widehat{\Delta}_{I_1}^\psi$ and they must anti-commute. In fact, if there were two commuting $\sigma_{\alpha\beta}$ contributing to the sum, then, as they would commute with $\sigma_{\mu\nu}$ and form a special quadruple Q_{00} contained in I which is excluded by hypothesis. Therefore, the $\sigma_{\alpha\beta}$ contributing to the sum must anti-commute and, from Lemma 5, cannot be no more than three. Suppose this is the case; denote by S_α , $\alpha = 1, 2, 3$, these three $\sigma_{\alpha\beta}$ such that $\{\sigma_{\alpha\beta}, \sigma_{\mu\nu}\} = 0$ and rewrite

$$\widehat{\Delta}_{I_1}^\psi = \frac{1}{4} |\psi\rangle \langle \psi| + \frac{1}{4} \sum_{\alpha=0}^3 S_\alpha |\psi\rangle \langle \psi| S_\alpha, \quad S_0 = \mathbb{1}_4.$$

Without restriction, we choose $|\psi\rangle$ such that $\sigma_{\mu\nu}|\psi\rangle = |\psi\rangle$. Each $S_\alpha|\psi\rangle$ is an eigenstate of $\sigma_{\mu\nu}$ belonging to the same twice degenerate eigenvalue 1. Let P project onto the corresponding eigenspace; then, $[S_\alpha, P] = 0$ and the rank 2 matrices $T_\alpha = P S_\alpha P = S_\alpha P = P S_\alpha$ satisfy the Pauli algebra (2.10) over \mathbb{C}^4 . Thus, (2.11) holds on \mathbb{C}^4 with T_α replacing σ_α , yielding

$$\widehat{\Delta}_{I_1}^\psi = \frac{1}{4} |\psi\rangle \langle \psi| + \frac{1}{4} \sum_{\alpha=0}^3 S_\alpha |\psi\rangle \langle \psi| S_\alpha = \frac{1}{4} |\psi\rangle \langle \psi| + \frac{1}{2} P.$$

If there are less than three anti-commuting contributions S_α , $\alpha \neq 0$, then the second equality becomes a strict inequality. Therefore, $\|\widehat{\Delta}_{I_1}^\psi\| \leq 3/4 < 1$. \square

Let us now consider the set of $\sigma_{\alpha\beta}$ indexed by the points (α, β) in the complement set I^c , that we list as (α_i, β_i) , $1 \leq i \leq N - N_I$. The following facts are a consequence of the structure of \mathcal{Q}_{00} studied in Lemma 5 and concern the points of I^c and the special quadruples in \mathcal{Q}_{00} they belong to.

1. Take the first point $(\alpha_1, \beta_1) \notin I$; then, it belongs to three quadruples in (6.40) which cannot be contained in I .
2. Also the second point $(\alpha_2, \beta_2) \in I^c$ may eliminate three quadruples from those contained in I ; it does so, only if it does not share any special quadruple with those of (α_1, β_1) : this can happen only if $\sigma_{\alpha_1\beta_1}$ and $\sigma_{\alpha_2\beta_2}$ anti-commute. If they commute, then (α_1, β_1) and (α_2, β_2) share one special quadruple. In this case, (α_2, β_2) eliminates only two special quadruples from those contained in I . It thus follows that the minimum cardinality of I^c complying with the hypothesis of Theorem 20, namely that no special quadruple of $(0, 0)$ is contained in I , is five with the corresponding $\sigma_{\alpha\beta}$ forming an anti-commuting set.
3. Consider the third point $(\alpha_3, \beta_3) \in I^c$: the number of special quadruples eliminated by this point from those contained in I is equal to three minus the number of previous points whose $\sigma_{\alpha\beta}$ commute with $\sigma_{\alpha_3\beta_3}$.
4. Moving to the fourth point (α_4, β_4) and further on, the rule is the same; only, one has to take into account that $\sigma_{\alpha_4\beta_4}$ does not commute with more than three $\sigma_{\alpha\beta}$. Therefore, if this happens, $(\alpha_4\beta_4)$ does not eliminate from those contained in I any further special quadruple with respect to those already eliminated by the previous points.

Based on these properties, we now distinguish the following cases.

Case 1. $\text{card}(I^c) = 5$: the matrices $\{\sigma_{\alpha_i\beta_i}\}_{i=1}^5$, with $(\alpha_i, \beta_i) \in I^c$ anti-commute.

Case 2. $\text{card}(I^c) > 5$ and there is a set of anti-commuting $\{\sigma_{\alpha_i\beta_i}\}_{i=1}^5$, with $(\alpha_i, \beta_i) \in I^c$: let $(\alpha_6, \beta_6) \in I^c$ not belong to the index set of the five anti-commuting σ 's. The corresponding $\sigma_{\alpha_6\beta_6}$ must commute with at least one of them and may commute with at most three of the $\sigma_{\alpha_i\beta_i}$. Therefore, there must exist at least two of them that anti-commute with $\sigma_{\alpha_6\beta_6}$. By putting together $\sigma_{\alpha_6\beta_6}$ with the one in the anti-commuting set which commutes with it and with the two which anti-commute with

it, then one can construct a set K of four $\sigma_{\alpha\beta}$ where 3 of them anti-commute among themselves and the fourth one commutes with only one of them.

Case 3. $\text{card}(I^c) > 5$, but there is no set of 5 anti-commuting $\sigma_{\alpha_i\beta_i}$ indexed by $(\alpha_i, \beta_i) \in I^c$. If there are 4 anti-commuting $\sigma_{\alpha\beta}$ indexed by points in I^c , these latter correspond to twelve special quadruples in \mathcal{Q}_{00} not contained in I . Therefore, there are three special quadruples of \mathcal{Q}_{00} left that also can not be contained in I . Thus, some of their points must be excluded from I . These three quadruples share a common point that cannot be excluded from I , otherwise the corresponding $\sigma_{\alpha\beta}$, together with the four which have already been assumed to anti-commute, would constitute a set of five anti-commuting σ 's contrary to the hypothesis of the present case. Therefore, in order to eliminate the three remaining special quadruples from being contained in I , one point for each of the three special quadruples must be excluded from I . The corresponding $\sigma_{\alpha\beta}$ will then anti-commute. Then, we have constructed two sets $U_{1,2}$ of σ 's, the first one containing four anti-commuting $\sigma_{\alpha\beta}$, the second one three anti-commuting $\sigma_{\alpha\beta}$. We already know that each element from U_2 commutes at least with one from U_1 ; further, it cannot commute with more than two of them. Indeed, if this happened, one would have two anti-commuting $\sigma_{\alpha\beta}$ in the same special quadruple which is impossible.

This makes it possible to construct a set K as in the previous case consisting of three anti-commuting $\sigma_{\alpha\beta}$ and a fourth one which commutes with only one of them. This set K can be constructed as follows: consider the set U_1 with $\sigma_{\alpha_i\beta_i}$, $i = 1, 2, 3, 4$, take the first three of them and $\sigma_{\alpha'\beta'}$ from U_2 : if $\sigma_{\alpha'\beta'}$ commutes with only one $\sigma_{\alpha_i\beta_i}$, $i = 1, 2, 3$, the set K consists of these four σ 's. Otherwise, if $\sigma_{\alpha'\beta'}$ commutes with two $\sigma_{\alpha_i\beta_i}$, then replace one of them with $\sigma_{\alpha_4\beta_4}$; as said before $\sigma_{\alpha'\beta'}$ does not commute with it because of the previous argument. Therefore, these four elements form the set K sought after.

The above procedure works also in the case of sets of anti-commuting σ 's with less than four elements.

The next two Lemmas concern Case 1 above, where I^c corresponds to a set of 5 anti-commuting $\sigma_{\alpha\beta}$: the first lemma specifies the structure of the anti-commuting set, while the second one is about the sub-space generated by these matrices acting on a vector state $|\psi\rangle$.

Lemma 10 *All sets of 5 anti-commuting $\sigma_{\alpha_\ell\beta_\ell}$, $(\alpha_\ell, \beta_\ell) \in I^c$, must be of the form*

$$K_1 = \{\sigma_{0i}, \sigma_{0j}, \sigma_{1k}, \sigma_{2k}, \sigma_{3k}\} \quad \text{or} \quad K_2 = \{\sigma_{i0}, \sigma_{j0}, \sigma_{k1}, \sigma_{k2}, \sigma_{k3}\}$$

with i, j, k such that the anti-symmetric tensor $\varepsilon_{ijk} \neq 0$.

Proof: Since we have 5 indices α_ℓ and β_ℓ to choose among 0, 1, 2, 3, at least two α s and two β s must be equal: let us consider $\alpha_1 = \alpha_2$.

If $\alpha_1 = \alpha_2 = 0$, in order to have $\{\sigma_{0\beta_1}, \sigma_{0\beta_2}\} = 0$, the corresponding β_1 and β_2 must be different and different from 0; therefore, $\beta_1 = i, \beta_2 = j$, with $i \neq j, i \neq 0, j \neq 0$, so that the first two anti-commuting matrices are σ_{0i} and σ_{0j} . In the three $(\alpha_\ell\beta_\ell)$ left, there cannot appear $\alpha_\ell = 0$, otherwise the corresponding β_ℓ , which cannot be 0 and must equal either i or j , would lead to a $\sigma_{\alpha_\ell\beta_\ell}$ violating anti-commutativity. Then, with the three remaining $\alpha_\ell \neq 0$, the three corresponding β_ℓ must be different from 0, i and j , otherwise $\sigma_{\alpha_\ell\beta_\ell}$ would commute with either σ_{0i} or σ_{0j} . Thus, $\beta_3 = \beta_4 = \beta_5 = \beta_k$ with $k \neq i, k \neq j$, while the corresponding α_ℓ must be different, namely $\alpha_3 = 1, \alpha_4 = 2$ and $\alpha_5 = 3$. This gives the set K_1 .

If $\alpha_1 = \alpha_2 = k \neq 0$, the corresponding $\beta_{1,2}$ cannot be equal and must be both different from 0. Thus, two $\sigma_{\alpha_\ell\beta_\ell}$ in the anti-commuting set are σ_{ki} and σ_{kj} , with $i \neq j = 1, 2, 3$. Only one of the remaining α_ℓ can be 0, otherwise we would be back to the previous case: for $\sigma_{0\beta_\ell}$ to anti-commute with σ_{ki} and σ_{kj} , β_ℓ must be equal to s with $s \neq i, s \neq j$. In order to anti-commute with σ_{ki}, σ_{kj} and σ_{0s} , $\sigma_{\alpha_4\beta_4}$ and $\sigma_{\alpha_5\beta_5}$, with $\alpha_{4,5} \neq 0$, must be of the form σ_{pi} and σ_{qj} with $p \neq q$ and both different from 0 and k . But then, they would commute among themselves; thus, $\alpha_{3,4,5} \neq 0$. At least one of them, say α_3 must equal k ; then, anti-commutativity only holds if $\beta_3 = r \neq 0$ with $i \neq r, j \neq r$. Finally, since at least two β 's must be equal, in order to anti-commute among themselves and with σ_{ki}, σ_{kj} and $\sigma_{kr}, \sigma_{\alpha_4\beta_4}$ and $\sigma_{\alpha_5\beta_5}$ must have $\beta_4 = \beta_5 = 0$ and $\alpha_4 = m, \alpha_5 = n$ such that the antisymmetric tensor $\varepsilon_{kmn} \neq 0$. This fixes the set K_2 . The same result would obtain if one started arguing with two equal β s instead of α s. \square

Lemma 11 *Let $K_{1,2}$ be the two sets of 5 anti-commuting $\sigma_{\alpha\beta}$ as described in the previous lemma. For any $|\psi\rangle \in \mathbb{C}^4$, let*

$$K_{1,2}^\psi = \text{Linear Span}\{\sigma_{\alpha\beta}|\psi\rangle : \sigma_{\alpha\beta} \in K_{1,2}\}.$$

Then, any vector orthogonal to $K_{1,2}^\psi$ is also orthogonal to $|\psi\rangle$.

Proof: Consider the set $\{\sigma_{0i}, \sigma_{0j}, \sigma_{1k}, \sigma_{2k}, \sigma_{3k}\}$ and let $|0\rangle_2$ and $|1\rangle_2$ be the eigenvectors of σ_k . Furthermore, fix i and j so that

$$\begin{aligned}\sigma_k|0\rangle_2 &= |0\rangle_2, & \sigma_k|1\rangle_2 &= |1\rangle_2; \\ \sigma_i|0\rangle_2 &= |1\rangle_2, & \sigma_i|1\rangle_2 &= |0\rangle_2; \\ \sigma_j|0\rangle_2 &= i|1\rangle_2, & \sigma_j|1\rangle_2 &= -i|0\rangle_2.\end{aligned}$$

Given $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^4$, consider their expansions with respect to the orthonormal basis $\{|ij\rangle = |i\rangle_1 \otimes |j\rangle_2\}_{i,j=0}^1$ where $|i\rangle_1, i = 0, 1$, are eigenvectors of σ_3 : $|\psi\rangle = \sum_{i,j=0}^1 \psi_{ij}|ij\rangle$ and $|\varphi\rangle = \sum_{i,j=0}^1 \varphi_{ij}|ij\rangle$. Acting with the first four $\sigma_{\alpha\beta}$ on $|\psi\rangle$, we have:

$$\begin{aligned}\sigma_{0i}|\psi\rangle &= \psi_{00}|01\rangle + \psi_{01}|00\rangle + \psi_{10}|11\rangle + \psi_{11}|10\rangle, \\ \sigma_{0j}|\psi\rangle &= i(\psi_{00}|01\rangle - \psi_{01}|00\rangle + \psi_{10}|11\rangle - \psi_{11}|10\rangle) \\ \sigma_{1k}|\psi\rangle &= \psi_{00}|10\rangle - \psi_{01}|11\rangle + \psi_{10}|00\rangle - \psi_{11}|01\rangle, \\ \sigma_{2k}|\psi\rangle &= i(\psi_{00}|10\rangle - \psi_{01}|11\rangle - \psi_{10}|00\rangle + \psi_{11}|01\rangle).\end{aligned}\tag{6.61}$$

If $|\varphi\rangle$ is orthogonal to each of the previous vectors, it follows that

$$\begin{aligned}\overline{\varphi_{01}}\psi_{00} + \overline{\varphi_{11}}\psi_{10} &= 0, & \overline{\varphi_{00}}\psi_{01} + \overline{\varphi_{10}}\psi_{11} &= 0 \\ \overline{\varphi_{10}}\psi_{00} - \overline{\varphi_{11}}\psi_{01} &= 0, & \overline{\varphi_{00}}\psi_{10} - \overline{\varphi_{01}}\psi_{11} &= 0.\end{aligned}$$

These relations recast in matrix equation read

$$\begin{bmatrix} 0 & \psi_{00} & 0 & \psi_{10} \\ \psi_{01} & 0 & \psi_{11} & 0 \\ 0 & 0 & \psi_{00} & -\psi_{01} \\ \psi_{10} & -\psi_{11} & 0 & 0 \end{bmatrix} \begin{bmatrix} \varphi_{00} \\ \varphi_{01} \\ \varphi_{10} \\ \varphi_{11} \end{bmatrix} = 0.$$

The determinant of the matrix is $2\psi_{00}\psi_{01}\psi_{10}\psi_{11}$; thus, $|\varphi\rangle$ orthogonal to the linear span of the vectors in (6.61) can only exist if all components of $|\psi\rangle$ are non-zero. Then,

$$\begin{aligned}\overline{\varphi_{01}} &= -\frac{\overline{\varphi_{11}}\psi_{10}}{\psi_{00}}, & \overline{\varphi_{00}} &= \frac{\overline{\varphi_{11}}\psi_{11}}{\psi_{00}}, & \overline{\varphi_{10}} &= \frac{\overline{\varphi_{11}}\psi_{01}}{\psi_{00}} & \text{and} \\ |\varphi\rangle &= \overline{\psi_{11}}|00\rangle + \overline{\psi_{10}}|01\rangle - \overline{\psi_{01}}|10\rangle - \overline{\psi_{00}}|11\rangle.\end{aligned}$$

Such a vector results orthogonal to both the fifth vector $\sigma_{3k}|\psi\rangle$ and $|\psi\rangle$ itself. Similar considerations hold for the set $\{\sigma_{i0}, \sigma_{j0}, \sigma_{k1}, \sigma_{k2}, \sigma_{k3}\}$. \square

The next Lemma concerns the dimensionality of the linear spans of vectors of the form $\sigma_{\alpha\beta}|\psi\rangle$ where the matrices belong to the sets discussed in Cases 2 and 3 in the proof of Theorem 20 where three anti-commute and the fourth one commutes with only one of them.

Lemma 12 Consider a sub-set $K = \{\sigma_{\alpha_i\beta_i} : i = 1, \dots, 4\}$ consisting of three anti-commuting matrices $\sigma_{\alpha\beta}$ plus a fourth one which commutes with only one of these three, say the first:

$$\{\sigma_{\alpha_i\beta_i}, \sigma_{\alpha_j\beta_j}\} = 0, \quad i, j = 1, 3 \quad [\sigma_{\alpha_4\beta_4}, \sigma_{\alpha_1\beta_1}] = 0. \quad (6.62)$$

Then, unless $|\psi\rangle \in \mathbb{C}^4$ is an eigenstate of some $\sigma_{\mu\nu}$, $V_K = \mathbb{C}^4$, where V_K is the linear span of $\{\sigma_{\alpha_i\beta_i}|\psi\rangle\}_{i=1}^4$.

Proof: Suppose $|\psi\rangle$ is not an eigenstate of any $\sigma_{\mu\nu}$, then the vectors $\sigma_{\alpha_1\beta_1}|\psi\rangle, \sigma_{\alpha_2\beta_2}|\psi\rangle$ cannot be proportional. For the same reason, the vectors $\sigma_{\alpha_1\beta_1}|\psi\rangle, \sigma_{\alpha_2\beta_2}|\psi\rangle$ and $\sigma_{\alpha_4\beta_4}|\psi\rangle$ are linearly independent. Indeed, suppose

$$\sigma_{\alpha_4\beta_4}|\psi\rangle = \alpha\sigma_{\alpha_1\beta_1}|\psi\rangle + \beta\sigma_{\alpha_2\beta_2}|\psi\rangle.$$

Then, acting on both sides with $\sigma_{\alpha_4\beta_4}$ we obtain $|\psi\rangle = \alpha S_1|\psi\rangle + \beta S_2|\psi\rangle$, where $S_i = \sigma_{\alpha_4\beta_4}\sigma_{\alpha_i\beta_i}$, $i = 1, 2$. When substituting this expression for $|\psi\rangle$ in the right hand side of the equality, the relations (6.62) yield

$$|\psi\rangle = (\alpha^2 - \beta^2)|\psi\rangle + \alpha\beta[\sigma_{\alpha_1\beta_1}, \sigma_{\alpha_2\beta_2}]|\psi\rangle,$$

which, for non-trivial $\alpha\beta$, is only possible if $|\psi\rangle$ is an eigenstate of the $\sigma_{\mu\nu}$ proportional to the commutator in the previous equality. The same conclusions can be drawn about the linear independence of the four vectors spanning V_K . Indeed, if

$$\sigma_{\alpha_3\beta_3}|\psi\rangle = \alpha\sigma_{\alpha_1\beta_1}|\psi\rangle + \beta\sigma_{\alpha_2\beta_2}|\psi\rangle + \gamma\sigma_{\alpha_4\beta_4}|\psi\rangle,$$

the same argument of before obtains

$$|\psi\rangle = -(\alpha^2 + \beta^2 + \gamma^2)|\psi\rangle + \alpha\gamma\{\sigma_{\alpha_1\beta_1}, \sigma_{\alpha_4\beta_4}\}|\psi\rangle.$$

This implies that, unless $|\psi\rangle$ is eigenstate of the $\sigma_{\mu\nu}$ arising from the anti-commutator in the above expression, the four vectors spanning V_K are linearly independent. \square

The previous results show that, as a consequence of the assumption that no special quadruple $Q \in \mathcal{Q}_{00}$ is contained in I , given a vector $|\psi\rangle \in \mathbb{C}^4$ the sub-space linearly generated by $\sigma_{\alpha\beta}|\psi\rangle$ with $(\alpha\beta) \in I^c$ is either \mathbb{C}^4 or contains $|\psi\rangle$. The proof of Theorem 20 is thus completed by using Lemma 8 and its corollary. \square

It might look like that, when all the points of the lattice have at least one special quadruple contained in I , the corresponding lattice state might be separable. But in the following examples, we will show that this is not in general true.

Example 39 Consider the following state:

$$N_I = 11 \quad \begin{array}{c|c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & & & & \times \\ \hline 1 & & \times & \times & \times \\ \hline 0 & \times & \times & \times & \times \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

This looks very similar to the state in example 6.52, where none of the special quadruples of $(0,0)$ were included in I . However in the above lattice state, $(0,0)$ has two special quadruples contained in I , which are:

$$\begin{array}{c|c|c|c|c} 3 & & & \times & \\ \hline 2 & & & & \times \\ \hline 1 & & \times & & \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} \quad \text{and} \quad \begin{array}{c|c|c|c|c} 3 & & \times & & \\ \hline 2 & & & & \times \\ \hline 1 & & \times & \times & \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array}$$

But from Proposition 1, we know that this state is NPT: the contribution to I from the row and the column for the point $(3,0)$ is $6 > \frac{11}{2}$.

Summary and Outlook

In this thesis work, we have studied the role of positive and completely positive maps in detecting entanglement. In the first chapters we have reviewed the necessary techniques that have been employed in the last chapter.

Indeed, in the final chapter of the thesis we have considered a particular class of bipartite states ρ_I on $\mathbb{C}^4 \otimes \mathbb{C}^4$, introduced in [4], called Lattice States. These are uniform mixtures of projections indexed by points (α, β) belonging to subsets I of the finite square lattice of cardinality 16. The projections are generated by the action of $\mathbb{1}_4 \otimes \sigma_{\alpha\beta}$ on the completely symmetric vector in $\mathbb{C}^4 \otimes \mathbb{C}^4$, where $\sigma_{\alpha\beta}$ is the tensor product of the Pauli matrices $\sigma_\alpha, \sigma_\beta$. We have generalized them to states on $\mathbb{C}^{2^n} \otimes \mathbb{C}^{2^n}$, referred to as σ -diagonal states.

One of the main issues was to decide whether a given σ -diagonal state, is entangled or separable. We have tackled this problem using the results of [65] and showed that, starting from a general non-diagonal positive map, possible entanglement of σ -diagonal states would be revealed using only a particularly simple sub-class of positive maps adapted to the diagonal structure of the states, that are combinations of elementary maps of the form $X \mapsto \sigma_{\alpha\beta} X \sigma_{\alpha\beta}$.

Back to the Lattice States in $\mathbb{C}^4 \otimes \mathbb{C}^4$, we have shown the compatibility of the results given in [5, 6], with ours.

As the next step, we have partially shown how the entanglement (respectively, separability) of the Lattice States can be explained through their geometrical structure. The results obtained are based on particular separable lattice states consisting of four points, called special quadruples, which play a crucial role in this game.

Using this notion, we have shown that if there exists a point in the set I , such that none of its special quadruples are contained in I , then the corresponding Lattice State ρ_I , is entangled. We have also provided a proper entanglement witness for such a state based on the results obtained in the first part of the chapter.

Also, using the notion of uniform covering by special quadruples con-

tained in the subset I , we could show that some of the Lattice States whose separability was left unknown in previous works, are indeed separable:

$$\begin{array}{c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & & \times & \times & \times \\ \hline 1 & & \times & \times & \times \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} , \quad \begin{array}{c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & & \times & & \times \\ \hline 1 & & \times & \times & \times \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} , \quad \begin{array}{c|c|c|c} 3 & & \times & \times & \times \\ \hline 2 & & \times & & \times \\ \hline 1 & & \times & & \times \\ \hline 0 & \times & & & \\ \hline & 0 & 1 & 2 & 3 \end{array} .$$

However, there are still some Lattice States whose separability could not be decided by the methods developed in this thesis; for instance,

$$\begin{array}{c|c|c|c} 3 & \times & & & \times \\ \hline 2 & \times & \times & & \times \\ \hline 1 & \times & \times & \times & \\ \hline 0 & \times & \times & \times & \\ \hline & 0 & 1 & 2 & 3 \end{array} .$$

For this Lattice State, all points have at least three special quadruples contained in I , but no uniform covering could be found, nor could be excluded.

Another interesting issue, still to be understood, is the relation between the special quadruples and partial transposition. The difficulties can be appreciated by looking at the following state:

$$\begin{array}{c|c|c|c} 3 & \times & & & \times \\ \hline 2 & \times & & & \times \\ \hline 1 & & & \times & \times \\ \hline 0 & \times & \times & \times & \times \\ \hline & 0 & 1 & 2 & 3 \end{array} ,$$

which is NPT entangled, nevertheless all points belong to at least one special quadruples contained in I . Obviously, in this case there does not exist a uniform covering of special quadruples as the state is entangled.

Further interesting issues to be tackled are whether separable Lattice States carry quantum discord and whether the structure of PPT entangled Lattice States could be investigated in terms of Edge States and Unextendible Product Bases.

Appendix A

Convexity

A good introduction of Convex Analysis is given in [1, 58].

Definition 30 *Convex Set*

Let S be a finite set of points in \mathbb{R}^d . S is said to be convex if

$$\alpha x + (1 - \alpha)y \in S \quad \forall x, y \in S \quad 0 \leq \alpha \leq 1. \quad (\text{A.1})$$

Consequently a point $y \in \mathbb{R}^d$ is said to be a convex combination of $\{x_i\}_{i=1}^n \subseteq \mathbb{R}^d$ if:

$$y = \sum_i p_i x_i, \quad \sum_i p_i = 1, \quad p_i \geq 0 \quad \text{for } i = 1, \dots, n. \quad (\text{A.2})$$

Example 40 The set of states and the subset of separable states $\rho_s \in M_n(\mathbb{C})$ are convex sets.

Definition 31 *Convex hull*

Convex hull of a convex set S , denoted by $\text{conv}(S)$ is the set of all the convex combinations of the elements of S :

$$\text{conv}(S) = \left\{ \sum_i p_i x_i, \quad \sum_i p_i = 1, \quad p_i \geq 0 \quad x_i \in S \right\}.$$

Convex hull of S is the smallest convex set containing S .

Let S be a convex set. Then its elements split into two subsets:

Definition 32 *Interior points*

The point $x \in S$ is an interior point if the line segment from any point in S to x can be extended within S .

Definition 33 *Extreme points*

A point $y \in S$ is said to be extreme if:

$$y = \alpha x_1 + (1 - \alpha)x_2, \quad x_1, x_2 \in S \implies (y = x_1 \wedge \alpha = 1) \vee (y = x_2 \wedge \alpha = 0).$$

In other words, extreme points of S do not belong to any proper segment defined by two distinct elements of S .

Example 41 *The pure states or projectors are extreme points for the set of density matrices, whereas the density states of mixed states are the interior points.*

When an inner product $\langle \cdot | \cdot \rangle$ is defined on \mathcal{C} , we have:

Definition 34 *Hyperplane*

Let a and x_0 be vectors in \mathbb{R}^d . Then a hyperplane is a set of the form $\{x | \langle a | (x - x_0) \rangle = 0\}$. The vector a is called the normal vector for the hyperplane.

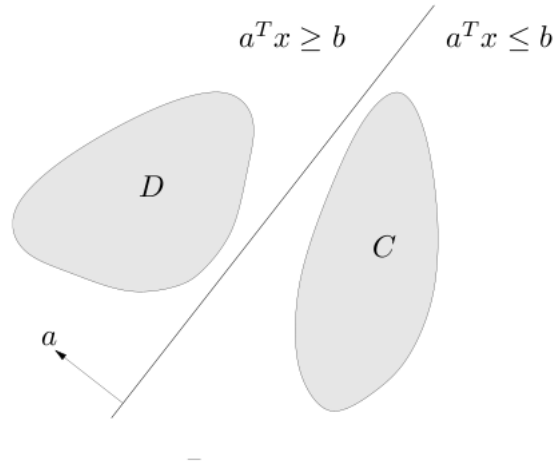
The hyperplane divides \mathbb{R}^d into two halfspaces:

Definition 35 *Halfspace* A halfspace is a set of the form:

$$\{x | \langle a | (x - x_0) \rangle \leq 0\}$$

The concept of hyperplanes and halfspaces are very useful as using them we can separate the convex sets which do not intersect:

Theorem 21 *Let C and D be two convex sets such that $C \cap D = \emptyset$. Then there exists $a \neq 0$ and x_0 such that $\langle a | (x - x_0) \rangle \leq b$ for all $x \in C$ and $\langle a | (x - x_0) \rangle \geq b$ for all $x \in D$. In another words, $\langle a | (x - x_0) \rangle$ is non-positive on C and non-negative on D .*



If a hyperplane is tangent to the set, at some extreme point x_0 , then it is called supporting hyperplane. Note also that the separating hyperplanes as well as supporting hyperplanes are not unique.

Definition 36 Cones

A set $\mathcal{C} \subseteq \mathbb{R}^d$ is a cone if

$$x \in \mathcal{C}, \quad \alpha \geq 0 \implies \alpha x \in \mathcal{C}.$$

\mathcal{C} is said to be a convex cone if:

$$x, y \in \mathcal{C}, \quad \alpha, \beta \geq 0 \implies \alpha x + \beta y \in \mathcal{C}.$$

To any convex cone one can associate a dual cone.

Definition 37 Dual Cone

The dual cone \mathcal{C}° is defined to be:

$$\mathcal{C}^\circ = \{y : \langle y|x \rangle \geq 0, \quad \forall x \in \mathcal{C}\}.$$

The dual cone \mathcal{C}° is always closed, even if \mathcal{C} is open.

Example 42

When the cone and dual cone coincide then the cone is said to be self-dual, i.e. :

$$\langle y|x \rangle \geq 0 \quad \forall x \in \mathcal{C} \iff y \in \mathcal{C}.$$

Example 43 *The cone of positive semidefinite $n \times n$ matrices is self-dual. This also holds for the cone of completely positive maps: $\mathcal{CP} = \mathcal{CP}^\circ$.*

Example 44 *All these concepts can be extended to the Hermitian operators and linear maps as well. Indeed one can easily verify that the set of positive operators is a convex set, and that positive (resp. complete positive) maps are unaffected by multiplication by positive scalars.*

Let \mathcal{C} denote the cone of (positive, completely positive) linear maps, the dual cone \mathcal{C}° in this case is defined via the Jamiolkowski Isomorphism. Let $\{E_{ij}\}$ be an orthonormal set of unit matrices, then the Choi matrix C_ϕ , for the map $\phi : M_n(\mathbb{C}) \longrightarrow M_n(\mathbb{C})$ is:

$$C_\phi = \sum E_{ij} \otimes \phi(E_{ij}). \quad (\text{A.3})$$

Using the Hilbert-Schmidt scalar product introduced in (2.4), the dual cone \mathcal{C}° is defined to be:

$$\mathcal{C}^\circ = \{\psi : M_n(\mathbb{C}) \longrightarrow M_n(\mathbb{C}) : \text{Tr}(C_\phi C_\psi) \geq 0, \quad \forall \phi \in \mathcal{C}\}. \quad (\text{A.4})$$

Let $P(\mathbb{C}^d)$ be the set of positive linear maps $\phi : M_n(\mathbb{C}) \longrightarrow M_n(\mathbb{C})$, and \mathcal{C} be a closed cone in $P(\mathbb{C}^d)$. Recall that the set of complete positive maps is denoted by \mathcal{CP} .

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