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The parts and the whole

how the tensor product affects Quantum Theory

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“Time keeps movin’ on,
Friends they turn away.
I keep movin’ on
But I never found out why
I keep pushing so hard the dream,
I keep tryin’ to make it right
Through another lonely day, whoaa..."
Janis Joplin, Kozmic Blues

”Once divided...nothing left to subtract...
Some words when spoken...can’t be taken back...
Walks on his own...with thoughts he can’t help thinking...
Future’s above...but in the past he’s slow and sinking...
Caught a bolt ’a lightnin’...cursed the day he let it go...
Nothingman...
Isn’t it something?
Nothingman...“
Pearl Jam, Nothingman

“If you’re reading this, it means I actually worked up the courage to mail it,
so good for me.
You don’t know me very well, but if you get me started I have a tendency to go on
and on about how hard the writing is for me.
But this,
this *is* the hardest thing I ever had to write.
There is no easy way to say this, so I’ll just say it...”
Hank Moody, Letter to Karen, Californication

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É... acho que é isso. Mais uma etapa que vai chegando ao fim. Essa em particular deixou muitas marcas, algumas permanentes... e permanentemente também serei grato. Aos meus pais primeiramente. Papai e Mamãe sempre estiveram do meu lado, e tenho toda certeza que muito perrengue foi passado pra que eu chegasse até aqui. Obrigado a ambos. Sem vocês nada do que foi feito aqui seria possível. Já que eu comecei pela família, também queria dizer um muito obrigado a toda ela. Dos dois lados! Coisa que eu normalmente não faço. Desse seleto conjunto gostaria de abraçar mais efusivamente Fia e Fabiano, vocês mesmo sem saber, eu imagino, me moldaram de uma maneira que é sem palavras. Obrigado por tudo!

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Queria fechar essa seção dizendo algumas palavras especiais para pessoas especiais. Thaís, eu não sei o que vai ser da gente, e eu não posso dizer que você deveria dar esse salto de fé que é gostar de mim, mas eu

[1] Aquele Ziggy Stardust vai ser inesquecível.
[2] Pesquisadora, já que Biólogo é conhecido por nadar com boto e abraçar Jequitibás Rei.
[3] Fora Temer!
[4] Ainda que eu discorde de você em alguns pontos, você também teve seu papel na minha formação.

Te Amo, e é só isso que me importa. Dudu, você não só me recebeu muito bem, como pela primeira vez me tratou como alguém que já sabia alguma coisa. Vou ser eternamente grato a você. Um dia, quem sabe, vou poder retribuir o que você fez por mim. Dutty...bicho, MUITO MUITO obrigado! Todas as nossas brigas, todas as nossas discussões, tudo só me fez crescer mais e mais. Não só academicamente, mas como pessoa, como ser humano. Você é o professor mais preocupado que eu já vi em vida, apesar de ser meio desatento (pô, quase 2 anos pra perceber que eu tinha tatuagem no braço!!). Do fundo do meu coração, obrigado! Marcelo Terra Cunha... orientador, professor, colaborador, amigo, ouvinte, chato as vezes, zeloso... você é isso tudo e muito mais. Sempre esteve querendo o nosso bem, e sempre lutou por isso. Mesmo quando essa batalha era travada contra nós mesmos. Você nunca me deixou desistir. Nunca vou cansar de repetir: Por me deixar pensar com minhas próprias pernas, ***Obrigado, bicho! Muito Obrigado!***

Published Works and Works in Preparation

The following works were published, or are in advanced stage of preparation:

- H. Bragança, E. Mascarenhas, G. I. Luiz, C. Duarte, et. al., Nonuniversality of entanglement convertibility. *Physical Review. B*, **89**, 235132-235137 (2014);
- R. Rabelo, C. Duarte, A. López-Tarrida, M. Terra Cunha, A. Cabello, Multigraph approach to quantum non-locality. *Journal of Physics. A*, **47**, 424021 (2014);
- C. Duarte, R. C. Drumond, M. Terra Cunha, Self-catalytic conversion of pure quantum states, *Journal of Physics. A*, **49**, 145303 (2016);
- R. C. Drumond, C. Duarte, M. Terra Cunha, M. C. Nemes, Universality of finite-time disentanglement. *Physical Review A*, **93**, 022313-1 (2016);
- R. C. Drumond, C. Duarte, R. I. Oliveira, *Typical Violations of Bell Inequalities* (in advanced preparation);
- C. Duarte, F. Brito, G. Carvalho and F. de Melo, *Emergent Dynamics from Quantum Mechanics* (in advanced preparation);
- N. Kolb Bernardes, C. Duarte, B. L. Amaral, M. França *Back Flow of information and CP-divisibility* (in early preparation)

Resumo

A proposta do presente trabalho é usar argumentos de Teoria dos Grafos; Topologia e Geometria; e Álgebra Multilinear para mostrar como a estrutura de produto tensorial afeta a Teoria Quântica. Dito de outra maneira, vamos usar seriamente a estrutura de partes na abordagem CSW voltada para Não-Localidade; estudar o fenômeno de Desemaranhamento a Tempo Finito para certas classes de dinâmicas quânticas; e analisar o comportamento de protocolos de Informação Quântica no paradigma LOCC quando estados emaranhados extras são permitidos, para mostrar como a estrutura de produto tensorial, enquanto inerente, afeta de maneira surpreendente a Teoria Quântica.

Palavras-Chave: Teoria Quântica, Teoria Quântica da Informação, ,Álgebra Linear, Produto Tensorial, Teoria dos Grafos, Não-Localidade e Desigualdades de Bell, Catálise, Auto-Catálise, LOCC, Dinâmica Quântica e Emaranhamento.

Abstract

The aim of the present work is to use arguments from Graph Theory, Topology and Geometry, and Multi-Linear Algebra in order to show how the tensor product structure affects Quantum Theory. Saying with other words, we will take seriously the idea of parts at the CSW approach; we will also study the Finite Time Disentanglement for certain classes of quantum dynamics; and by the end we will analyse the behaviour of Quantum Information Protocols (in the LOCC paradigm) when an extra entangled is allowed, all of that to show how the structure of tensor product, albeit inherent, brings striking features to Quantum Theory.

Key-Words: Quantum Theory, Quantum Information Theory, Linear Algebra, Tensor Product, Graph Theory, Non-Locality and Bell-Inequalities, Cataysis, Self-Catalysis, LOCC, Quantum Dynamics and Entanglement.

Contents

Introduction

Why:

- Adverb

  1. for what? for what reason, cause, or purpose?: Why did you behave so badly?

- Conjunction

  2. for what cause or reason: I don't know for sure why composite systems is described by tensor product.

  3. for which; on account of which (usually after reason to introduce a relative clause): the reason why he refused to go.

  4.the reason for which: That is why he returned.

- Noun, plural whys.

  5. a question concerning the cause or reason for which something is done, achieved, etc.: a child's unending hows and whys.

  6.the cause or reason: the whys and wherefores of a troublesome situation.

How:

- Adverb

  1. in what way or manner; by what means?: How tensor product affects QM?

  2. to what extent, degree, etc.?: How damaged is the car?

  3. in what state or condition?: How are you?

  4. to what effect; with what meaning?: How is one to interpret his action?

  5. by what amount or in what measure or quantity?: How do you sell these tomatoes?

- Conjunction

  6. the manner or way in which: He couldn't figure out how to solve the problem.

  7. a question concerning the way or manner in which something is done, achieved, etc.: a child's unending whys and hows.

Yes, I've opened my Ph.D. thesis discussing the difference between *How* and *Why*. And I'm doing that just to clarify the unwary reader that in the core of the thesis I won't talk about *why* the tensor product has been used in Quantum Theory. My emphasis is going to be about *how*, in which extent, the tensor product affects it. The main aim of this work will be fulfilled if right after the Chapter 4 the readers are convinced that the structure of parts dictated by that product affects not only more applied branches of Quantum Mechanics, as Quantum Computation and Quantum Information Protocols for instance, but also how it could be used to shed light on foundational aspects of Quantum Theory itself. Indeed, as we are going to see, even today, astonishing novel phenomena, connected with tensor product, are discovered. And they highlight the striking and fascinating aspect of Quantum Theory... **no**, I'm not reinventing Entanglement, I'm being deeper and talking about the mathematical structure that allows it, or going further, the physical structure behind it.

But wait, even now some atypical words have already appeared, right!? What is, or what do I mean by Quantum Theory? and why should such a purely algebraic structure, as Tensor Product, affect it? Entanglement? Even more, why should Quantum Mechanics, and its implications, call attention of somebody? So, it's not a simple task to address those questions, of course, in particular is quite hard to say anything about what Quantum Mechanics really is, but we can try, at least, to give naive arguments to excite the reader's curiosity and motivate the subject of this thesis. Let us start with the following Feynman's quote [1]:

> *"Quantum Mechanics is the description of the behaviour of matter in all its details and, in particular, of the happenings on an atomic scale. Things on a very small scale behave like nothing that you have any direct experience about. They don't behave like waves, they don't behave like particles, they do not behave like clouds, or billiard balls... or like anything that you have ever seen... even experts do not understand it the way they would like to...*

Roughly speaking, and being a little bit more pragmatic than the Feynman's point of view, Quantum Theory is a framework used to describe phenomena, usually associated with tiny components of the matter, that the Classical Mechanics cannot[5] to deal with. Historically Quantum Theory has been taught as something strictly connected with atoms and molecules, but today is a common point that

> *"Quantum Theory tells about atoms and molecules the same that Probability Theory does about dices and coins."*

Such as Probability is an alive and beautiful Theory [4–6], Quantum Theory is broad, and walks by its own feet too. Nevertheless, to hold ourselves in things more visual and tangible, it's good keep on mind a prototype[6] of a simplified physical situation:

The (usually simplified) Stern-Gerlach's apparatus.

[5] For a historical account we suggest [1–3] and references therein.
[6] We suggest to the reader the Appendix A

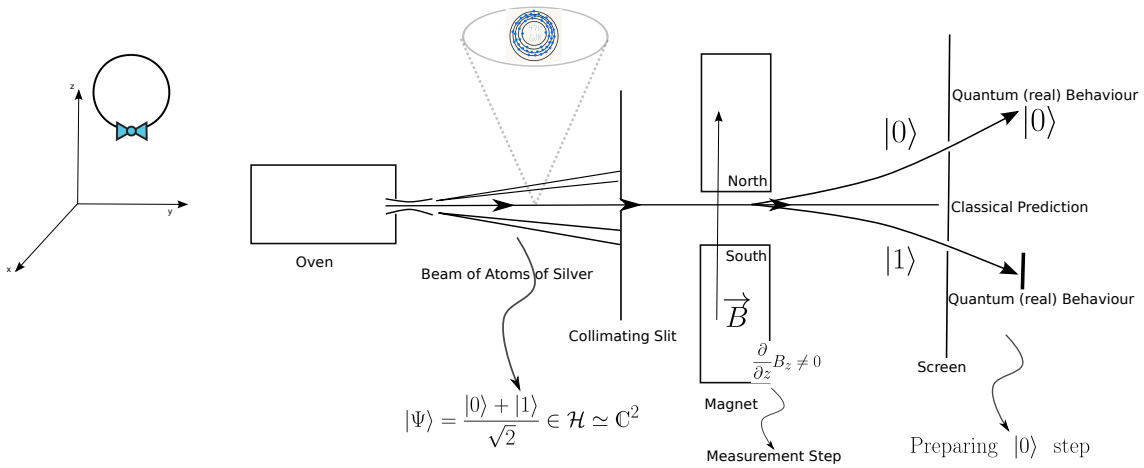


Figure 1: Schematic drawing of Stern and Gerlach's experiment [12–14]. Classically as the magnetic moment of each atom is isotropically distributed, and since $\boldsymbol{F} = -grad(-\mu \cdot \boldsymbol{B}) = \mu \cdot \partial_z B_z$, then the beam of atoms of silver should form only one symmetrical pattern at the screen. However, the results of the experiment cannot not be explained with the previous discussion. Performed the experiment, one did not observe a single spot centered at the screen, but actually 2 symmetrical spots. There are a bunch of good explanations [1, 2, 13, 14] of how quantum theory explains the phenomenon, and we will not enter into the details. All we need to know here is the classical description fails in explain it, and we are entering into the Quantum Realm.

In fact, the figure above contains almost all necessary elements to promote our discussion. Let us see: to a given system $\mathcal{S}$ (in our prototype represented by the atoms of silver) that one would like to describe mathematically using quantum theory, some sort of object must be associated to it. And of course, this object should lie in some set with desired properties[7]. So,

Axiom 1. To each quantum system $\mathcal{S}$ is associated a Hilbert space $\mathcal{H}_S$, and each state of $\mathcal{S}$ is described by a normalized vector $|\psi\rangle \in \mathcal{H}_S$.

Well, since we know how to represent a quantum system $\mathcal{S}$, it is interesting to investigate some properties of it. The possibility to ask questions like "is its energy between 3.50 Joules and 4.78 Joules? ", "what is its polarization? ", or "in what direction is pointing its spin-z component? "... and so on, must be codified in the theory. Therefore, it is natural to postulate something along this lines:

Axiom 2. Given a quantum system $\mathcal{S}$, to a measurement process (or a test) $\mathcal{M}$ with d classically distinct alternatives $a_1, a_2, ..., a_d$, it is associated an orthonormal basis $\{|a_1\rangle, |a_2\rangle, ..., |a_d\rangle\}$. Applying the test $\mathcal{M}$ is viewed as a decomposition of each vector with respect to that basis. Furthermore, if the quantum system $\mathcal{S}$ is in a state represented for $|\psi\rangle \in \text{span}(|a_1\rangle, ..., |a_d\rangle)$, then when the test $\mathcal{M}$ is performed, the probability to obtain the $j-$th answer a_j is $|\alpha_j|^2$, where[8] $|\psi\rangle = \sum_{i=1}^{d} \alpha_i |a_i\rangle$.

In our example, all the experimental setup has to do with the test $\mathcal{M}$, connected with the question "what is the spin-z component? ", but actually is it the Stern-Gerlach Magnet that plays the role of "measurer". And after the measurement? What can we say about the state of the system?

[7] As we are going to see, i)linearity; ii) inner product; and iii) freedom to work with the complex field, will be these "desired properties".

[8] Note that $\sum_{i=1}^{d} |\alpha_i|^2 = 1$.

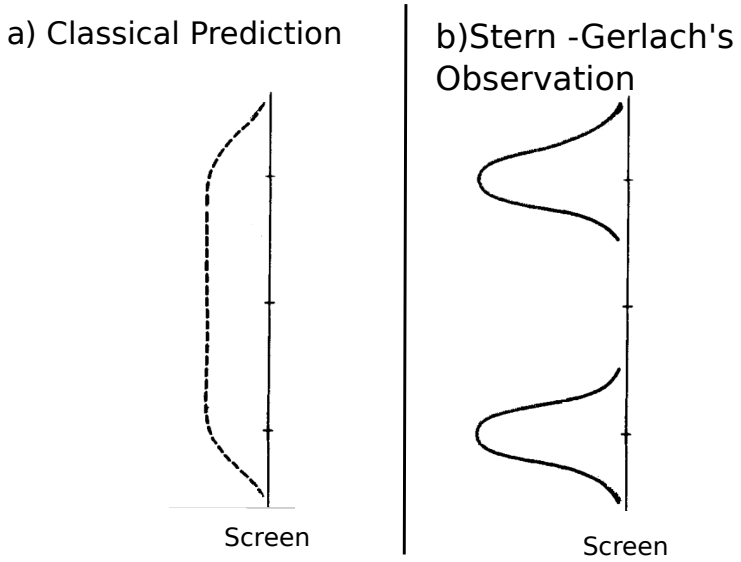


Figure 2: Schematic drawing of Stern and Gerlach's results. Classically should be noted a symmetrical spot at the screen, with equal probability for all possible values of magnetic moment $\mathcal{M}_z$, but what was actually seen were 2 spots, meaning that the angular momentum is somehow quantized [13, 14, 16]

Axiom 3. Performed a test $\mathcal{M}$, with d classically distinct alternatives $a_1, a_2, ..., a_d$, and associated orthonormal basis $\{|a_1\rangle, |a_2\rangle, ..., |a_d\rangle\}$, if the $j-$th alternative, labelled by a_j, is obtained then the system will be described by $|\psi'\rangle = |a_j\rangle$.

The Axiom 3 above is saying that our best description for the system *changes* when new information is added to the game [17–19]. (Un)Fortunately I will not discuss interpretations of Quantum Theory, it is a quite delicate subject and pages and pages would be needed to do so. Instead we refer to [16, 19–21] for accounts on the issue.

Finally we need to talk about *parts* right? So, probably the best way to start that discussion is thinking that we would like to describe collectively the behaviour of two, or more, quantum systems which are spatially[9] separated. For instance suppose two experimentalists, sharing each one an atom of silver coming from the furnace at Stern-Gerlach's experiment, would like to describe jointly the behaviour of their systems. Since they are holding quantum systems (which may have previously interacted), should be possible (in principle) to treat mathematically that situation. In fact,

Axiom 4. Given two quantum systems $\mathcal{S}_A$ and $\mathcal{S}_B$ each one associated with $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively, then the Hilbert space $\mathcal{H}_{AB}$ associated to the composite system $\mathcal{S}_A + \mathcal{S}_B$ is

$$\mathcal{H}_A \otimes \mathcal{H}_B \tag{1}$$

The beauty behind that axiom is the strict relationship between *parts* and *factors* of the tensor product. Each physical system, corresponding to a part to be described, contributes with one factor in the tensor product, and conversely each factor is associated with one system. Multiple

[9] Actually the idea of spatial separation is not necessary, see [22]. We do need to consider just two, or more, distinct properties to be jointly described by quantum theory.

systems $\mathcal{S}_1, ..., \mathcal{S}_N$, meaning multiple parts, ensure a Hilbert space $\mathcal{H} = \bigotimes_{i=1}^{N} \mathcal{H}_i$, and then $\dim(\mathcal{H}) = \Pi_{i=1}^{N} \dim(\mathcal{H}_i)$. It is quite obvious, but what is less obvious is the situation where $\dim\mathcal{H}$ is prime and don't matter how much effort you do, the system $\mathcal{S}$ associated with that Hilbert space can not be viewed as being composed of different parts. For instance, when $\mathcal{H} = \mathbb{C}^{11}$, then on the one hand there is no pair $\mathcal{H}_A, \mathcal{H}_B$ with $\dim(\mathcal{H}_A) \geq 2$ and $\dim(\mathcal{H}_B) \geq 2$, such that $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. On the other hand, it is always true that $\mathbb{C}^{11} = \mathbb{C}^2 \oplus \mathbb{C}^2 \oplus \mathbb{C}^2 \oplus \mathbb{C}^2 \oplus \mathbb{C}^3$, showing that, while possible, the description of composite systems by means of other mathematical structures than $\otimes$ will fail in order to capture the idea of *parts*. Both Chapter 2 and Chapter 3 explore this striking phenomenon, called Entanglement, associated with this idea of how parts are treated into Quantum Realm. In fact, at Chapter 3 we are concerned with the temporal evolution of quantum systems:

Axiom 5. A temporal evolution for a closed quantum system $\mathcal{S}$ with associated Hilbert space $\mathcal{H}_S$ is a family of unitaries $\{U_t : \mathcal{H}_S \longrightarrow \mathcal{H}_S\}_{t\geq 0}$ such that:

$$U_0 = \mathbb{1}_{\mathcal{H}_S} \tag{2}$$

$$U_{t+s} = U_t \circ U_s, \ \forall \ t \geq s \geq 0 \tag{3}$$

All the axioms above represent a first and naive approach to Quantum Theory, we reinforce that the Appendix A is strongly suggested to those readers unfamiliar with Quantum Physics.

A framework a little bit more abstract, whereas modern[10], to discuss, or to introduce some features of Quantum Theory is also liable to be cited. This one has more to do with the device-independent (or black-box) point of view, and it explores more directly the "non-classicality" and its relationship with the concept of locality (highly connected with the concept of parts). Roughly speaking, consider *two spatially separated and distant* experimentalists/observers, Alice and Bob, sharing physical systems[11] (which may have previously interacted).

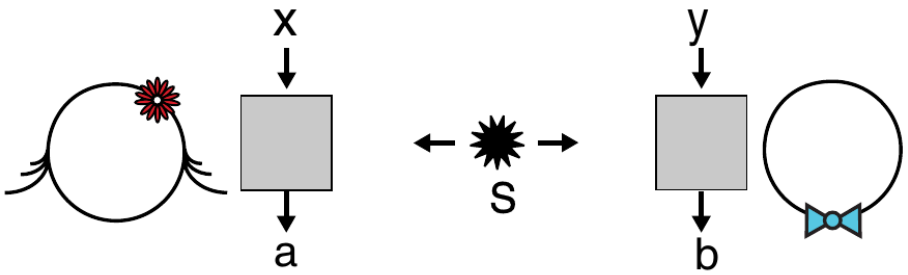


Figure 3: Alice and Bob sharing a physical system enclosed in 2 black-boxes.

[10] See [7–9]

[11] The physical nature of the systems does not matter in this scenario. The only thing that is important is how the boxes behave.

Each part of the system can be imagined to be enclosed into a black-box, of which neither Alice nor Bob [12] knows its operating details. They are only able to pull some buttons on their respective the boxes, and once the buttons were pressed, they yield an answer (pictorially representing the paradigm measurement/outcome). These answers, provided by pressing buttons, are in general governed by a probability distribution $p(ab|xy)$, meaning *the probability of Alice obtain the answer labelled by "a" given she has pressed the button x and Bob obtain "b" given he has pressed y*. When the experiment is performed, no matter what the system is enclosed into those black-boxes, they will found in general that $p(ab|xy) \neq p(a|x)p(b|y)$. But it is ok, since the shared physical systems may have interacted in some instant of time. If they had had control of all variables involved in the whole process, condensed and represented by a label λ, certainly $p(ab|xy,\lambda) = p(a|x,\lambda)p(b|y,\lambda)$. This factorization is simply expressing that the local experiment performed on Alice's side is independent of that performed on Bob's side (and vice-versa). The knowledge of that *hidden variable* λ allows to derive deterministic distributions for the parts, that is $p(a|x,\lambda),\ p(b|y,\lambda) \in \{0,1\}$.

Naively, if λ is not deterministic, but follows a probability distribution $q(\lambda)$ such that[13] $q(\lambda|x,y) = q(\lambda)$, then:

$$p(ab|xy) = \int_\Lambda q(\lambda)p(a|x,\lambda)p(b|y,\lambda)d\mu(\lambda),\ \forall\ a,b,x,y. \tag{4}$$

Now, defining the expected value of the product ab for a particular choice of buttons xy as $\langle a_x b_y\rangle = \sum_{a,b} abp(ab|xy)$, and

$$S = \langle a_0 b_0\rangle + \langle a_1 b_0\rangle + \langle a_0 b_1\rangle - \langle a_1 b_1\rangle, \tag{5}$$

it's a simple fact [7] that all probability distributions $\{p(ab|xy)\}$, with outcomes $a,b \in \{\pm 1\}$, that obey Eq.4 above, known as *locality decomposition*, satisfy[14]

$$S \leq 2. \tag{6}$$

On the other hand, if Alice shares with Bob a Quantum System described by (a Bell State) $|\psi^+\rangle$ [12–14], and if we allow the buttons x and y be associated with vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ corresponding to measurements of $\boldsymbol{x}\cdot\boldsymbol{\sigma} = \sum_{i=1}^3 x_i\sigma_i$ on Alice's system and $\boldsymbol{y}\cdot\boldsymbol{\sigma} = \sum_{i=1}^3 y_i\sigma_i$ on Bob's system, where $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$ denotes a vector composed by Pauli Matrices [13, 15], such that

$$\text{for } x \in \{0,1\} : \begin{cases} x = 0 \text{ corresponds to } \boldsymbol{e_1} \\ x = 1 \text{ to } \boldsymbol{e_2} \end{cases} \tag{7a}$$

$$\text{for } y \in \{0,1\} : \begin{cases} y = 0 \text{ corresponds to } \frac{\boldsymbol{e_1}+\boldsymbol{e_2}}{\sqrt{2}} \\ y = 1 \text{ to } \frac{\boldsymbol{e_1}-\boldsymbol{e_2}}{\sqrt{2}}, \end{cases} \tag{7b}$$

[12] We thank D. Cavalcanti for these broadly used drawings of Alice and Bob.

[13] This condition is extremely important. In fact it's saying that Alice and Bob can choose freely which experiment will be performed. It is a sort of freedom of choice. In many reviews, or discussion on the topic this condition is left aside, or even hidden, but in fact it's of extreme and philosophical importance.

[14] Clauser-Horne-Shimony-Holt inequality [59]. Just an example of a Bell-Inequality [7, 23].

then $S = \langle a_0 b_0 \rangle + \langle a_1 b_0 \rangle + \langle a_0 b_1 \rangle - \langle a_1 b_1 \rangle = \frac{3}{\sqrt{2}} - \frac{1}{\sqrt{2}} = 2\sqrt{2} > 2$, and therefore we have designed a physical situation that is non-local, for it violates the $CHSH$ inequality. We should stress that here was the peculiar notion of parts brought by Quantum Theory that allowed us to violate that Bell-Inequality. In fact, as we are going to see, Chapter 1 addresses this issue, and also shows how one can take the concept of parts seriously, and use it to find better upper bounds for those Inequalities.

The thesis is organized as follows: in Chapter 1 we begin our discussion stressing the fact that Non-Contextuality (NC) and Bell inequalities can be expressed as bounds Ω for positive linear combinations S of probabilities of events, $S \leq \Omega$. Exclusive events in S can be represented as adjacent vertices of a graph called the *exclusivity graph* of S. In the case that events correspond to the outcomes of quantum projective measurements, quantum probabilities are intimately related to the *Grötschel-Lovász-Schrijver theta body* of the exclusivity graph. Then, one can efficiently compute an upper bound to the maximum quantum violation of any NC or Bell inequality by optimizing S over the theta body and calculating the *Lovász number* of the corresponding exclusivity graph. In some cases, this upper bound is tight and gives the exact maximum quantum violation. However, in general, this is not the case. The reason is that the exclusivity graph does not distinguish among the different ways exclusivity can occur in Bell-inequality (and similar) scenarios. An interesting question is whether there is a graph-theoretical concept which accounts for this problem. There we show that, for any given N-partite Bell inequality, an edge-coloured multigraph composed of N single-colour graphs can be used to encode the relationships of exclusivity between each party's parts of the events. Then, the maximum quantum violation of the Bell inequality is *exactly* given by a refinement of the Lovász number that applies to these edge-coloured multigraphs. We show how to calculate upper bounds for this number using a hierarchy of semi-definite programs and calculate upper bounds for I_3, I_{3322} and the three bipartite Bell inequalities whose exclusivity graph is a pentagon. In Chapter 2 we analyse the conversion of entangled pure states under (Stochastic) Local Operations and Classical Communication, and since we know it admits the phenomenon of catalysis, as shown by D. Jonathan and M. Plenio, there we explore the possibility of a copy of the initial state itself to perform as a catalyst, which we call a self-catalytic process. We show explicit examples of self-catalysis. Necessary and sufficient conditions for the phenomenon to take place are discussed. We numerically estimate how frequent it is, and for some cases we show that increasing the number of copies used as catalyst can increases the probability of conversion, but do not make the process deterministic. By the end we conjecture that under LOCC the probability of finding a self-catalytic reaction *does not* increase monotonically with the dimensions whereas SLOCC *does* increase. We close the thesis with Chapter 3, investigating how common is the phenomenon of Finite Time Disentanglement (FTD) with respect to the set of quantum dynamics of bipartite quantum states with finite dimensional Hilbert spaces. Considering a quantum dynamics from a general sense (see Appendix A), as just a continuous family of Completely Positive Trace Preserving maps (parametrized by the time variable) acting on the space of the bipartite systems, we conjecture that FTD happens for all dynamics but those when all maps of the family are induced by local unitary operations. We prove this conjecture

valid for two important cases: i) when all maps are induced by unitaries; ii) for pairs of qbits, when all maps are unital. Moreover, we prove some general results about unitaries/CPTP maps preserving product/pure states.

Before embarking into the core of the thesis, I think a little disclaimer is necessary: Since the present text contains essentially[15] (some of) the works that I published during my years spent as Ph.D candidate at UFMG, I've chosen write this entire Introduction using that friendly and softly way, almost talking directly to you The Reader. And I've done that just because I think this is the best way to introduce whichever subject, preparing the ears and warming up the engines. In fact, I think, this is the optimal way to convince anyone to read the hard things that are coming. So, whilst what is written here is kindly informal, the main text of the thesis is formal, methodical, and as far as I could, it is rigorous and precise. Well... I hope you enjoy it. Have fun! ;)

[15] With minor modifications in order to improve them a little more, or in some cases to fit them in a more mathematical form.

Chapter 1

Graphs and Colours: Parts and Foundations of Quantum Theory

1.1 Introduction

John Bell proved the impossibility of reproducing quantum theory (QT) with hidden variables in two different ways. The first, in a paper [23] submitted in the summer of 1964 but not published until 1966 [24, 25], shows the impossibility of explaining QT with non-contextual hidden variables. Roughly speaking, non-contextual hidden variable (NCHV) theories are those in which every observable has a predefined outcome that is independent of the context (i.e., the set of co-measurable observables) in which the observable is measured. The second way, in a paper submitted and published in 1964 [26], shows the impossibility of explaining QT with local hidden variables in a simplified version of the bipartite scenario considered by Einstein, Podolsky and Rosen. Local hidden variable (LHV) theories are those in which outcomes are independent of spacelike separated measurements. Nowadays, by "quantum contextuality" and "quantum non-locality" we refer to the impossibility of explaining QT with NCHV and LHV theories, respectively. Two key observations that connect both Bell's papers are that quantum probabilities cannot, in general, be reproduced by a joint probability distribution over a single probability space and that quantum non-locality follows from quantum contextuality when the contexts are made of observables measured on spacelike separated regions. This means that Bell-inequality scenarios (where a pre-established set of parties, measurements for each party and outcomes for each measurement is assumed) involve extra constraints with respect to more abstract scenarios (where no such assumptions are made).

This chapter discusses how to deal with these extra constraints. The approach presented here refines the graph-theoretical approach introduced by Cabello, Severini and Winter (CSW) to study quantum correlations without these extra constraints [27, 28] (a different refinement has been presented in Ref. [29]). By *quantum correlations* we mean correlations between the outcomes of co-measurable quantum observables as defined in Ref. [30], i.e., via quantum projective measurements. Here we introduce a novel graph-based method for characterizing the set of quantum correlations for experimental scenarios such as specific non-contextuality-

inequality [31, 32] and Bell-inequality scenarios. The name non-contextuality (NC) inequality was introduced in Ref. [33].

The CSW graph-theoretical approach to quantum correlations aims at singling out quantum correlations among correlations in general probabilistic theories (here understood as those that specify the joint probabilities of each possible set of outcomes of each possible set of co-measurable observables given each possible state, but not necessarily they specify anything else [34, 35]) and is based on the following ideas and results:

(i) An *experimental scenario* is defined by a set of observables (each with a certain number of outcomes) and their relationships of co-measurability. A *context* is a set of observables that are co-measurable. Typical experimental scenarios involve observables belonging to two or more contexts. By *event*, CSW mean a proposition such as "outcomes $a, \ldots, c$ are respectively obtained when observables $x, \ldots, z$ are jointly measured", which is denoted as $a \ldots c|x \ldots z$. Two events are *exclusive* if both include one measurement x with distinct outcomes $a \neq a'$. For more precise definitions of events and exclusive events, see Ref. [40] or Appendix C. To any experimental scenario, CSW associate a graph $\mathcal{G}$ in which events are represented by vertices and pairs of exclusive events are represented by adjacent vertices. $\mathcal{G}$ is called the *exclusivity graph of the experimental scenario*.

(ii) An NC inequality is a constraint on a linear combination of probabilities of a subset of events of the corresponding scenario. Normalization of probability distributions can be used to express this linear combination as a *positive* linear combination of probabilities of events, $S = \sum_i w_i P(e_i)$, with $w_i > 0$. Therefore, any NC inequality can be expressed as

$$S \overset{\text{NCHV}}{\leq} \Omega, \tag{1.1}$$

where Ω is the maximum value attainable with NCHV theories (or with LHV theories in the case of a Bell inequality). The fact that any NC inequality can be written in different forms which are related to each other by adding multiples of normalization and/or co-measurability conditions implies that each of these forms may lead to a different S. Recall that co-measurability implies that marginal probabilities are independent of other co-measurable observables (see Appendix C) and, in this sense, co-measurability generalizes the notion of no-signalling invoked in Bell-inequality scenarios (see Appendix C).

(iii) CSW associate to S a vertex-weighted graph (G, w) with vertex set V, where $G \subseteq \mathcal{G}$ (in fact, G is an induced subgraph of $\mathcal{G}$) and $i \in V$ represents event e_i such that $P(e_i)$ is in S, adjacent vertices represent exclusive events and the corresponding vertex weights are the coefficient w_i. CSW refer to (G, w) as the *exclusivity graph of* S.

(iv) CSW prove that the maximum of S in QT is upper bounded by the *Lovász number* of (G, w), denoted as $\vartheta(G, w)$. The Lovász number was introduced by Lovász, for non-weighted graphs, as an upper bound to the Shannon capacity of a graph [41] and then extended to vertex-weighted graphs in Ref. [42]. The Lovász number of (G, w) can be defined [43] as

$$\vartheta(G, w) := \max \sum_{i \in V} w_i |\langle \psi | v_i \rangle|^2, \tag{1.2}$$

where the maximum is taken over all orthonormal representations of $\overline{G}$ and handles in any (finite or infinite) dimension. The *complement* $\overline{G}$ of a graph G with vertex set V is the graph with the same vertex set such that two vertices i, j are adjacent in $\overline{G}$ if and only if i, j are not adjacent in G. An *orthonormal representation* in $\mathbb{R}^d$ of $\overline{G}$ assigns a unit vector $|v_i\rangle \in \mathbb{R}^d$ to each $i \in V$ such that $\langle v_i|v_j\rangle = 0$, for all pairs i, j of non-adjacent vertices in $\overline{G}$ (i.e., adjacent in G). A further unit vector $|\psi\rangle \in \mathbb{R}^d$, called *handle*, is usually specified together with the orthonormal representation.

The set of all vectors of probabilities of the form $|\langle\psi|v_i\rangle|^2$, where $\{|v_i\rangle\}$ is an orthonormal representation of $\overline{G}$ and $|\psi\rangle$ is a handle, is the *Grötschel-Lovász-Schrijver (GLS) theta body* of G [42] (or see the Appendix D), denoted as $\mathrm{TH}(G)$, and represents the *set of quantum correlations associated to* G, defined as the set of vectors of probabilities of events attainable through quantum projective measurements (without any further constraint) satisfying the relationships of exclusivity encoded in G. We will denote this set as $Q^{\mathrm{CSW}}(G)$.

(v) CSW also show that, for any graph (G, w), there is always an NC inequality (but not necessarily a Bell inequality) such that its maximum in QT is exactly $\vartheta(G, w)$ and a quantum system and an experimental scenario spanning exactly $\mathrm{TH}(G)$. This result identifies $\vartheta(G, w)$ as a fundamental physical limit for quantum correlations associated to G and $\mathrm{TH}(G)$ as the set of quantum correlations for a given G.

A problem of the CSW approach is that, for a given NC or Bell inequality (expressed as a specific S), $\vartheta(G, w)$ *may only give an upper bound* to the maximum quantum value of S. As noticed in Ref. [44], this occurs because (G, w) does not contain information about some additional constraints that may exist in S. For example, if S refers to a bipartite Bell-inequality scenario, two events $ab|xy$ (denoting "Alice measures x and obtains a, and Bob measures y and obtains b") and $a'b'|x'y'$ can be exclusive because Alice's parts of the events are exclusive (i.e., because $x = x'$ and $a \neq a'$), because Bob's parts of the events are exclusive (i.e., because $y = y'$ and $b \neq b'$) or because both Alice's and Bob's parts of the events are exclusive. S tells us in which of these three cases we are. However, this information is lost when we represent S by (G, w). This problem does not only affect Bell inequalities, but also many NC inequalities (e.g., NC inequalities resulting from those discussed in section 1.5 by identifying each party with a different degree of freedom of a single physical system).

In Ref. [45] we solve this problem by encoding these extra constraints in a multigraph (G, w) composed of n simple graphs sharing the same vertex set, and introduce a novel multigraph number, denoted as $\theta(\mathsf{G}, w)$, that gives the quantum maximum for any S. In this present text, our idea is to discuss those results.

The structure of this first chapter is the following: In section 1.2 we define (G, w), which refines (G, w). In section 1.3 we define $\theta(\mathsf{G}, w)$, which refines $\vartheta(G, w)$, and $\hat{Q}(\mathsf{G})$, which refines $Q^{\mathrm{CSW}}(G)$. Unlike $\vartheta(G, w)$, which can be computed to any desired precision in polynomial time [42] using a single semi-definite program (SDP), we can only compute upper bounds to $\theta(\mathsf{G}, w)$ by means of a hierarchy of SDPs which progressively implement extra restrictions. In section 1.4 we show how to compute upper bounds to $\theta(\mathsf{G}, w)$ using the ideas developed by Navascués, Pironio and Acín (NPA) [48, 49]. In section 1.5 we compute upper bounds to $\theta(\mathsf{G}, w)$ for some Bell inequalities

that are important for different reasons. All of them have in common the fact that $\vartheta(G,w)$ does not provide their quantum maxima but $\theta(\mathsf{G},w)$ does. Discussions will be presented in Chapter 4, there we discuss the relation between $\theta(\mathsf{G},w)$ and $\vartheta(G,w)$, and between $\hat{Q}(\mathsf{G})$ and $Q^{\mathrm{CSW}}(G)$, and their significance within the program of understanding quantum correlations from first principles. The Appendix B gives details about the NPA method and how we adapt it to bound $\theta(\mathsf{G},w)$.

1.2 The edge-coloured exclusivity multigraph

A *multigraph* $\Gamma = (V,E)$ is special kind of a Graph [56–58] with vertex set V and edge set E such that multiple edges between two vertices are allowed (see Appendix D for more details). A vertex-weighted multigraph $(\Gamma,w) = (V,E,w)$ is a multigraph endowed with a weight assignment $w : V \to \mathbb{R}_+$. In this text we will focus on a special type of multigraphs (and vertex-weighted multigraphs): N-colour edge-coloured (vertex-weighted) multigraphs $(\mathsf{G},w) = (V,E,w)$ composed of N simple graphs $(G_A,w) = (V,E_A,w),\ldots,(G_N,w) = (V,E_N,w)$ that have a common vertex set V with a common weight assignment w and have mutually disjoint edge sets $E_A,\ldots,E_N$, such that $E = E_A \sqcup \ldots \sqcup E_N$ (where $\sqcup$ stands for disjoint union) and each E_j is of a different colour. That is, we will focus on multigraphs (G,w) that can be factorized into N simple subgraphs $(G_A,w),\ldots,(G_N,w)$, called *factors*, each of which spans the entire set of vertices of (G,w), and such that all together collectively exhaust the set of edges of (G,w).

As a refinement of point (i) in the CSW approach, to any given experimental scenario we can associate an *edge-coloured exclusivity multigraph of the experimental scenario*, $\mathbf{G}$. As a refinement of point (iii), to any given S we can associate an *edge-coloured vertex-weighted exclusivity multigraph of* S, (G,w), where $\mathsf{G} \subseteq \mathbf{G}$ (in fact, G is an induced subgraph of $\mathbf{G}$). For the sake of simplicity, we will refer to (G,w) as the *exclusivity multigraph of* S. The idea is that (G,w) can encode all the restrictions built in the relationships of exclusivity between the events in S that are missing in the CSW graph when dealing with N-party scenarios. The number of colours in (G,w) is determined by the number of parties and the graph (G_J,w) encodes the relationships of exclusivity between party J's parts of the events. We will refer to (G_J,w) as the *exclusivity factor of party* J. Party J's exclusivity factor has several connected components, one for each of her settings. The minimum number of outcomes of a given setting appearing in S is equal to the clique number of the corresponding connected component.

Here, parties are defined as entities that perform measurements that are co-measurable with any other measurement performed by any other party. Notice that this notion of parties includes the one used in Bell-inequality scenarios (in which measurements of different parties are mutually spacelike separated), but is less restrictive (e.g., measurements of different parties may be timelike separated). Notice also that not all NC inequalities allow us to distribute the measurements between a given number of parties in such a way that each experiment only involves measurements performed by different parties and each party can choose between different measurements (examples of NC inequalities in which this distribution is not possible can be found in Refs. [31, 32]).

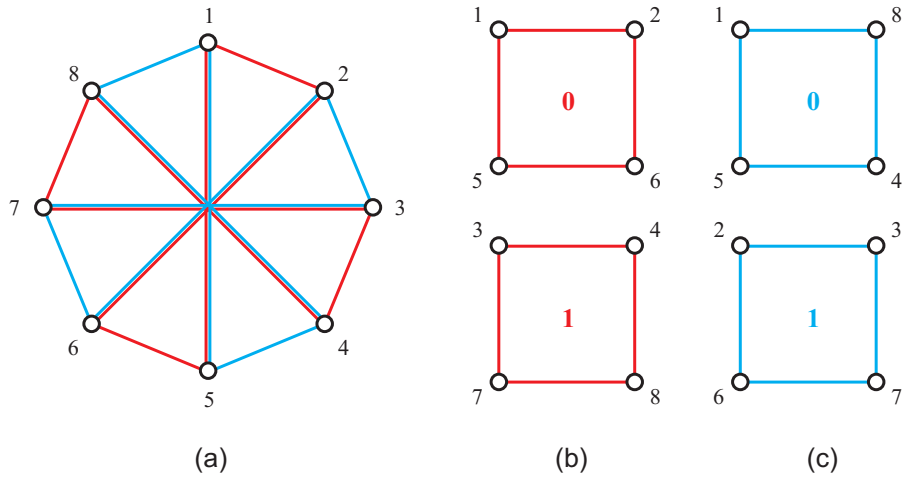


Figure 1.1: (a) Exclusivity multigraph $(\mathsf{G}^{(S_{\text{CHSH}})}, w)$, (b) exclusivity factor of Alice, $(G_A^{(S_{\text{CHSH}})}, w)$, and (c) exclusivity factor of Bob, $(G_B^{(S_{\text{CHSH}})}, w)$, for the CHSH Bell inequality (1.3). Notice that each factor has two connected components, each of them corresponding to a local observable. This observable is indicated with a bold letter. All vertices have weight 1. See Table 1.1 for the correspondence between the vertices of $(\mathsf{G}^{(S_{\text{CHSH}})}, w)$ and the events of S_{CHSH}.

As an example of an exclusivity multigraph of S, consider the Clauser-Horne-Shimony-Holt (CHSH) Bell inequality [59] written as

$$\begin{aligned} S_{\text{CHSH}} =& P(00|00) + P(11|00) + P(00|01) + P(11|01) + P(00|10) \\ &+ P(11|10) + P(01|11) + P(10|11) \overset{\text{LHV}}{\leq} 3, \end{aligned} \tag{1.3}$$

where $P(ab|xy)$ is the joint probability of obtaining the results a and b for, respectively, the measurements x (in Alice's side) and y (in Bob's) and LHV denotes local hidden variables. In Fig. 1.1 we show the exclusivity multigraph $(\mathsf{G}^{(S_{\text{CHSH}})}, w)$ and the corresponding exclusivity factors of Alice and Bob.

Table 1.1: Enumeration of the 8 events involved in the CHSH Bell inequality (1.3) and whose relationships of exclusivity are represented in Fig. 1.1.

Vertex	Event	Vertex	Event
1	00|00	5	11|00
2	11|01	6	00|01
3	10|11	7	01|11
4	00|10	8	11|10

We should stress how useful is the CHSH example depicted above[1]. Given the already coloured-graph of Figure 1.1, we are able to associate with it an inequality[2]. Indeed, since there are two colours we are talking about with a scenario with 2 parts. Furthermore there are two connected components for each colour, then each part has 2 (available) questions to do. Keeping the simplest scenario so far as possible, all the exclusivity relations could be reach with two

[1] In fact, we are going to see that far to be useful, this particular example is surprisingly, since the quantum bound given by the ordinary Lovász number already coincides with our new bound. The explanation for that fact is an open problem, and it will be discussed at Chapter 4.

[2] Again, see 4 for open problems on that association.

outcomes per measurement. Putting all these facts together, and remembering that all vertices has the same weight, we obtain both Table 1.1 and Ineq. (1.3).

1.3 The multigraph Lovász number

We define an *orthogonal projective representation* of $\overline{G}$ as an assignment to each $i \in V$ of a projector Π_i (not necessarily of rank-one) onto a subspace of a d-dimensional Hilbert space, such that $\Pi_i\Pi_j = 0 = \Pi_j\Pi_i$ (i.e., the subspaces onto which Π_i and Π_j project are orthogonal), for all pairs i, j of non-adjacent vertices in $\overline{G}$ (i.e., adjacent in G). There is a vague connection between this concept and the multigraphs defined in Ref. [60], which are supposed to encode orthonormal relations between vectors belonging to different parties.

We define the *factor-constrained Lovász number* of a multigraph (G, w) composed of simple graphs $(G_A, w) = (V, E_A, w), \ldots, (G_N, w) = (V, E_N, w)$ as

$$\theta(\mathsf{G}, w) = \sup \sum_{i \in V} w_i \langle\psi|\Pi_i|\psi\rangle, \tag{1.4}$$

with

$$\Pi_i = \Pi_i^A \otimes \cdots \otimes \Pi_i^N, \tag{1.5}$$

where $\otimes$ denotes tensor product and $\{\Pi_i^J : i \in V\}$ constitutes an orthogonal projective representation of $\overline{G_J}$, for all parties J, and the supremum in (1.4) is taken over all orthogonal projective representations of $\overline{G_1}, \ldots, \overline{G_n}$, unit vectors $|\psi\rangle \in \mathbb{R}^D$ (not necessarily product vectors) and dimensions D. Throughout the chapter, and for the sake of simplicity, we will refer to $\theta(\mathsf{G}, w)$ as the *multigraph Lovász number* of (G, w).

Let us denote as (G, w) the (simple) graph obtained from (G, w) when all edges between each two vertices are merged into a single edge connecting them (i.e., the exclusivity graph considered in the CSW approach [27, 28]). As it is clear from the definitions, $\theta(\mathsf{G}, w) \leq \vartheta(G, w)$. For S_{CHSH}, defined in (1.3), $\theta(\mathsf{G}^{(S_{\text{CHSH}})}, w) = \vartheta(G^{(S_{\text{CHSH}})}, w) = 2 + \sqrt{2}$. In section 1.5 we discuss some examples in which $\theta(\mathsf{G}, w) < \vartheta(G, w)$.

Now we define the *set of quantum correlations of the multigraph* G *composed of simple graphs* $G_A, \ldots, G_N$, denoted as $\hat{Q}(\mathsf{G})$, as the set whose elements are vectors $\hat{\mathbf{P}} \in \mathbb{R}^{|V|}$ with components

$$\hat{P}(i) = \langle\psi|\Pi_i^A \otimes \cdots \otimes \Pi_i^N|\psi\rangle, \quad \forall\, i \in V. \tag{1.6}$$

This set refines $Q^{\text{CSW}}(G)$. At first sight, this definition may look too restrictive since, to be general, one should consider mixed states and positive operator valued measures (POVMs)[3]. Notice, however, that any vector of quantum probabilities in a Bell-inequality scenario can be obtained from a pure state and a tensor product of orthogonal projectors in a higher dimensional Hilbert space. We do not suffer the problem of loss of co-measurability of POVMs under arbitrary Neumark's dilations [61] discussed in Ref. [62], since, in our approach, G indicates which events involve exclusive outcomes of a local observable: We assume that, in each exclusivity factor G_J of G, the events associated to cliques correspond to exclusive outcomes of a local observable.

[3] See Appendix A.

1.4 Bounding $\theta(\mathbf{G}, w)$

Contrary to $\vartheta(G, w)$, which can be efficiently computed to any desired precision in polynomial time [42] using a single SDP [63, 64], it is not known for which (G, w) can the multigraph Lovász number $\theta(\mathsf{G}, w)$ be computed efficiently. However, it is possible to obtain upper bounds to $\theta(\mathsf{G}, w)$ by means of SDPs using the ideas developed by NPA [48, 49].

We define a *multipartite quantum behaviour* of an edge-coloured exclusivity multigraph G as a vector $\mathbf{P} \in \mathbb{R}^{|V|^N}$ whose entries are joint probabilities $P(a, \ldots, n)$ for which there exist orthogonal projective representations of $\overline{G_1}, \ldots, \overline{G_n}$, $\{\Pi_a^A : a \in V\}, \ldots, \{\Pi_n^N : n \in V\}$, respectively, and a normalized vector $|\psi\rangle$ in a Hilbert space such that

$$P(a, \ldots, n) = \langle\psi|\Pi_a^A \otimes \cdots \otimes \Pi_n^N|\psi\rangle, \quad \forall\, a, \ldots, n \in V, \tag{1.7}$$

where V is the vertex set of G. Let $Q(\mathsf{G})$ denote the set of multipartite quantum behaviours of G.

It follows that the multigraph Lovász number $\theta(\mathsf{G}, w)$ can be seen as the maximum value of a linear function of probabilities, where optimisation is performed over $\hat{Q}(\mathsf{G})$. Let us remark that, since S only involves $\hat{P}(i)$, optimising S over $\hat{Q}(\mathsf{G})$ is the same as optimising S over $Q(\mathsf{G})$ under the identification $\hat{P}(i) = P(i, \ldots, i)$. For convenience, we will adopt optimisation over $Q(\mathsf{G})$ as the standard throughout this text. The reason is that the set $Q(\mathsf{G})$, as defined here, is in direct analogy to the set of quantum non-local correlations, a set known to be hard to completely characterize, but which can be efficiently outer-approximated by means of a hierarchy of SDPs, as proven by NPA [48, 49]. We will not discuss in this thesis neither the NPA method, nor SDPs. For accounts on these subjects we strongly suggest the already cited [48, 49] and [8, 50–53].

To bound the multigraph Lovász number of a given (G, w), we adapt the method developed by NPA to the situation in which no experimental scenario is assumed a priori and the only information we have is the relationships of exclusivity given by (G, w). Details on how our method works are given in the Appendix B. In the usual NPA method, the relationships of exclusivity are given by the assumed *Bell scenario* (i.e., the pre-established number of parties, measurements per party and outcomes per measurement). In our version of the method, it is not necessary to assume, *a priori*, a Bell scenario or a particular labelling of events. The multigraph Lovász number is a graph-theoretical quantity, and, for this reason, our method is general in the sense that it can be applied not only to exclusivity multigraphs that represent specific NC or Bell inequalities, but also to any conceivable N-colour edge-coloured vertex-weighted multigraph. Note that any such multigraph is physically realizable in QT, in the sense that there is always a Bell inequality such that its maximum in QT is exactly $\theta(\mathsf{G}, w)$ and a quantum system and an experimental scenario spanning exactly $\hat{Q}(\mathsf{G})$.

1.5 Examples

As indicated before, in general, $\theta(\mathsf{G}, w) \leq \vartheta(G, w)$, where (G, w) is the simple graph obtained from (G, w) when multiple edges between two vertices are merged into a single edge and colours

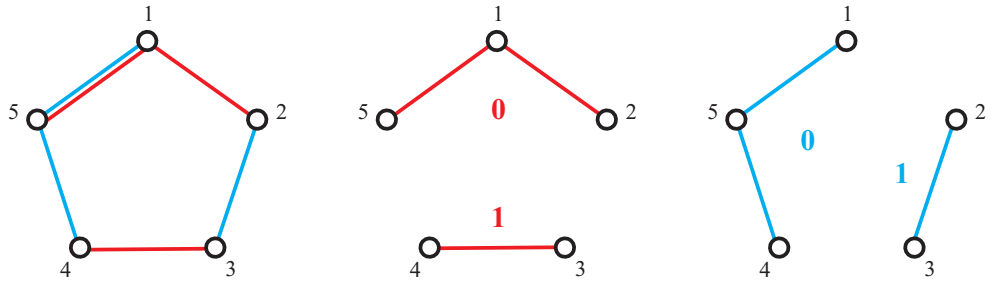


Figure 1.2: (a) Exclusivity multigraph $(\mathsf{G}^{(I_1^{\mathrm{P}})}, w)$, (b) exclusivity factor of Alice, $(G_A^{(I_1^{\mathrm{P}})}, w)$, and (c) exclusivity factor of Bob, $(G_B^{(I_1^{\mathrm{P}})}, w)$, for the first pentagonal Bell inequality (1.8). All vertices have weight 1. See Table 1.2 for the correspondence between the vertices of $(\mathsf{G}^{(I_1^{\mathrm{P}})}, w)$ and the events of I_1^{P}.

are ignored. The equality occurs[4] for some NC and Bell inequalities. In this section we focus on three relevant cases in which $\vartheta(G, w)$ does *not* provide the quantum maximum. Each of them is interesting for a different reason.

1.5.1 Pentagonal Bell inequalities

The pentagonal Bell inequalities introduced in Ref. [44] are the Bell inequalities with quantum violation with the simplest exclusivity graph. There are three non-equivalent pentagonal Bell inequalities and none of them is tight. The point is that they provide the simplest platform to understand why, in some cases, $\vartheta(G, w)$ does not give the quantum maximum.

Following [44], the first, second and third pentagonal Bell inequalities are, respectively,

$$I_1^{\mathrm{P}} = P(00|00) + P(11|01) + P(10|11) + P(00|10) + P(11|00) \overset{\mathrm{LHV}}{\leq} 2, \tag{1.8}$$

$$I_2^{\mathrm{P}} = P(00|00) + P(11|01) + P(10|11) + P(00|10) + P(\_1|\_0) \overset{\mathrm{LHV}}{\leq} 2, \tag{1.9}$$

$$I_3^{\mathrm{P}} = P(00|00) + P(11|01) + P(10|11) + P(00|10) + P(11|20) \overset{\mathrm{LHV}}{\leq} 2, \tag{1.10}$$

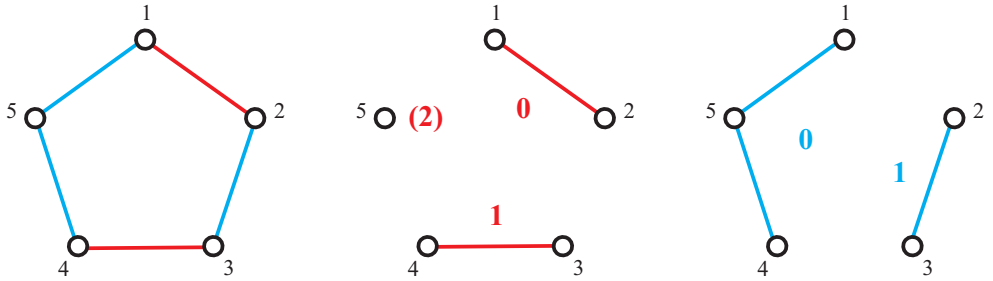
where $P(ab|xy)$ is the joint probability of obtaining the results a and b for, respectively, the measurements x (in Alice's side) and y (in Bob's), and $P(\_b|\_y)$ is the probability of the result b for Bob's measurement y irrespectively of Alice. Note that, in I_2^{P}, Alice chooses among two measurements, while in I_3^{P} she chooses among three.

Figure 1.2 shows the exclusivity multigraph $(\mathsf{G}^{(I_1^{\mathrm{P}})}, w)$ and the corresponding exclusivity factors of Alice and Bob for the first pentagonal Bell inequality, given by (1.8). Figure 1.3 shows the exclusivity multigraph $(\mathsf{G}^{(I_2^{\mathrm{P}}, I_3^{\mathrm{P}})}, w)$ and the corresponding exclusivity factors of Alice and Bob for the second and third pentagonal Bell inequalities, given by (1.9) and (1.10), respectively. Both inequalities are represented by the same exclusivity multigraph and factors; the only difference is the labelling of vertex 5 in the exclusivity factor of Alice's parts of the events: For I_2^{P}, there is no labelling; for I_3^{P}, it is labeled after Alice's observable 2.

[4] See the discussion in Chapter 4.

Table 1.2: Enumeration of the 5 events involved in the first pentagonal Bell inequality (1.8) and whose relationships of exclusivity are represented in Fig. 1.2.

Vertex	Event
1	00|00
2	11|01
3	10|11
4	00|10
5	11|00



(a) (b) (c)

Figure 1.3: (a) Exclusivity multigraph $(\mathsf{G}^{(I_2^{\mathrm{P}},I_3^{\mathrm{P}})},w)$, (b) exclusivity factor of Alice, $(G_A^{(I_2^{\mathrm{P}},I_3^{\mathrm{P}})},w)$, and (c) exclusivity factor of Bob, $(G_B^{(I_2^{\mathrm{P}},I_3^{\mathrm{P}})},w)$, both for the second and for the third pentagonal Bell inequalities, (1.9) and (1.10), respectively. All vertices have weight 1. See Table 1.3 for the correspondence between the vertices of $(\mathsf{G}^{(I_2^{\mathrm{P}},I_3^{\mathrm{P}})},w)$ and the events of I_2^{P} and I_3^{P}.

Table 1.3: Enumeration of the 5 events involved in the second (second column) and third (third column) pentagonal Bell inequalities and whose relationships of exclusivity are represented in Fig. 1.3.

Vertex	Event	Event
1	00|00	00|00
2	11|01	11|01
3	10|11	10|11
4	00|10	00|10
5	_1|_0	11|20

To test our approach, we have computed an upper bound to $\theta(\mathsf{G},w)$ for these two exclusivity multigraphs using our SDP method. Already in level $Q_{1+AB}(\mathsf{G})$ of the hierarchy (see the Appendix B for details) the results obtained coincide, up to the third digit, with the values obtained in Ref. [44] for the maximum quantum violation of the corresponding Bell inequalities. That is, we obtained

$$\theta(\mathsf{G}^{(I_1^{\mathrm{P}})},w) \leq 2.178, \tag{1.11}$$

$$\theta(\mathsf{G}^{(I_2^{\mathrm{P}},I_3^{\mathrm{P}})},w) \leq 2.207, \tag{1.12}$$

while the values obtained in Ref. [44] are 2.178 and $\frac{3+\sqrt{2}}{2} \approx 2.207$, respectively. Notice that, in both cases, the maximum quantum non-local violation is smaller than the Lovász number of the corresponding CSW exclusivity graph, i.e., the pentagon, namely, $\sqrt{5} \approx 2.236$.

1.5.2 CGLMP I_3 Bell inequality

The Collins-Gisin-Linden-Massar-Popescu (CGLMP) Bell inequalities [65], which can be written as

$$I_d^{\text{CGLMP}} \overset{\text{LHV}}{\leq} 2, \tag{1.13}$$

with $d = 2, 3, \ldots$, constitute a family of tight [66] bipartite 2-setting d-outcome Bell inequalities which, for $d > 2$, are maximally violated by pairs of qudits in non-maximally entangled states [67–69]. This family is in one-to-one correspondence with a generalized version of Hardy's paradox proposed in Ref. [70]. Chen et al. have recently shown that $\vartheta(G, w)$ provides the maximum quantum non-local value of I_d for $d = 2, 4, 5$, but, curiously, not for $d = 3$ [71]. Here we construct the exclusivity multigraph corresponding to the Bell inequality I_3 and calculate its multigraph Lovász number $\theta(\mathsf{G}, w)$.

The general form of I_d, as defined in Ref. [65], is the following:

$$\begin{aligned} I_d^{\text{CGLMP}} = \sum_{k=0}^{\lfloor d/2 \rfloor - 1} \left(1 - \frac{2k}{d-1}\right) [&P(A_0 = B_0 + k) + P(B_0 = A_1 + k + 1) \\ &+ P(A_1 = B_1 + k) + P(B_1 = A_0 + k) - P(A_0 = B_0 - k - 1) \\ &- P(B_0 = A_1 - k) - P(A_1 = B_1 - k - 1) - P(B_1 = A_0 - k - 1)], \end{aligned} \tag{1.14}$$

where $P(A_x = B_y + k)$ stands for the probability that the measurements A_x and B_y have outcomes that differ, modulo d, by k. The relation between the notation used here and the one used in other parts of this thesis is the following: $P(ab|xy) = P(A_x = a, B_y = b)$.

In order to construct the corresponding CSW graph (G, w) and the exclusivity multigraph (G, w), we have to express I_d as a positive linear combination of joint probabilities. For this purpose, we make the following transformations in I_d^{CGLMP}:

$$-P(A_x = a, B_x = b) = -1 + \sum_{(a',b') \neq (a,b)} P(A_x = a', B_y = b'). \tag{1.15}$$

Then, we obtain

$$\begin{aligned} I_d^{\text{CSW}} = \sum_{k=0}^{d-1} (d - 1 - k) [&P(A_0 = B_0 + k) + P(B_0 = A_1 + k + 1) \\ &+ P(A_1 = B_1 + k) + P(B_1 = A_0 + k)] \overset{\text{LHV}}{\leq} 3(d-1). \end{aligned} \tag{1.16}$$

The relation between both expressions is

$$I_d^{\text{CSW}} = \frac{d-1}{2} (I_d^{\text{CGLMP}} + 4). \tag{1.17}$$

In particular, for $d = 3$ we obtain

$$\begin{aligned} I_3^{\text{CSW}} =& 2P(00|00) + P(01|00) + 2P(11|00) + P(12|00) + P(20|00) \\ &+ 2P(22|00) + 2P(00|01) + P(02|01) + P(10|01) + 2P(11|01) \\ &+ P(21|01) + 2P(22|01) + P(01|10) + 2P(02|10) + 2P(10|10) \\ &+ P(12|10) + P(20|10) + 2P(21|10) + 2P(00|11) + P(01|11) \\ &+ 2P(11|11) + P(12|11) + P(20|11) + 2P(22|11) \overset{\text{LHV}}{\leq} 6. \end{aligned} \tag{1.18}$$

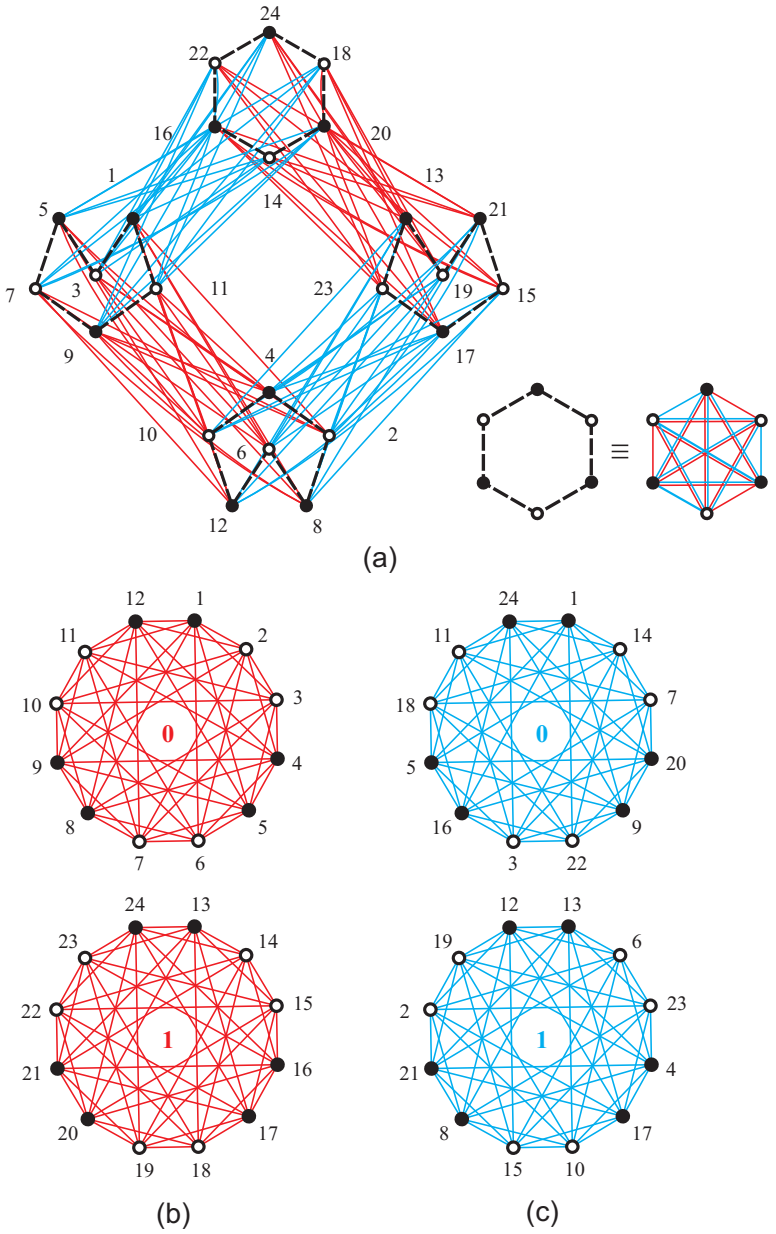


Figure 1.4: (a) Exclusivity multigraph $(\mathsf{G}^{(I_3)}, w)$, (b) exclusivity factor of Alice, $(G_A^{(I_3)}, w)$ and (c) exclusivity factor of Bob, $(G_B^{(I_3)}, w)$, for the Bell inequality associated to I_3^{CSW} given in (1.18). The graphs in (b) and (c) are isomorphic to the circulant graph $Ci_{12}(1,2,4,5)$ under different vertex orderings. See Table 1.4 for the correspondence between the vertices of $(\mathsf{G}^{(I_3)}, w)$ and the events of I_3^{CSW}. Vertices in white correspond to events whose probability appears in I_3^{CSW} with weight 1. Vertices in black correspond to events whose probability appears in I_3^{CSW} with weight 2.

The corresponding exclusivity multigraph, $(\mathsf{G}^{(I_3)}, w)$, and the exclusivity factors of Alice and Bob are shown in Fig. 1.4 (a), (b) and (c), respectively.

For the exclusivity multigraph corresponding to I_3^{CSW} we have obtained that

$$\theta(\mathsf{G}^{(I_3)}, w) \leq 6.9149, \tag{1.19}$$

for level $Q_{1.11}(\mathsf{G})$, an intermediate level between $Q_1(\mathsf{G})$ and $Q_{1+AB}(\mathsf{G})$ in the SDP hierarchy

Table 1.4: Enumeration of the 24 events involved in I_3^{CSW} and whose relationships of exclusivity are represented in Fig. 1.4.

Vertex	Event	Vertex	Event	Vertex	Event	Vertex	Event
1	00|00	7	01|00	13	00|11	19	01|11
2	10|01	8	11|01	14	12|10	20	10|10
3	20|00	9	22|00	15	20|11	21	22|11
4	00|01	10	02|01	16	02|10	22	01|10
5	11|00	11	12|00	17	11|11	23	12|11
6	21|01	12	22|01	18	20|10	24	21|10

(see the Appendix B for details). This result coincides, up to the fifth digit, with previous numerical [49, 67] and analytical [68] results for the maximum quantum violation of the I_3 Bell inequality, which is $5+\sqrt{\frac{11}{3}} \approx 6.9149$. This value is clearly smaller than the Lovász number of the corresponding CSW graph, which is $4\sqrt{3} \approx 6.9282$ [71].

1.5.3 I_{3322} Bell inequality

The I_{3322} inequality, first considered in Ref. [72], is, after the CHSH Bell inequality, the simplest tight Bell inequality violated by QT [73]. I_{3322} is also an interesting inequality because it has been conjectured that its maximum quantum violation only occurs for infinite dimensional local quantum systems [74]. In Ref. [27], CSW noticed that, for I_{3322}, the Lovász number is higher than the upper bound to the maximum quantum value calculated in Ref. [74].

Here we construct the exclusivity multigraph corresponding to the symmetric version of I_{3322} presented in Ref. [75]. Then, we compute an upper bound to its multigraph Lovász number.

The symmetric version of the I_{3322} inequality in Ref. [75] is

$$\begin{aligned} I_{3322}^{\mathrm{BG}} =& P(00|01)+P(00|02)+P(00|10)+P(00|12)+P(00|20)+P(00|21) \\ & -P(00|11)-P(00|22)-P(0\_|0\_)-P(0\_|1\_)-P(\_0|\_0)-P(\_0|\_1) \overset{\mathrm{LHV}}{\leq} 0. \end{aligned} \tag{1.20}$$

Using transformations like (1.15) to replace probabilities with minus signs by the corresponding positive probabilities, we obtain

$$I_{3322}^{\mathrm{BG}} = I_{3322}^{\mathrm{CSW}} - 6, \tag{1.21}$$

where

$$\begin{aligned} I_{3322}^{\mathrm{CSW}} =& P(00|01)+P(00|02)+P(00|10)+P(00|12)+P(00|20)+P(00|21) \\ & +P(01|11)+P(10|11)+P(11|11)+P(01|22)+P(10|22)+P(11|22) \\ & +P(1\_|0\_)+P(1\_|1\_)+P(\_1|\_0)+P(\_1|\_1) \overset{\mathrm{LHV}}{\leq} 6. \end{aligned} \tag{1.22}$$

The corresponding exclusivity multigraph and the exclusivity factors of Alice and Bob are shown in Fig. 1.5 (a), (b) and (c), respectively.

For the exclusivity multigraph corresponding to I_{3322}^{CSW}, we have obtained

$$\theta(\mathsf{G}^{(I_{3322})}, w) \leq 6.2515, \tag{1.23}$$

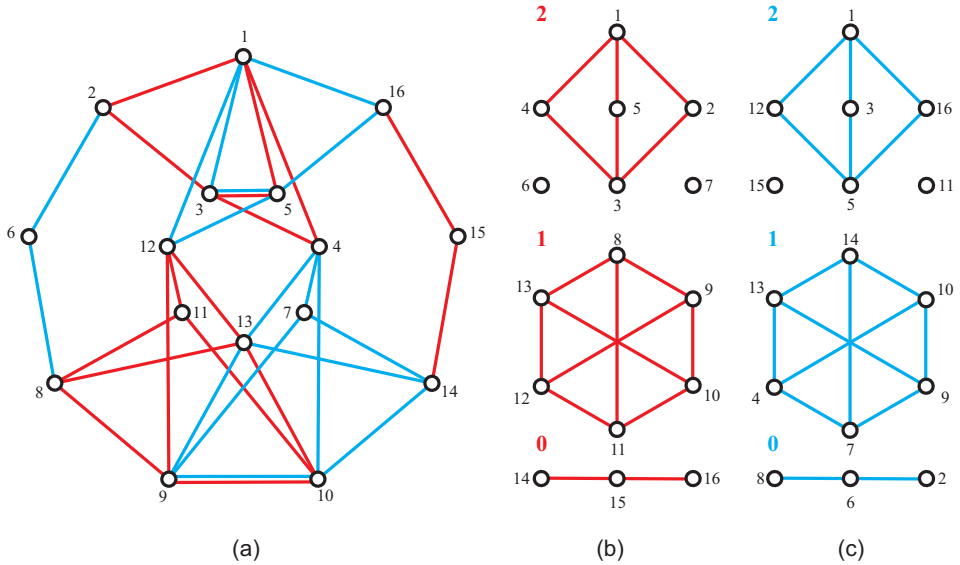


Figure 1.5: (a) Exclusivity multigraph $(\mathsf{G}^{(I_{3322})}, w)$, (b) exclusivity factor of Alice, $(G_A^{(I_{3322})}, w)$ and (c) exclusivity factor of Bob $(G_B^{(I_{3322})}, w)$ for the Bell inequality associated to I_{3322}^{CSW} given in (1.22). See Table 1.5 for the correspondence between the vertices of $(\mathsf{G}^{(I_{3322})}, w)$ and the events of I_{3322}^{CSW}.

Table 1.5: Enumeration of the 16 events involved in I_{3322}^{CSW} and whose relationships of exclusivity are represented in Fig. 1.5.

Vertex	Event	Vertex	Event	Vertex	Event	Vertex	Event
1	11|22	5	01|22	9	10|11	13	11|11
2	00|20	6	_1|_0	10	01|11	14	00|01
3	10|22	7	_1|_1	11	1_|1_	15	1_|0_
4	00|21	8	00|10	12	00|12	16	00|02

for level $Q_{1.13}(\mathsf{G})$ of the hierarchy (see the Appendix B for an explanation). This result is in agreement with the result obtained in Ref. [49] for the maximum quantum violation of I_{3322} Bell inequality, where they obtained ≤ 6.2515 for level Q_{1+AB} in the NPA hierarchy. It would be interesting to go higher in our hierarchy in order to reproduce the results obtained in Ref. [74] for level Q_4 in the NPA hierarchy. However, our methods are less efficient and even the resources required to reach level $Q_2(\mathsf{G})$ are beyond our possibilities. Notice that the value obtained is clearly smaller than the Lovász number of the corresponding CSW graph, which is 6.588412879 (the uncertainty is in the last two digits).

Table 1.6 summarizes the results obtained in this section and their relation with previous results.

Table 1.6: Results obtained for $\theta(\mathsf{G}, w)$ for the exclusivity multigraphs associated to the Bell inequalities studied here. The column $\vartheta(G, w)$ lists the Lovász number of the corresponding CSW graph. The column $\theta(\mathsf{G}, w)$ lists the computed bound for the Lovász number of the corresponding exclusivity multigraph and, in brackets, the level in the hierarchy in which the results were obtained. The column Maximum quantum value lists the maximum quantum value or upper bounds to it previously known, the level in the hierarchy in which these bounds were obtained, in brackets, and the reference where they were reported. The uncertainty is in the last digits.

Inequality	$\vartheta(G, w)$	$\theta(\mathsf{G}, w)$	Maximum quantum value
I_1^{P}	$\sqrt{5} \approx 2.236$	2.178 $(1 + AB)$	2.178 [44]
I_2^{P}, I_3^{P}	$\sqrt{5} \approx 2.236$	2.207 $(1 + AB)$	$\frac{3+\sqrt{2}}{2} \approx 2.207$ [44]
I_3	$4\sqrt{3} \approx 6.9282$ [71]	6.9149 (1.11)	$5 + \sqrt{\frac{11}{3}} \approx 6.9149$ [68]
I_{3322}	6.588412879	6.2515 (1.13)	6.2515 $(1 + AB)$ [49], 6.25087538 (4) [74]

Chapter 2

Self-Catalysis: Parts and Quantum Information

2.1 Introduction

The conversion between bipartite or multipartite quantum states through local operations is a central concept of entanglement theory. For instance, it is the criterion used to classify entanglement, namely, two states have equivalent entanglement if they can be converted to each other [15]. Moreover, it is usual and natural to consider a state more entangled than other when the first can *access* the former by the allowed transformations [97]. Two important sets of allowed transformations are the deterministic *local operations and classical communication* (LOCC) and its stochastic version (SLOCC), where the transformation only needs to succeed with positive probability [98]. Although this hierarchisation is relatively simple for bipartite pure states [97, 99], it is quite involved if mixed or multipartite states are considered [100–102].

The problem of convertibility of bipartite pure states has been solved by Nielsen [97], using the concept of majorisation [103]. However, Jonathan and Plenio discovered a surprising effect [104]. They have shown the existence of pairs of states which are not directly inter-convertible but such that their conversion is possible if another (necessarily entangled) state is attached to them. That is, the pair of states have incomparable entanglement but they may become ordered if an extra system is attached to the original ones. Such extra state that makes a transformation possible, without being consumed, is called a *catalyst*. More recently, the problem of convertibility has received experimental attention [105] and has also been connected to basic results in thermodynamics [106] and phase transitions [107].

In this chapter we explore the following question: can one of the states of a non inter-convertible pair be used as a catalyst? We answer this question positively, providing explicit examples. We also explore how common such processes are for low dimensional systems. An interesting situation is when a state $|\Psi\rangle$ is not able of self-catalysing a transformation, but a number of copies, $|\Psi\rangle^{\otimes n}$, is. We exhibit examples where more than one copy is required and study how augmenting the number of copies can increase the probability of conversion.

In section 2.2 we review basic notions of state conversion and catalysis under LOCC. In

section 2.3 we show explicit examples of self-catalytic processes, explore, through numerical analysis, how frequent they are under random samples of incomparable pairs and how it depends on the size of the systems. Section 2.4 review the notions of probabilistic catalysis under SLOCC, while the natural questions of self-catalysis under SLOCC are discussed in section 2.5. Our discussions, further problems and final remarks on the subject will be presented in Chapter 4.

2.2 Catalisys

We say that a bipartite state $|\alpha\rangle \in H_A \otimes H_B$ *access* a state $|\beta\rangle \in H'_A \otimes H'_B$, if there is some LOCC operation, represented by a completely positive trace preserving (CPTP) map Λ, such that $\Lambda(|\alpha\rangle\langle\alpha|) = |\beta\rangle\langle\beta|$, where H_A, H'_A, H_B and H'_B are finite dimensional Hilbert spaces and Λ maps density operators acting on $H_A \otimes H_B$ to density operators acting on $H'_A \otimes H'_B$. In such case, we write $|\alpha\rangle \to |\beta\rangle$. If there is no LOCC operation able to convert $|\alpha\rangle$ to $|\beta\rangle$, we write $|\alpha\rangle \nrightarrow |\beta\rangle$.

For example, for a pair of qbits, the Bell state $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ can access all other two-qbit pure states. Indeed, naming our qbits A and B, and writing the target state as $|\beta\rangle = a|00\rangle + b|11\rangle$, we can, for example, make A unitarily interact with an auxiliary qbit A', so that $|0_A 0_{A'}\rangle \mapsto a|0_A 0_{A'}\rangle + b|1_A 1_{A'}\rangle$ and $|1_A 0_{A'}\rangle \mapsto a|0_A 1_{A'}\rangle + b|1_A 0_{A'}\rangle$. Then, $[(|0_A 0_B\rangle + |1_A 1_B\rangle)/\sqrt{2}]|0_{A'}\rangle \mapsto (1/\sqrt{2})(a|0_A 0_B\rangle + b|1_A 1_B\rangle)|0_{A'}\rangle + (1/\sqrt{2})(a|0_A 1_B\rangle + b|1_A 0_B\rangle)|1_{A'}\rangle$. The lab with qbit A can make a measurement on the computational basis of the auxiliary A' and send the result to the lab holding qbit B. If the result is 0, they already share the desired state, while the result being 1, a NOT operation, $|0_B\rangle \mapsto |1_B\rangle, |1_B\rangle \mapsto |0_B\rangle$, can be applied to qbit B to also leave the system AB in the desired state. This result generalises for a pair of qu*d*its in the state $|\Phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |ii\rangle$, which justifies $|\Phi_d^+\rangle$ to be called a maximally entangled state.

Nielsen, in his seminal paper [97], provided a simple necessary and sufficient condition for determining whether a general bipartite state $|\alpha\rangle$ can access a state $|\beta\rangle$ in terms of their corresponding Schmidt vectors [15]:

Theorem 2.1 (Nielsen Criterion). *If $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n)$ and $\boldsymbol{\beta} = (\beta_1, ..., \beta_m)$ are the (non-increasing) ordered Schmidt vectors of $|\alpha\rangle$ and $|\beta\rangle$, respectively, we have $|\alpha\rangle \to |\beta\rangle$ if, and only if,*

$$\sum_{l=1}^{k} \alpha_l \leq \sum_{l=1}^{k} \beta_l \tag{2.1}$$

for all $1 \leq k \leq \min\{n, m\}$.

By an ordered Schmidt vector $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_n)$, we mean that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. In this work, we shall always assume that Schmidt vectors are ordered. When vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ satisfy conditions (2.1) we say that $\boldsymbol{\alpha}$ is majorised by $\boldsymbol{\beta}$ and write $\boldsymbol{\alpha} \preceq \boldsymbol{\beta}$.

Revisiting the example above, we have $(1/2, 1/2)$ for the ordered Schmidt vector of $|\Phi^+\rangle$ and $(|a|^2, |b|^2)$ for $a|00\rangle + b|11\rangle$, assuming $|a| \geq |b|$, it is straightforward to apply the criterion and verify that $|\Phi^+\rangle \to [a|00\rangle + b|11\rangle]$.

A consequence of the criterion is the existence of pair of states $|\alpha\rangle$ and $|\beta\rangle$ such that $|\alpha\rangle \nrightarrow |\beta\rangle$ and $|\beta\rangle \nrightarrow |\alpha\rangle$. Actually, the only case where such an order is total is for two qbits. For instance,

consider a state of two four-level systems with Schmidt vector $(0.4, 0.4, 0.1, 0.1)$ and a two-qutrit state with Schmidt vector $(0.5, 0.25, 0.25)$. Indeed,

$$0.4 = \alpha_1 < \beta_1 = 0.5, \tag{2.2a}$$

$$0.4 + 0.4 = \alpha_1 + \alpha_2 > \beta_1 + \beta_2 = 0.5 + 0.25. \tag{2.2b}$$

In Ref. [104], the authors surprisingly show that it is possible to circumvent such non-accessibility between these states by making the parts to share an entangled state $|\kappa\rangle$ such that $|\alpha\rangle \otimes |\kappa\rangle \to |\beta\rangle \otimes |\kappa\rangle$ (see Figure 2.1). Since the state $|\kappa\rangle$ allows for a previously forbidden conversion, but at the end of the process it remains unaltered, it is called a *catalyst*. In this sense, we say that $|\alpha\rangle$ $\boldsymbol{\kappa}$*-access* $|\beta\rangle$ when $|\alpha\rangle \nrightarrow |\beta\rangle$, but $|\alpha\rangle \otimes |\kappa\rangle \to |\beta\rangle \otimes |\kappa\rangle$. In this specific example, the two-qbit state $|\kappa\rangle$ with Schmidt vector $\boldsymbol{\kappa} = (0.6, 0.4)$ is a catalyst.

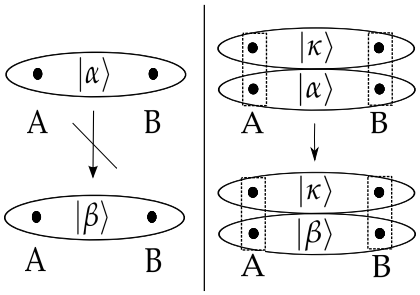


Figure 2.1: Although the conversion $|\alpha\rangle \to |\beta\rangle$ is not allowed under LOCC, the state $|\kappa\rangle$ can be used (but not consumed) to make it viable.

Nielsen's criterion ensures that all information about the (possibility of) conversion is contained in the Schmidt vectors. Therefore, we can explore our knowledge regarding probability vectors to provide more examples of catalysts. If $\boldsymbol{\alpha} = (0.5, 0.4, 0.05, 0.05)$, $\boldsymbol{\beta} = (0.7, 0.15, 0.15)$, $\boldsymbol{\kappa_1} = (0.7, 0.3)$, and $\boldsymbol{\kappa_2} = (0.75, 0.25)$, we obtain:

$$\boldsymbol{\alpha} \nrightarrow \boldsymbol{\beta} \tag{2.3a}$$

$$\boldsymbol{\alpha} \otimes \boldsymbol{\kappa_1} \to \boldsymbol{\beta} \otimes \boldsymbol{\kappa_1} \tag{2.3b}$$

$$\boldsymbol{\alpha} \otimes \boldsymbol{\kappa_2} \to \boldsymbol{\beta} \otimes \boldsymbol{\kappa_2}. \tag{2.3c}$$

This is a good example of non-unicity of catalysts. Indeed, for a given forbidden transition, $|\alpha\rangle \nrightarrow |\beta\rangle$, and fixed local dimensions for the catalysts, the set of allowed vectors $\boldsymbol{\kappa}$ is a polytope [108].

Remark 2.2. *Another interesting geometric fact is that catalysis is possible for every bipartite scenario, starting from* 4×3, i.e. *for all effective dimensions* $m \geq n$, $m \geq 4$, *and* $n \geq 3$ *it is possible to choose* $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_m) \nrightarrow (\beta_1, ..., \beta_n) = \boldsymbol{\beta}$ *with a catalyst* $\boldsymbol{\kappa}$. *The essential step, after the previously described examples, is that given* $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, *and* $\boldsymbol{\kappa}$, *we generically can increase dimensions by one and construct a forbidden transition* $\boldsymbol{\alpha'} \nrightarrow \boldsymbol{\beta'}$ *with the same catalyst* $\boldsymbol{\kappa}$, *by using* $\boldsymbol{\alpha'} = (\alpha_1, ..., \alpha_n - \epsilon, \epsilon)$ *and* $\boldsymbol{\beta'} = (\beta_1, ..., \beta_n - \epsilon', \epsilon')$ *with small enough* $\epsilon > 0$ *and* $\epsilon' \geq 0$. *This allow us to construct examples for all such* m *and* n.

$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$	♯Copies (N)
$(0.900, 0.081, 0.010, 0.009)$	(0.950,0.030,0.020)	$N = 1$
$(0.900, 0.088, 0.006, 0.006)$		$N = 2$
$(0.908, 0.080, 0.006, 0.006)$		$N = 3$
$(0.918, 0.070, 0.006, 0.006)$	$(0.950, 0.030, 0.020)$	$N = 4$
$(0.925, 0.063, 0.006, 0.006)$		$N = 5$
$(0.928, 0.060, 0.006, 0.006)$		$N = 6$
$(0.900, 0.081, 0.010, 0.009)$	(0.950,0.030,0.019,0.001)	$N = 1$

Table 2.1: Number N of copies required to make $|\alpha\rangle^{\otimes N}$ a deterministic catalyst for the process $|\alpha\rangle \to |\beta\rangle$.

2.3 Self-Catalysis

In this section we address our main question for the case of LOCC convertibility: can a bipartite quantum state be itself the catalyst of a forbidden conversion? To be more precise, is there a forbidden conversion $|\alpha\rangle \nrightarrow |\beta\rangle$, such that $|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle$? Refining a little bit more, is it possible that we still have $|\alpha\rangle \otimes |\alpha\rangle \nrightarrow |\beta\rangle \otimes |\alpha\rangle$, but a larger number of copies of $|\alpha\rangle$ would do the job, *i.e.* $|\alpha\rangle \otimes |\alpha\rangle^{\otimes N} \to |\beta\rangle \otimes |\alpha\rangle^{\otimes N}$ for some $N > 1$?

In Table 2.1 we list examples to answer affirmatively these questions. The first is an example of self-catalysis from a two-ququart state to a two-qutrit state. Then, for the same scenario, there is a list of multi-copy self-catalysis, with the corresponding minimal number of copies. At the last row, we come back to single-copy self-catalysis from a two-ququart state to another two-ququart state.

Remark 2.3. *When $|\alpha\rangle$ has 4 non-zero Schmidt coefficients and $|\beta\rangle$ has 3 non-zero Schmidt coefficients, the phenomenon of self-catalysis can be noted, that is, even in the minimal dimensions to occur catalysis (see [104]) the self-catalysis can also carry out. Geometrically, this mean that even in the smallest dimension (most restrictive) scenario, there are cases where the source state $\boldsymbol{\alpha}$ belongs to the polytope of catalysts for the reaction $\boldsymbol{\alpha} \nrightarrow \boldsymbol{\beta}$. Moreover, it is possible to construct examples for any higher-dimensional scenario through a similar argument presented at the Section 2.2.*

2.3.1 Stability under small perturbations

It is important to mention that the phenomenon of self-catalysis, as it happens with catalysis, is generically robust against small perturbations of the state vectors involved. That is, suppose that one is aiming to perform a self-catalytic process $|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle$, but it actually implements states $|\alpha'\rangle$, $|\beta'\rangle$, where $|\alpha'\rangle \approx |\alpha\rangle$ and $|\beta'\rangle \approx |\beta\rangle$. Our claim is: *generically, if $|\alpha\rangle$ α-access $|\beta\rangle$, then $|\alpha'\rangle$ α'-access β'*. It is easy to see that this will be true, depending only on the inequalities implying that $|\alpha\rangle \nrightarrow |\beta\rangle$, as well as those assuring that $|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle$, all be strict (except the last one, which is granted by normalisation). Denote by $|\boldsymbol{\lambda}|$ some norm (*e.g.* Euclidean) of the vector $\boldsymbol{\lambda}$ and n, m the sizes of Schmidt vectors $\boldsymbol{\alpha}, \boldsymbol{\beta}$. Now, assuming that we have, for some l, $\sum_{j=1}^{k} \alpha_j < \sum_{j=1}^{k} \beta_j$ for $1 \leq k \leq l$ and $\sum_{j=1}^{k} \alpha_j > \sum_{j=1}^{k} \beta_j$ for $l < k \leq n-1$, the same set of inequalities will hold for the entries of vectors $\boldsymbol{\alpha'}$ and $\boldsymbol{\beta'}$ if $|\boldsymbol{\alpha} - \boldsymbol{\alpha'}|, |\boldsymbol{\beta} - \boldsymbol{\beta'}| < \epsilon$, as long as

ϵ is small enough. This implies that $|\alpha'\rangle$ and $|\beta'\rangle$ are still incomparable. A similar reasoning can be applied when the incomparability of vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ is due to two or more changes of signs in the inequalities. In the same way, $\sum_{j=1}^{k}(\alpha\otimes\alpha)_j^{\downarrow} < \sum_{j=1}^{k}(\beta\otimes\alpha)_j^{\downarrow}$ for $k < nm-1$, imply $\sum_{j=1}^{k}(\alpha'\otimes\alpha')_j^{\downarrow} < \sum_{j=1}^{k}(\beta'\otimes\alpha')_j^{\downarrow}$, if $|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|, |\boldsymbol{\beta}-\boldsymbol{\beta}'| < \epsilon$, for small enough ϵ, which proves the claim. Naturally, the argument includes the well-motivated situation when $|\beta'\rangle = |\beta\rangle$ as a special case.

2.3.2 Self-Catalysis under LOCC for random Schmidt vectors

We have numerically investigated how usual the phenomenon of self-catalysis among pairs of incomparable bipartite states is. Fixing the sizes of $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, we randomly sample pairs of such vectors until we find incomparable ones. The sampling of each vector is done by uniformly sorting unitary vectors in $\mathbb{C}^n\otimes\mathbb{C}^n$, *i.e.* sorting according to the *Haar Measure* in the respective state spaces [116, 133], and then calculating the correspondent Schmidt vector. After finding a pair of incomparable states, we test whether the first of the vectors can be used as a catalyst for the conversion. The results show that for this method of sampling and for small dimensional systems, the phenomenon is actually *atypical*. Moreover, the numerical estimations seem to imply that the phenomenon of self-catalysis is atypical in any dimension.

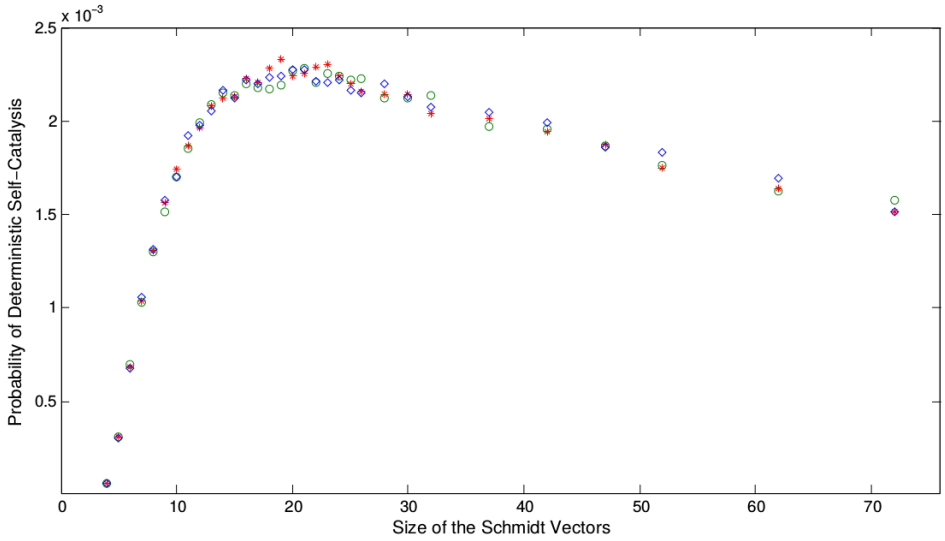


Figure 2.2: Probability of finding a pair of states exhibiting self-catalysis as function of the dimension of each system, that is $\mathbb{P}(|\alpha\rangle\otimes|\alpha\rangle \to |\beta\rangle\otimes|\alpha\rangle \mid |\alpha\rangle \nleftrightarrow |\beta\rangle)$. Each symbol means an average over a distinct set of random choices. For each size explored there are three different symbols, which indicates a reasonable stability in this sampling process.

Figure 2.2 shows a numerical estimation for $\mathbb{P}(|\alpha\rangle\otimes|\alpha\rangle \to |\beta\rangle\otimes|\alpha\rangle \mid |\alpha\rangle \nleftrightarrow |\beta\rangle)$, that is, the conditional probability of self-catalysis given a pair of incomparable Schmidt vectors, as a function of their sizes. Note that this probability increases with the size of the Schmidt vectors, until sizes about 20 and then starts to slowly decrease, but in fact for any dimension its order of magnitude shows that the phenomenon is present, but rare.

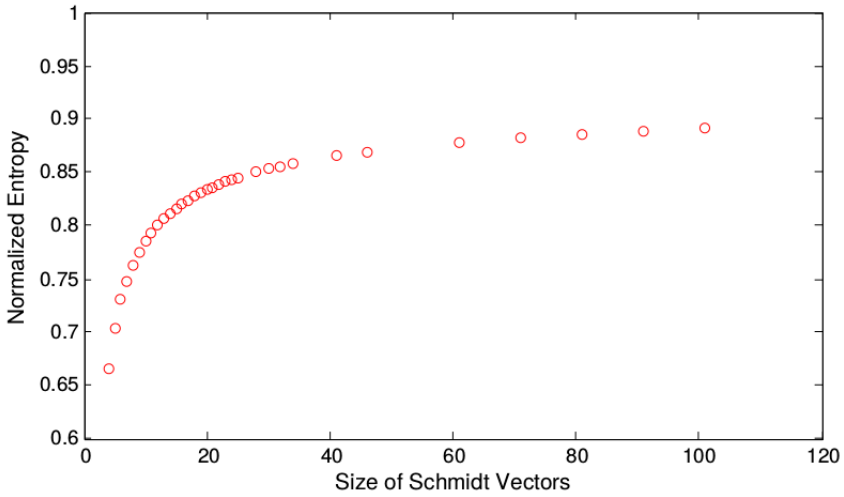


Figure 2.3: Mean normalized entropy for Schmidt vectors sorted by Haar measure. Here we have explored the behavior of the entropy until effective dimension 100.

We believe the global maximum present in the Figure 2.2 can be explained by the algebraic character of the comparison between vectors and the concentration of measure phenomenon. In order to $|\alpha\rangle \otimes |\alpha\rangle$ access $|\alpha\rangle \otimes |\beta\rangle$, all the corresponding inequalities of Eq. (2.1) must be satisfied. Then, in one hand, by increasing the dimension of the vectors, this comparison become harder to be valid (more inequalities have to be obeyed). On the other hand, it is known that a measure concentration phenomenon takes place for increasing dimensionality, in the sense that the Schmidt vectors become typically closer and closer to the constant vector $(\frac{1}{d}, ..., \frac{1}{d})$. This phenomenon can be highlighted by the average normalized entropy of the sorted vectors: if this average is close to 1, it means that most vectors are close to the constant vector. This average value is know to be exactly $\frac{1}{\ln d}[\sum_{k=d+1}^{d^2} \frac{1}{k} - \frac{d-1}{2d}]$, as conjectured by Page [114] and latter proved by Foong and Kanno [115]

If the vectors of the pair are incomparable, that is, some inequalities of Eq. (2.1) are not satisfied, but both are close to the constant vector, it will be easier for the catalyst to make the transition possible, since the corresponding inequalities for the vectors with the catalyst attached will be easier to be satisfied.

We can note that the concentration of measure increases very fast at low dimensions (see Figure 2.3), helping the possibility of "organising" the Schmidt vectors with the catalyst attached, which justifies the corresponding increasing in the probability for self-catalysis. However, around dimension 20 the concentration happens much slower and presumably is not fast enough to overcome the size effect (which makes majorisation more difficult), so the probability of finding a self-catalytic pair decreases after this point.

Summing up, the probability seems to be a smooth function of the dimension, reaching its higher value for dimensions of each Schmidt vector close to 20 and, apparently, converging to a value considerably smaller than 1.

Remark 2.4. *We have restricted the analysis above to events where* $|\alpha\rangle \nleftrightarrow |\beta\rangle$. *For large dimensions*

we have checked that this event is *typical. Indeed, in such regime the entries of vectors* $\boldsymbol{\alpha}$ *and* $\boldsymbol{\beta}$*, before ordering, are essentially concentrated random variables fluctuating around a fixed value. If we look, then, to Eq.* (2.1) *we see that there is a good chance for the sign of the inequality to change as we vary the index* k*, implying that the states are incomparable. Therefore, we expect that* $\mathbb{P}(|\alpha\rangle \nleftrightarrow |\beta\rangle) \approx 1$*, for* $n \gg 1$.

2.4 Catalysis under SLOCC

It is possible to generalize the concept of accessibility if we allow for non-deterministic processes. In this case, we can look for the probability $P_{SLOCC}(|\alpha\rangle \to |\beta\rangle)$, or $P_S(|\alpha\rangle \to |\beta\rangle)$ for short, of having the state conversion $|\alpha\rangle \to |\beta\rangle$ under the best local strategy, *i.e.* optimizing P under the conditions defining SLOCC. It is interesting to recall that the famous result on inconvertibility between W and GHZ states refers to such conditions on the multipartite scenario [109].

As shown by Vidal [110], for the bipartite case, the Schmidt vectors also encode this maximal probability of conversion, $P_S(|\alpha\rangle \to |\beta\rangle)$ through

Theorem 2.5. *Let* $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n)$ *and* $\boldsymbol{\beta} = (\beta_1, ..., \beta_n)$ *be ordered Schmidt vectors for states* $|\alpha\rangle$ *and* $|\beta\rangle$*, assuming* $\alpha_n, \beta_n > 0$*. Define* $E_k(\lambda) = 1 - \sum_{l=1}^{k-1} \lambda_l$*. Then, the optimal transformation probability is given by*

$$P_S(|\alpha\rangle \to |\beta\rangle) = \min_{1 \leq k \leq n} \left\{ \frac{E_k(\alpha)}{E_k(\beta)} \right\}. \tag{2.4}$$

For instance, if

$$\boldsymbol{\alpha} = (0.6, 0.2, 0.2) \text{ and } \boldsymbol{\beta} = (0.5, 0.4, 0.1) \tag{2.5}$$

are the Schmidt vectors for the two-qutrit states $|\alpha\rangle$ and $|\beta\rangle$, respectively, we get:

$$P_S(|\alpha\rangle \to |\beta\rangle) = 0.8, \tag{2.6a}$$

$$P_S(|\beta\rangle \to |\alpha\rangle) = 0.5. \tag{2.6b}$$

The following Proposition shows that the optimal probability of conversion P_S attains 1 precisely when $|\alpha\rangle$ access $|\beta\rangle$.

Proposition 2.6. *Let* $\boldsymbol{\alpha}$ *and* $\boldsymbol{\beta}$ *be a pair of random independent Schmidt vectors with same size* n*, then the event* $\{|\alpha\rangle \to |\beta\rangle\}$ *is equal to event* $\{P_S(|\alpha\rangle \to |\beta\rangle) = 1\}$*. In particular* $\mathbb{P}(|\alpha\rangle \to |\beta\rangle) = \mathbb{P}(P_S(|\alpha\rangle \to |\beta\rangle) = 1)$.

Proof. Suppose that $|\alpha\rangle \to |\beta\rangle$, thus:

$$\sum_{i=1}^{k} \alpha_i \leq \sum_{i=1}^{k} \beta_i, \ \forall k \ \in \{1, 2, ..., n\}. \tag{2.7}$$

Then $E_k(\alpha) = 1 - \sum_{i=1}^{k-1} \alpha_k \geq 1 - \sum_{i=1}^{k-1} \beta_k = E_k(\beta), \ \forall \ k \in \{1, 2, ..., n-1\}$ with the equality holding if $k = 1$, therefore $P_S(|\alpha\rangle \to |\beta\rangle) = 1$. The converse is similar. □

Note that from our considerations at the end of section 2.3.2 we expect that $\mathbb{P}(|\alpha\rangle \to |\beta\rangle) \approx 0$ (using LOCC) for large n, since the event $\{|\alpha\rangle \to |\beta\rangle\}$ is in the complement of $\{|\alpha\rangle \nleftrightarrow |\beta\rangle\}$.

We numerically estimate the SLOCC average rate of conversion between random states. For this, we generate incomparable Schmidt vectors following the *Haar measure* and calculate the probabilities of conversion from the first to the second and also the maximum conversion probability. The results shown in Figure 2.4 clearly shows that, given a random pair α, β, it is very common to have a large probability of conversion from some of them to the other, that is $\mathbb{E}[\max\{P_S(|\alpha\rangle \to |\beta\rangle, P_S(|\beta\rangle \to |\alpha\rangle)\}] \gtrsim 0.8$. Moreover we have a smaller, but still significant, average probability of conversion $\mathbb{E}[P_S(|\alpha\rangle \to |\beta\rangle)]$, slightly below 0.6.

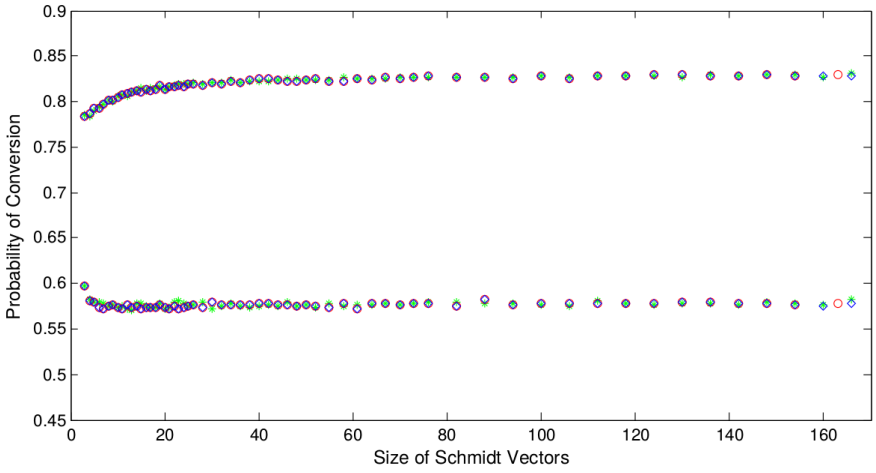


Figure 2.4: Sampled probability of conversion under SLOCC for randomly chosen (following the Haar measure) incomparable states as function of the dimension of each system. Each symbol represents an average over a distinct set of randomly chosen pairs. There are two sets of three symbols for each explored dimension. For each dimension, the smaller results consider conversion from the first to the second $\mathbb{E}[P_S(|\alpha\rangle \to |\beta\rangle)]$, and the larger the maximum conversion rate $\mathbb{E}[\max\{P_S(|\alpha\rangle \to |\beta\rangle, P_S(|\beta\rangle \to |\alpha\rangle)\}]$.

Also in the probabilistic scenario the presence of an extra state can improve the probability of conversion between two states [111]. As a chemical catalyst, this extra state is used, but not consumed, to increase the rate (probability) of a reaction (conversion). In the above example, if $\boldsymbol{\kappa} = (0.65, 0.35)$, we arrive at:

$$\boldsymbol{\alpha} \otimes \boldsymbol{\kappa} = (0.39, 0.21, 0.13, 0.13, 0.07, 0.07), \tag{2.8a}$$

$$\boldsymbol{\beta} \otimes \boldsymbol{\kappa} = (0.325, 0.26, 0.175, 0.14, 0.065, 0.035). \tag{2.8b}$$

Therefore $P_S(|\alpha\rangle \otimes |\kappa\rangle \to |\beta\rangle \otimes |\kappa\rangle) \simeq 0.904$, and $|\kappa\rangle$ can be viewed as a *probabilistic-catalyst* in the stochastic scenario for the conversion that starts in α and ends in β, despite the fact that $P_S(|\beta\rangle \otimes |\kappa\rangle \to |\alpha\rangle \otimes |\kappa\rangle) = 0.5$, and then $|\kappa\rangle$ does not increases the probability of conversion for the transformation that starts in β and ends in α. In this sense Jonathan and Plenio pointed out [104] that if $P_S(|\alpha\rangle \to |\beta\rangle)$, under the best local strategy, is equal to α_n / β_n, then this probability can not be increased by the presence of any catalyst state. Feng *et. al.* [111] improved this result, obtaining the following theorem:

Theorem 2.7. *Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ be two n–dimensional probability vectors written in non-increasing order. There is a probability vector $\boldsymbol{\kappa}$ such that $P_S(\boldsymbol{\alpha}\otimes\boldsymbol{\kappa}\to\boldsymbol{\beta}\otimes\boldsymbol{\kappa}) > P_S(\boldsymbol{\alpha}\to\boldsymbol{\beta})$ if, and only if,*

$$P_S(\boldsymbol{\alpha}\to\boldsymbol{\beta}) < \min\left\{\frac{\alpha_n}{\beta_n}, 1\right\}. \tag{2.9}$$

A deeper connection between LOCC catalysis and its stochastic counterpart connects the probability of occurrence of the event $\{\alpha\to\beta\}$ and the maximal probability of stochastic conversion, $P_S(|\alpha\rangle\otimes|\phi\rangle\to|\beta\rangle\otimes|\phi\rangle)$.

Proposition 2.8. *Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ be a pair of random independent Schmidt vectors with same size n. Then*

$$\mathbb{P}[\sup_{\phi}\{P_S(|\alpha\rangle\otimes|\phi\rangle\to|\beta\rangle\otimes|\phi\rangle)\} > P_S(|\alpha\rangle\to|\beta\rangle)] \quad\geq\quad \frac{1}{2} - \mathbb{P}(|\alpha\rangle\to|\beta\rangle). \tag{2.10}$$

Proof.

$$\mathbb{P}[P_S(|\alpha\rangle\otimes|\phi\rangle\to|\beta\rangle\otimes|\phi\rangle) > P_S(|\alpha\rangle\to|\beta\rangle)] = \tag{2.11a}$$

$$= 1 - \mathbb{P}\{P_S(|\alpha\rangle\to|\beta\rangle) = \min(\alpha_n/\beta_n, 1)\} \tag{2.11b}$$

$$\geq 1 - \mathbb{P}\{P_S(|\alpha\rangle\to|\beta\rangle) = \alpha_n/\beta_n\} - \mathbb{P}\{|\alpha\rangle\to|\beta\rangle\} \tag{2.11c}$$

$$\geq \frac{1}{2} - \mathbb{P}\{|\alpha\rangle\to|\beta\rangle\}. \tag{2.11d}$$

Where (2.11b) comes from Thm 2.7, (2.11c) from set theory and Proposition 2.6, and finally (2.11d) from $\{P_S(|\alpha\rangle\to|\beta\rangle) = \alpha_n/\beta_n\}\subseteq\{\alpha_n\leq\beta_n\}$. □

Remark 2.9. *From Remark 2.4 we know that as n grows, $\mathbb{P}(|\alpha\rangle\to|\beta\rangle)\approx 0$, so we conclude from Proposition 2.8 that $\mathbb{P}[P_S(\boldsymbol{\alpha}\to\boldsymbol{\beta}) < \min\left\{\frac{\alpha_n}{\beta_n}, 1\right\}]\gtrsim 1/2$.*

In Ref. [112] a necessary and sufficient condition for a state $|\kappa\rangle$ works as a probabilistic catalyst was provided:

Theorem 2.10. *Suppose that $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are two non-increasingly ordered n–dimensional probability vectors, and $P(\boldsymbol{\alpha}\to\boldsymbol{\beta}) < \min\left\{\frac{\alpha_n}{\beta_n}, 1\right\}$. Define*

$$L = \left\{l; 1 < l < n, \text{ and } P(\boldsymbol{\alpha}\to\boldsymbol{\beta}) = \frac{E_l(\boldsymbol{\alpha})}{E_l(\boldsymbol{\beta})}\right\}. \tag{2.12}$$

Then a non-increasingly ordered k-dimensional probability vector $\boldsymbol{\kappa}$ serves as a probabilistic catalyst for the conversion from $|\alpha\rangle$ to $|\beta\rangle$ if, and only if, for all $r_1, r_2, ..., r_k \in L\cup\{n+1\}$ satisfying $r_1\geq r_2\geq ...\geq r_k\neq n+1$, there exist i and j, with $1\leq j<i\leq k$, such that

$$\frac{\kappa_i}{\kappa_j} < \frac{\beta_{r_j}}{\beta_{r_i-1}} \text{ or } \frac{\kappa_i}{\kappa_j} > \frac{\beta_{r_j-1}}{\beta_{r_i}}. \tag{2.13}$$

By definition, whenever one of the inequalities (2.13) includes an index $n+1$, it is considered to be violated, so the other one must necessarily be satisfied.

We should stress a couple of facts about the set L: first of all, note that it is a key ingredient for identifying catalysts for a given conversion, since in a certain sense it determines which indexes are really important for the comparison between $\boldsymbol{\beta}$ and $\boldsymbol{\kappa}$. Secondly observe that typically L has only one element l, *i.e.* the minimum which determines the probability of conversion (see Thm. 2) is non-degenerate.

2.5 Self-Catalysis under SLOCC

The phenomenon of self-catalysis can also take place when considering conversions under SLOCC. Namely, if a conversion $|\alpha\rangle \to |\beta\rangle$ takes place with optimal probability $0 < p < 1$, it can be the case that the optimal probability for $|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle$ be $p' > p$. Indeed, for the same Schmidt vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ given by Eq. (2.5), there is a gain in the probability of conversion if we use the state $|\alpha\rangle$ itself as a catalyst. Using Eq. (2.4), we have:

$$P_S(|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle) \simeq 0.889 > 0.800 = P_S(|\alpha\rangle \to |\beta\rangle). \tag{2.14}$$

As it happens in the context of LOCC operations, the conversion between states can depend on the number of attached copies of $|\alpha\rangle$. Table 2.2 shows, for the example we are considering (given by Eq. (2.5)), how the probability of conversion increases with the number of copies of $|\alpha\rangle$ to be used as catalyst.

This example may suggest that, by increasing the number of copies of $|\alpha\rangle$, the probability of conversion approaches one. This is not always the case, however. Note that we can bound from above the probability in Thm. 2.5 for the pair $|\alpha\rangle \otimes |\alpha\rangle^{\otimes N}$ and $|\beta\rangle \otimes |\alpha\rangle^{\otimes N}$, since $P_S(|\alpha\rangle \otimes |\alpha\rangle^{\otimes N} \to |\beta\rangle \otimes |\alpha\rangle^{\otimes N}) \leq \alpha_n/\beta_n$, for all $N \geq 1$. Therefore, as long as $\alpha_n/\beta_n < 1$, no matter how many copies of $|\alpha\rangle$ we have, the probability of conversion will not exceed α_n/β_n. The previous reasoning allows us to state the following Proposition:

Proposition 2.11. *Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ be a pair of ordered Schmidt vectors with n non-null components. If $\alpha_n/\beta_n < 1$, then*

$$P_S(|\alpha\rangle \otimes |\alpha\rangle^{\otimes N} \to |\beta\rangle \otimes |\alpha\rangle^{\otimes N}) \leq \frac{\alpha_n}{\beta_n}, \ \forall\ N \geq 0. \tag{2.15}$$

For example, given $\boldsymbol{\alpha} = (0.60, 0.21, 0.10, 0.09)$ and $\boldsymbol{\beta} = (0.55, 0.25, 0.10, 0.10)$, we have a pair of states with $P_S(|\alpha\rangle \to |\beta\rangle) = 0.88$, but since $\alpha_4/\beta_4 = 0.9$, the probability of conversion under SLOCC using self-catalysis is limited by 0.9 and indeed, for this case, $N = 1$ is already optimal, since $P_S(|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle) = 0.9$. Analogously, for the pair $\boldsymbol{\alpha'} = (0.40, 0.34, 0.15, 0.11)$ and $\boldsymbol{\beta'} = (0.50, 0.21, 0.17, 0.12)$, Table 2.3 shows the behavior of $P_S(|\alpha'\rangle \otimes |\alpha'\rangle^{\otimes N} \to |\beta'\rangle \otimes |\alpha'\rangle^{\otimes N})$ with the number N of copies of $|\alpha'\rangle$, and since $\alpha'_n/\beta'_n = 0.91667 < 1$ the probability of conversion may increase, but can not reach 1. Moreover, there is the case (see Table 2.4) where, for a given pair $\boldsymbol{\alpha}, \boldsymbol{\beta}$ of incomparable Schmidt vectors, the probability of conversion increases monotonically with respect to N and, for an $N_0 < \infty$, $P_S(|\alpha\rangle \otimes |\alpha\rangle^{\otimes N_0} \to |\beta\rangle \otimes |\alpha\rangle^{\otimes N_0}) = 1$ and, by Proposition 2.6, $|\alpha\rangle \otimes |\alpha\rangle^{\otimes N_0} \to |\beta\rangle \otimes |\alpha\rangle^{\otimes N_0}$.

A particular case of Theorem 2.10 allows us to obtain a necessary and sufficient condition to exist probabilistic self-catalysis for a single copy:

Criterion *Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ be two n–dimensional Schmidt vectors with $P_S(\boldsymbol{\alpha} \to \boldsymbol{\beta}) < \min\left\{\frac{\alpha_n}{\beta_n}, 1\right\}$ and*

$$L = \left\{l; 1 < l < n, \text{ and } P_S(\boldsymbol{\alpha} \to \boldsymbol{\beta}) = \frac{E_l(\boldsymbol{\alpha})}{E_l(\boldsymbol{\beta})}\right\}. \tag{2.16}$$

The vector $\boldsymbol{\alpha}$ serves as a probabilistic self-catalyst for the transformation from $|\alpha\rangle$ to $|\beta\rangle$ if, and only if, for all $r_1, r_2, ..., r_n \in L \cup \{n+1\}$ satisfying $r_1 \geq r_2 \geq ... \geq r_n \neq n+1$, there exist i and j, with

♯ Copies (N)	$P_S(\|\alpha\rangle \otimes \|\alpha\rangle^{\otimes N} \to \|\beta\rangle \otimes \|\alpha\rangle^{\otimes N})$
0	$\simeq 0.800$
1	$\simeq 0.889$
2	$\simeq 0.907$
3	$\simeq 0.926$
4	$\simeq 0.932$
5	$\simeq 0.940$
6	$\simeq 0.944$
7	$\simeq 0.947$
8	$\simeq 0.950$
9	$\simeq 0.952$
10	$\simeq 0.955$

Table 2.2: Increase of optimal probability for the conversion $|\alpha\rangle \to |\beta\rangle$, where $\boldsymbol{\alpha} = (0.6, 0.2, 0.2)$ and $\boldsymbol{\beta} = (0.5, 0.4, 0.1)$, with the number of copies N of $|\alpha\rangle$ used as a catalyst.

♯ Copies (N)	$P_S(\|\alpha'\rangle \otimes \|\alpha'\rangle^{\otimes N} \to \|\beta'\rangle \otimes \|\alpha'\rangle^{\otimes N})$
0	$\simeq 0.8965$
1	$\simeq 0.9038$
2	$\simeq 0.9072$
3	$\simeq 0.9092$
4	$\simeq 0.9105$
5	$\simeq 0.9109$
6	$\simeq 0.9110$

Table 2.3: Increase of optimal probability for the conversion $|\alpha'\rangle \to |\beta'\rangle$, where $\boldsymbol{\alpha'} = (0.40, 0.34, 0.15, 0.11)$ and $\boldsymbol{\beta} = (0.50, 0.21, 0.17, 0.12)$, with the number of copies N of $|\alpha'\rangle$ used as a catalyst.

♯ Copies (N)	$P_S(\|\alpha\rangle \otimes \|\alpha\rangle^{\otimes N} \to \|\beta\rangle \otimes \|\alpha\rangle^{\otimes N})$
0	$\simeq 0.600$
1	$\simeq 0.818$
2	$\simeq 0.911$
3	$\simeq 0.957$
4	$\simeq 0.981$
5	$\simeq 0.994$
6	$= 1$

Table 2.4: Increase of optimal probability for the conversion $|\alpha\rangle \to |\beta\rangle$, where $\boldsymbol{\alpha} = (0.928, 0.060, 0.006, 0.006)$ and $\boldsymbol{\beta} = (0.950, 0.030, 0.0195, 0.0005)$, with the number of copies N of $|\alpha\rangle$ used as a catalyst.

$1 \leq j < i \leq n$, *such that*

$$\frac{\alpha_i}{\alpha_j} < \frac{\beta_{r_j}}{\beta_{r_i-1}} \tag{2.17}$$

or

$$\frac{\alpha_i}{\alpha_j} > \frac{\beta_{r_j-1}}{\beta_{r_i}}. \tag{2.18}$$

Whenever one of the inequalities (2.17) *or* (2.18) *has an index* $n+1$*, it is considered to be violated, so the other one must necessarily be satisfied.*

Remark 2.12. *Again, we observe that typically* L *has only one element* l*, since the minimum which determines the probability of conversion is non-degenerate with probability* 1*.*

2.5.1 Self-Catalysis under SLOCC for random Schmidt vectors

The criterion above, together with Proposition 2.8 and the behaviour of L, have interesting consequences for the probability of occurrence of self-catalysis.

From Remark 2.9, we know that the event $[P_S(|\alpha\rangle \to |\beta\rangle) < \min\{\frac{\alpha_n}{\beta_n}, 1\}]$ has probability $\gtrsim 1/2$. Conditioning on this event we can then analyze the validity of Ineqs. (2.17) and (2.18). With probability 1 we must have $L = \{l\}$, for some $1 < l < n$. Therefore, we can choose the indexes r_i in only two ways: either $r_1 = r_2 = ... = r_n = l$ or $r_1 = r_2 = ... = r_j = n+1$ and $r_{j+1} = ... = r_n = l$, for some j. For the second case, one can always satisfy one of the inequalities using the index $n+1$. For the first case, the r.h.s of the inequalities always have index l and we can lower bound the probability for at least one of Inequalities (2.18) to be valid:

$$\mathbb{P}[\max_{1\leq j<i\leq n}\{\frac{\alpha_i}{\alpha_j}\} > \frac{\beta_{l-1}}{\beta_l}] \geq \mathbb{P}[\max_{1<j\leq n}\{\frac{\alpha_{j-1}}{\alpha_j}\} > \max_{1<j\leq n}\{\frac{\beta_{j-1}}{\beta_j}\}] = 1/2, \tag{2.19}$$

using that $\max_{1\leq j<i\leq n}\{\frac{\alpha_i}{\alpha_j}\} = \max_{1<j\leq n}\{\frac{\alpha_{j-1}}{\alpha_j}\}$, since $\boldsymbol{\alpha}$ is ordered, and the fact that the two random variables on the second term are independent and identically distributed. Putting these together we get that the probability for having SLOCC self-catalysis is $\gtrsim \frac{1}{4}$.

We have also numerically investigated the typicality of probabilistic self-catalysis by 1) sorting a pair of incomparable Schmidt vectors with a same fixed dimension; 2) counting how many of them show the effect; and 3) computing the average gain in probability. To be more specific, we consider as a success case the situation where the pairs are such that $p_1 = P_S(|\alpha\rangle \to |\beta\rangle) < P_S(|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle) = p_2$ and we compute the average value of $p_2 - p_1$. In order to avoid counting cases where $p_1 < p_2$ due to numerical fluctuations, we only consider as valid those vectors where $p_2 > (1 + 10^{-5})p_1$. The results are shown in Figures 2.5 and 2.6.

First note that they are consistent with the lower bound of $1/4$ estimated before. Comparing with the deterministic case, probabilistic self-catalysis is much more frequent, as expected. Even more, here we *do not* have the same qualitative behaviour: the probability of having a pair of incomparable states exhibiting self-catalysis increases monotonically with the size of the Schmidt vectors and seems to be converging to a value around 0.6. Meanwhile, this is not the behaviour of the average probability gain, shown in Figure 2.6. The average gain in probability is relatively

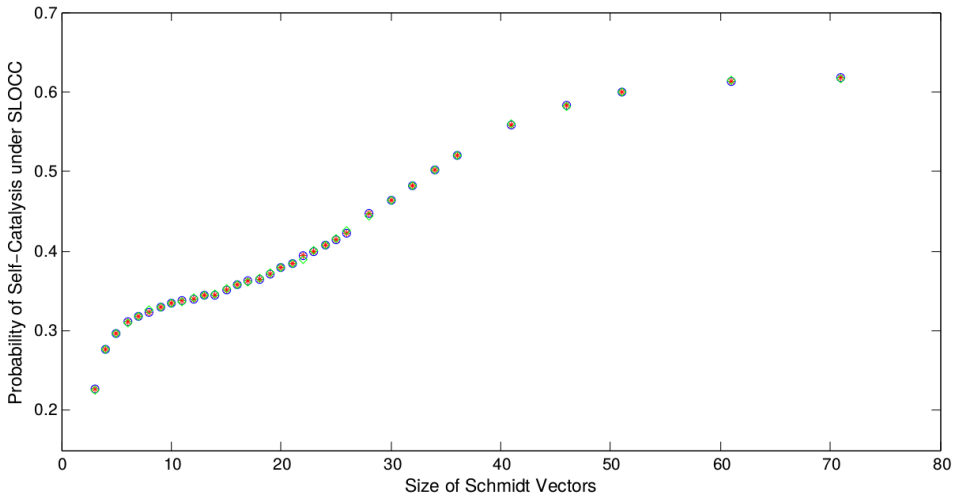


Figure 2.5: Probability of finding a pair of states exhibiting self-catalysis under SLOCC, $\mathbb{P}[P_S(|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle) > \mathbb{P}(|\alpha\rangle \to |\beta\rangle)]$, as function of the dimension of each system. Each symbol represents an average over a new set of randomly (Haar) chosen pairs. There are three symbols for each explored dimension.

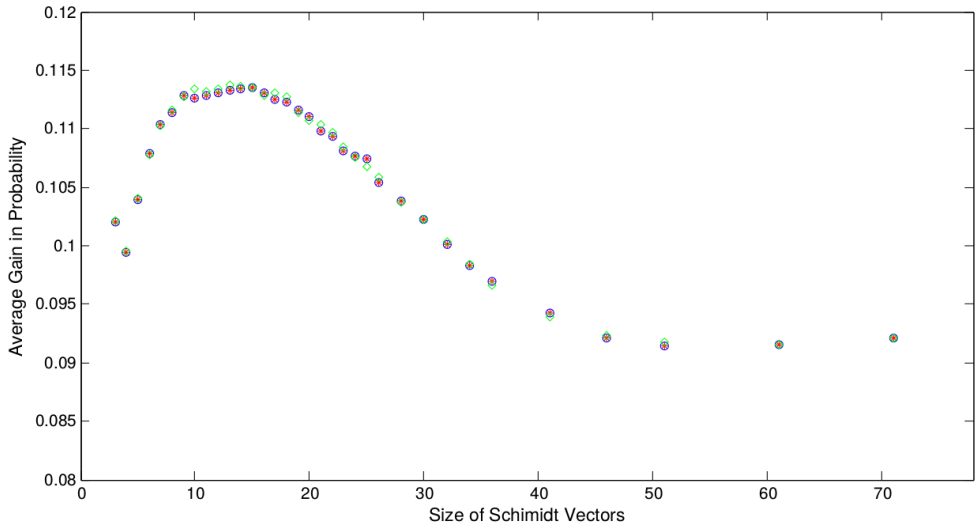


Figure 2.6: Average gain of probability, $\mathbb{E}[P_S(|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle) - P_S(|\alpha\rangle \to |\beta\rangle)]$, as a function of the size of Schmidt vectors (sampled following Haar measure), considered only those pairs where self-catalysis occurs, *i.e.* $P_S(|\alpha\rangle \otimes |\alpha\rangle \to |\beta\rangle \otimes |\alpha\rangle) > P_S(|\alpha\rangle \to |\beta\rangle)$.

small for all system sizes, and decreases even more for larger sizes. But note that we consider only one copy of $|\alpha\rangle$ attached, in fact we expect that in the regime of many more copies, the average gain shall be greater. It is important to recall Fig. 2.4, however, which tell us that a pair $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ has, on average, a probability of direct conversion close to 0.6, which naturally bounds the catalytic gain to about 0.4.

Finally, Figure 2.7 represents, for randomly chosen pairs of incomparable Schmidt vectors with size $n = 45$, the self-catalytic probability gain *versus* direct conversion rates, *i.e.* without a catalyst state. The diagonal straight line just represents saturation of probability. Some concentration

close to the horizontal axis is natural, representing the cases where self-catalysis does not happen. However it is not clear why there is the bold concentrated cloud in red, where the majority of the pairs fit. It empirically means that the most typical situation for a pair of Schmidt vectors of the same size is to have a large probability of conversion and to have a considerable (but not maximal) self-catalytical gain.

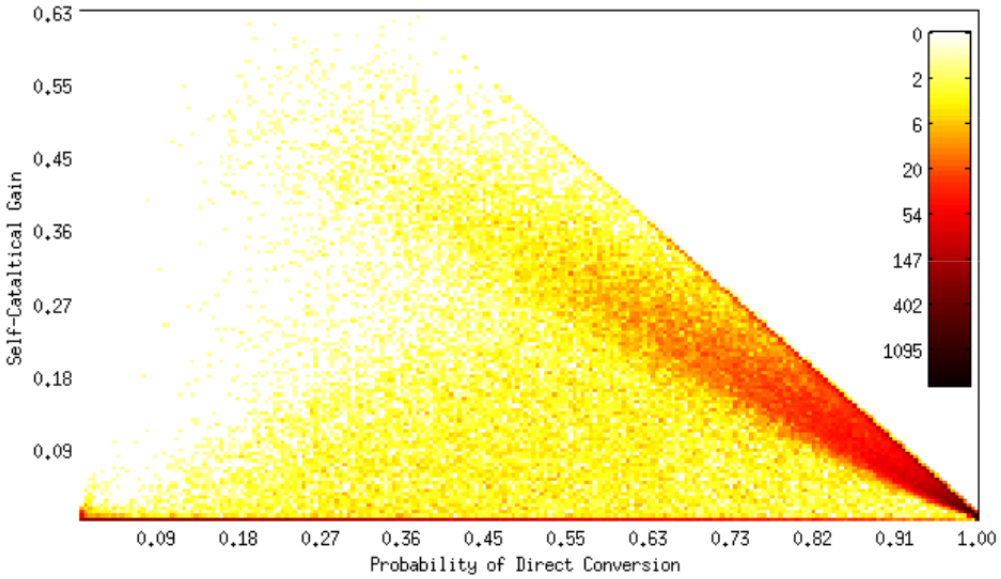


Figure 2.7: Self-catalytic probability gain and direct conversion rates for randomly (Haar) chosen pairs of incomparable Schmidt vectors with size $n = 45$. The colour represents the number of pairs per pixel.

Chapter 3

Finite Time Disentanglement: Parts and Quantum Dynamics

3.1 Introduction

Following the definition of entanglement as a resource for non-local tasks, as a consequence being quantified [117], the time evolution of this quantity was the subject of intense interest. Typically a composite system will lose its entanglement whenever its parts interact with an environment. It is of great interest then for practical implementations of quantum information protocols, that require entanglement, to understand how the amount of entanglement behaves in time [118].

One characteristic of entanglement dynamics that drew a lot of attention was the possibility of an initially entangled state to lose all its entanglement in a finite time, instead of asymptotically. The phenomenon was initially called "entanglement sudden death" [119], or Finite Time Disentanglement (FTD). The simplest explanation for this fact is essentially topological: for finite dimensional Hilbert spaces, the set $\mathcal{S}$ of separable states, where entanglement is null, has non-empty interior, *i.e.*, there are "balls" entirely consisted of separable states. Therefore, whenever an initially entangled state approaches a separable state in the interior of $\mathcal{S}$, and given that the dynamics of the state is continuous, it must spend at least a finite amount of time inside the set, so entanglement will be null during this time interval [120].

In references [121, 122], the authors explored how typical the phenomenon is (for several paradigmatic dynamics of two qbits and two harmonic oscillators) when one varies the initial states for a fixed dynamics. Here we shall explore how typical it is with respect to the dynamics themselves. More explicitly, given a dynamics for a composite system, should one expect to find some initially entangled state exhibiting FTD? Here we argue that the answer is generally positive.

The chapter is organized as follows. In Section 3.2 we discuss about the generic existence of FTD and illustrate this discussion with a well-known example of a family of maps. In Section 3.3 we go to the technical Lemmas and Theorems already used on Section 3.2. Discussions closing this present work are shown in Chapter 4, there we stress further questions and open problems.

3.2 Finite time disentanglement

In a very broad sense, we can think a *(continuous time) quantum dynamical system* as given by a family of completely positive trace preserving (CPTP) maps Λ_t, parametrized by the real time variable t for, say, $t \geq 0$. If a quantum system is in some state given by a density operator ρ_0 at $t = 0$, for any $t \geq 0$ we have the system at the quantum state $\rho(t) = \Lambda_t(\rho_0)$. Of course, one must have $\Lambda_0 = I$, where I is the identity map. Although in some cases a discontinuous family of maps can be a good approximation to describe a process (for example, when a very fast operation is performed on a system, or when the system will not be accessed during some time interval), strictly speaking the family of maps should be at least continuous.

Generally speaking, fixed some dynamics Λ_t, we say that it shows *finite time disentanglement* (FTD) if there exists an entangled state ρ_{ent} and a time interval (a, b), with $0 < a < b \leq \infty$ such that $\Lambda_t(\rho_{\text{ent}})$ is a separable state for all $t \in (a, b)$. In Refs. [120, 121], the authors point out that the occurrence of such effect is a natural consequence of the set of separable states $\mathcal{S}$ having a non-empty interior. Indeed, if an initially entangled state is mapped at some time $\bar{t}$ to a state in the interior of $\mathcal{S}$, given the dynamics continuity, it must spend some finite time inside S to reach that state. During that time interval entanglement is null, although initially the system had some entanglement. We shall formally state this fact for future reference:

Proposition 3.1. *If a bipartite quantum dynamical system is such that, for some $\bar{t} > 0$, there exists an initially entangled state ρ_{ent} where its evolved state at time $\bar{t}$ is in the interior of the separable states, there is FTD.*

This proposition is one of the main reasons of why we believe the following general conjecture is valid:

Conjecture 3.2. *Given a bipartite quantum dynamical system with finite dimensional Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ and a continuous family of CPTP maps Λ_t, there is no finite time disentanglement if, and only if, for all $t > 0$ there exists unitary operations $U_{A,t}$ and $U_{B,t}$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, such that $\Lambda_t(\cdot) = (U_{A,t} \otimes U_{B,t})(\cdot)(U_{A,t} \otimes U_{B,t})^*$.*

In physical terms, this says that FTD do not takes place only in the extremely special situation where the pair of systems is closed (or at most interacting with a classical external field) *and* non-interacting. That is, whatever interaction they may have, with each other *or* with a third quantum system (such as a reservoir), FTD takes place for some entangled state. From now on, we denote the family of dynamics contained in Conjecture 3.2 by $\mathcal{F}_{\mathcal{H}_A,\mathcal{H}_B}$, that is:

$$\begin{aligned}\mathcal{F}_{\mathcal{H}_A,\mathcal{H}_B} = \{\{\Lambda_t(.)\}_{t\geq 0};\ \{\Lambda_t(.)\}_{t\geq 0} \text{ is continuous and} \\ \Lambda_t(\cdot) = (U_{A,t} \otimes U_{B,t})(\cdot)(U_{A,t} \otimes U_{B,t})^*\}. \end{aligned} \tag{3.1}$$

Once again, the intuition behind Conjecture 3.2 is geometrical. Figure 3.1 shows a pictorial representation of the set of quantum states when the Hilbert space is finite dimensional, with the distinguishing property of the set of separable states having non-empty interior. In Figure 3.2 the arrows indicates the mapping of initial states to their corresponding evolved ones, on an instant

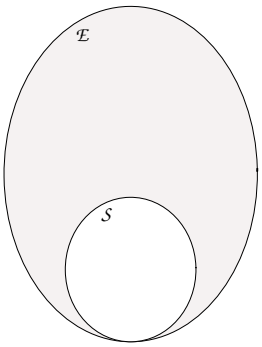
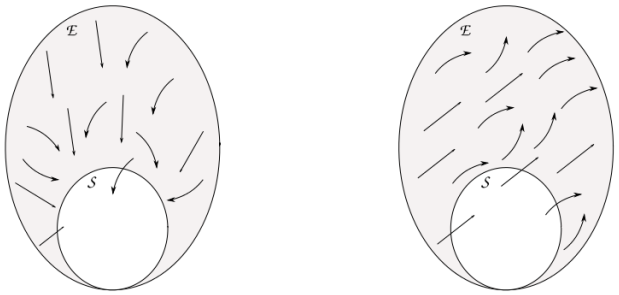


Figure 3.1: Pictorial representation of set of quantum states when $\dim(\mathcal{H}) < \infty$.



(a) (b)

Figure 3.2: The arrows represent how initial states are mapped to time evolved ones. Figure (a) shows a flow directed towards a separable state, while the figure (b) shows the flow directed towards an entangled one. In fact, we should stress that it is not always true that the whole family keeps fixed some ρ, *i.e.*, $\Lambda_t(\rho) = \rho, \forall t \geq 0$ for some state ρ.

of time $\bar{t} > 0$. Note that all CPTP maps must have at least one fixed point, and all other states can not increase their distance to that fixed one, therefore for each instant of time $t \geq 0$ we can identify a "direction" for the flow of states. It is expected that if the flow is directed towards a separable state, some entangled states will be mapped inside the separable set (3.2a). But even in the case where the flow is directed towards an entangled one, if the displacement is small enough, some entangled state located "behind" the set of separable states will be mapped inside it (3.2b). Below we prove this statement under some special conditions.

Closed systems

We start with the additional assumption that the bipartite system dynamics is induced by unitary operations for all $t > 0$ [there is some U_t acting on $\mathcal{H}_{AB}$ such that $\Lambda_t(\cdot) = U_t(\cdot)U_t^*$]. That is, the pair of systems may have any interaction with each other and they can even interact with classical external sources (for instance, their Hamiltonian may vary in time due to an external control of some of its parameters). Under such conditions, FTD is a consequence of Proposition 3.1 above and Theorem 3.11 (discussed in Section 3.3):

Theorem 3.3. *If a bipartite system have dynamics given by $\Lambda_t(\cdot) = U_t(\cdot)U_t^*$ for all $t > 0$, there is no FTD if, and only if, $\{\Lambda_t\}_{t\geq 0} \in \mathcal{F}_{\mathcal{H}_A,\mathcal{H}_B}$.*

Proof. Indeed, if the family Λ_t is such that, for some $\bar{t} > 0$, $U_{\bar{t}}$ is not a local unitary operation,

there exists an entangled state $|\psi_E\rangle$ such that $|\psi_P\rangle = U_{\bar{t}}|\psi_E\rangle$ is a product state (see Corollary 3.12). Take small enough $0 < \lambda < 1$ such that $\rho_E = \lambda\frac{I}{d_A d_B} + (1-\lambda)|\psi_E\rangle\langle\psi_E|$ is still an entangled state. We then have that $\Lambda(\rho_E) = \lambda\frac{I}{d_A d_B} + (1-\lambda)|\psi_P\rangle\langle\psi_P|$ is a state *in the interior* of the set of separable states (a convex combination of an arbitrary point of a convex set with a point in the interior of it, results in an element also in its interior [54]). By Proposition 3.1, FTD takes place. □

Pair of qbits

Physically, although Theorem 3.3 allows for very general interactions between the systems, it is restrictive with respect to their interaction with their environment, since this environment must be effectively classic. Here we greatly relax this restriction, on the expense of diminishing the range of quantum systems considered.

Theorem 3.4. *If a bipartite system with Hilbert space $\mathcal{H}_{AB}$, where* $\dim(\mathcal{H}_A) = \dim(\mathcal{H}_B) = 2$, *have a dynamics such that $\Lambda_t(\mathbb{1}) = \mathbb{1}$ for all $t \geq 0$* (i.e. *each map is unital), there is no FTD if, and only if, $\{\Lambda_t\}_{t\geq 0} \in \mathcal{F}_{\mathcal{H}_A,\mathcal{H}_B}$.*

Proof. For an arbitrary instant of time t, we have the following four possibilities for the corresponding CPTP map Λ_t: *i*) it is induced by a local unitary operation; *ii*) it is induced by a composition of a local unitary operation with the SWAP operator; *iii*) it is induced by a unitary operation which is neither local nor the composition of a local unitary with the SWAP operator; *iv*) it is not induced by any unitary. Let us look to each situation:

i) Of course, if this holds for all $t > 0$, we do not have FTD.

iii) Here we can just apply Theorem 3.3 to show that there is FTD.

iv) We can find a maximally entangled state ρ_E such that $\Lambda_{\bar{t}}(\rho_E)$ is mixed (see Theorem 3.10). If $\lambda_-(\rho)$ is the smallest eigenvalue of the partial transposition of ρ, we have that $\lambda_-(\rho_E) = -\frac{1}{2}$ and $\lambda_-[\Lambda(\rho_E)] = \delta > -\frac{1}{2}$ (see Ref. [123]). We can choose $0 < p < 1$ such that $\lambda_-[p\rho_E + (1-p)\frac{\mathbb{1}}{4}] = p(-\frac{1}{2} - \frac{1}{4}) + \frac{1}{4} < 0$ and $\lambda_-[p\Lambda(\rho_E) + (1-p)\frac{\mathbb{1}}{4}] = p(\delta - \frac{1}{4}) + \frac{1}{4} > 0$. That is, the initial state

$p\rho_E + (1-p)\frac{\mathbb{1}}{4}$ is entangled but its time evolved state at $\bar{t}$, $p\Lambda(\rho_E) + (1-p)\frac{\mathbb{1}}{4}$ is in the interior of the set of separable states. By Proposition 3.1, we have FTD.

ii) Finally, if this is the case, the continuity of the family of maps allows us to conclude for the existence of a $0 < \bar{t} < t$ where $\Lambda_{\bar{t}}$ fits in either cases *iii*) or *iv*), since the set of CPTP maps induced by such unitaries is disjoint from the set induced by local unitaries (a continuous path between two disjoint sets must necessarily pass trough the complement of them).

□

Example: Markovian dynamics

A Markovian dynamics [124] is distinguished by a semi-group property satisfied by the family of CPTP maps:

$$\Lambda_{t+t'} = \Lambda_t \circ \Lambda_{t'}, \tag{3.2}$$

for all $t, t' \geq 0$. It holds then [125] that the dynamics can be equivalently described by a differential equation (a Lindblad equation):

$$\frac{d\rho(t)}{dt} = -i[H,\rho] + \sum_{i=1}^{N}\left(A_i\rho A_i^* - \frac{1}{2}\{A_i^*A_i,\rho\}\right), \tag{3.3}$$

where H is self-adjoint while A_i are linear operators. Lindbladian equations can describe a plethora of physical phenomena, such as the dissipation of electromagnetic field modes of a cavity, spontaneous emission of atoms, spin dephasing due to a random magnetic field and so on. Therefore, despite the fact that the semi-group condition is somewhat restrictive, it is satisfied by many relevant quantum systems. The first term in the r.h.s. generates a unitary evolution and can usually be interpreted as the Hamiltonian evolution of the *isolated* system. The term involving the operators A_i is usually called *dissipator*, being responsible for the contractive part of the dynamics.

When an operator A_i is proportional to the identity it does not contribute to the dynamics. Moreover, the dynamics will preserve the purity of initial states if, and only if, all operators A_i are of such kind (that is, the dynamics is Hamiltonian):

Lemma 3.5. *For $\rho(t)$, a solution of Eq. (3.3) with initial condition $|\psi\rangle\langle\psi|$, it holds that $\lim_{t\to 0}\frac{d\mathrm{Tr}[\rho^2(t)]}{dt} = 0$ for all $|\psi\rangle$ if, and only if, $A_i = \lambda_i I$ for $i = 1, ..., N$.*

Proof. Indeed, for $t > 0$

$$\begin{aligned}\frac{d\mathrm{Tr}[\rho^2]}{dt} &= 2\mathrm{Tr}[\frac{d\rho}{dt}\rho] \\ &= 2\mathrm{Tr}(-i[H,\rho]\rho + \sum_{i=1}^{N} A_i\rho A_i^*\rho - \frac{1}{2}\{A_i^*A_i,\rho\}\rho)\end{aligned}$$

Since $\lim_{t\to 0}\rho = |\psi\rangle\langle\psi|$, it follows that:

$$\lim_{t\to 0}\frac{d\mathrm{Tr}[\rho^2(t)]}{dt} = 2\sum_{i=1}^{N}(|\langle\psi|A_i|\psi\rangle|^2 - ||A_i|\psi\rangle||^2). \tag{3.4}$$

By the Cauchy-Schwarz inequality,

$$|\langle\psi|A_i|\psi||\rangle^2 \leq |||\psi\rangle||^2||A_i|\psi\rangle||^2 = ||A_i|\psi\rangle||^2,$$

we can conclude the r.h.s of eq. (3.4) is zero iff all terms in the sum are zero and $|\psi\rangle \propto A_i|\psi\rangle$ for every $i = 1, ..., N$. These proportionality relations holds for all $|\psi\rangle$ if, and only if, all A_i are proportional to the identity operator. □

The above lemma shows that, for every $t > 0$, the CPTP map defined by Eq. (3.3) is not induced by a unitary operation. It is also easy to check that every CPTP maps given by Eq. (3.3) is unital as long as $\sum_{i=1}^{N}(A_iA_i^* - A_i^*A_i) = 0$. With this in hand, by Theorem 3.4, we can state:

Corollary 3.6. *If a bipartite system with Hilbert space $\mathcal{H}_{AB}$, where* $\dim(\mathcal{H}_A) = \dim(\mathcal{H}_B) = 2$, have a dynamics described by eq. (3.3), where some A_i is not a multiple of the identity and $\sum_{i=1}^{N}(A_iA_i^* - A_i^*A_i) = 0$, there is FTD.

3.3 Unital pure state preserving maps and product preserving unitaries

In this section we prove some results about CPTP maps, such as the characterization of unital and pure state preserving ones, which were used in the Section 3.2.

Consider a bipartite quantum system with finite dimensional Hilbert space $\mathcal{H}$. We say that a CPTP map Λ, acting on the set of all density operators $\mathcal{D}(\mathcal{H})$, is *pure state preserving* if $\Lambda(|\psi\rangle\langle\psi|)$ is a pure state for every pure state $|\psi\rangle$. Trivial examples of such maps are those induced by unitary operations [$\Lambda(\rho) = U\rho U^\dagger$, for U unitary acting on $\mathcal{H}$] and the constant maps $\Lambda(\rho) = |\phi_0\rangle\langle\phi_0|$ where $|\phi_0\rangle$ is a fixed state. Moreover a CPTP map is said to be *Unital* if it maps the maximally mixed state on itself.

Theorem 3.7. *Every pure state preserving unital map $\Lambda : \mathcal{D}(\mathcal{H}) \to \mathcal{D}(\mathcal{H})$, where* $\dim(\mathcal{H}) = d < \infty$, is induced by a unitary operation.

Proof. Take a Naimark dilation of Λ, that is, a unitary U acting on a larger space $\mathcal{H} \otimes \mathcal{R}$ and a fixed vector $|R\rangle \in \mathcal{R}$, such that $\Lambda(\rho) = \mathrm{Tr}_{\mathcal{R}}[U(\rho \otimes |R\rangle\langle R|)U^*]$ for all $\rho \in \mathcal{D}(\mathcal{H})$.

It must be the case that $U|\phi\rangle \otimes |R\rangle$ is a product vector for all $|\phi\rangle \in \mathcal{H}$, since otherwise $\mathrm{Tr}_{\mathcal{R}}[U(|\phi\rangle\langle\phi| \otimes |R\rangle\langle R|)U^*]$ would not be a one-dimensional projector and Λ would not preserve pure states.

Now, if $\{|\phi_j\rangle\}_{j=1}^d$ is an orthonormal basis, we have that $\Lambda(|\phi_j\rangle\langle\phi_j|) = P_j$ for some one-dimensional projectors P_j. From Λ being unital, it holds that $\Lambda(\sum_{j=1}^d |\phi_j\rangle\langle\phi_j|) = \sum_{j=1}^d P_j = I$, so the projectors P_j must be mutually orthogonal.

With the last two paragraphs in mind it must be true that, for $j = 1, ..., d$, there are normalized vectors $|\psi_j\rangle \in \mathcal{H}$ and $|R_j\rangle \in \mathcal{R}$, such that $U|\phi_j\rangle \otimes |R\rangle = |\psi_j\rangle \otimes |R_j\rangle$. Moreover, the set $\{|\psi_j\rangle\}_{j=1}^d$ must be orthonormal. On the other hand, for $j = 2, ..., d$,

$$U(|\phi_1\rangle + |\phi_j\rangle) \otimes |R\rangle = |\psi_1\rangle \otimes |R_1\rangle + |\psi_j\rangle \otimes |R_j\rangle.$$

For the vectors on the r.h.s of this equation being product, given that $|\phi_1\rangle$ is orthogonal to $|\phi_j\rangle$, it must hold that $|R_j\rangle = z_j|R_1\rangle$ for some $z_j \in \mathbb{C}$ of unity modulus. If we define a unitary V acting on $\mathcal{H}$ by $V|\phi_j\rangle = z_j|\psi_j\rangle$ for $j = 1, ..., d$, we get $\Lambda(\rho) = V\rho V^*$ for all density operators ρ. □

Lemma 3.8. *Let $\mathcal{H}_A, \mathcal{H}_B$ be two bi-dimensional Hilbert spaces. If $|\phi\rangle, |\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, and $|\phi\rangle + e^{i\theta}|\psi\rangle$ is a product vector for all $\theta \in \mathbb{R}$, then $|\phi\rangle$ and $|\psi\rangle$ are product too.*

Proof. Let be $|\psi\rangle = a|00\rangle + b|11\rangle$ a Schmidt decomposition for $|\psi\rangle$, and $|\phi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$ the expression for $|\phi\rangle$ with respect to the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. For arbitrary $z \in \mathbb{C}$, we can define the family of vectors:

$$|z\rangle = |\phi\rangle + z|\psi\rangle = (az + \alpha)|00\rangle + (bz + \delta)|11\rangle + \\ + \beta|01\rangle + \gamma|10\rangle.$$

For each z, the above state factorizes if, and only if, the following determinant is zero:

$$D = \begin{vmatrix} (az + \alpha) & \beta \\ \gamma & (bz + \delta) \end{vmatrix} = abz^2 + (a\delta + b\alpha)z + \alpha\delta + \beta\gamma.$$

If $a, b \neq 0$ (*i.e.*, $|\psi\rangle$ is entangled), D can not be identically zero for all values of z. Therefore, $|\psi\rangle$ must be product. By similar reasoning, we conclude $|\phi\rangle$ is also product. □

Lemma 3.9. *Let $\mathcal{H}_A, \mathcal{H}_B$ be two Hilbert spaces with dimension $d \geq 2$. If $|\phi\rangle, |\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, and $|\phi\rangle + e^{i\theta}|\psi\rangle$ is a product state for all $\theta \in \mathbb{R}$, then $|\phi\rangle$ and $|\psi\rangle$ are product too.*

Proof. Let us argue by contradiction. Suppose that $|\psi\rangle$ is entangled, thus in the Schmidt decomposition $|\psi\rangle = \sum_{l=1}^{d} \psi_l|ll\rangle$ there are, at least two indexes l_1, l_2 such that $\psi_{l_1}, \psi_{l_2} \neq 0$. Writing $|\phi\rangle = \sum_{k,j} \phi_{k,j}|kj\rangle$ in the same basis as $|\psi\rangle$, and defining $\psi_{k,j} = \psi_k \delta_{k,j}$ we get:

$$\forall\theta \in \mathbb{R} : |\theta\rangle = |\psi\rangle + e^{i\theta}|\phi\rangle = \sum_{k,j}(\psi_{k,j} + e^{i\theta}\phi_{k,j})|kj\rangle.$$

Therefore $|\theta\rangle$ is product, by hypothesis, for all $\theta \in \mathbb{R}$. Projecting $|\theta\rangle$ at the subspace generated by $\{|l_1l_1\rangle, |l_1l_2\rangle, |l_2l_1\rangle, |l_2l_2\rangle\}$ we obtain:

$$|\xi_\theta\rangle = \sum_{k,j \in \{l_1,l_2\}} (\psi_{k,j} + e^{i\theta}\phi_{k,j})|kj\rangle.$$

Since $|\xi_\theta\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is product for all values of θ, we can apply Lemma 3.8 and obtain the desired contradiction. □

Theorem 3.10. *If Λ is a unital map acting on $\mathcal{H}_{AB} = \mathbb{C}^2 \otimes \mathbb{C}^2$ and preserves the purity of maximally entangled states, then Λ is induced by an unitary operation.*

Proof. Take a representation of Λ in terms of a unitary U acting on a larger space $\mathcal{H}_{AB} \otimes \mathcal{H}_R$, such that

$$\Lambda(\rho) = \mathrm{Tr}_R[U(\rho \otimes |R\rangle\langle R|)U^*],$$

where $|R\rangle \in \mathcal{H}_R$. With $U(|00\rangle \otimes |R\rangle) = |\psi\rangle$ and $U(|11\rangle \otimes |R\rangle) = |\phi\rangle$, we have, for all $\theta \in \mathbb{R}$:

$$(|00\rangle + e^{i\theta}|11\rangle) \otimes |R\rangle \overset{U}{\mapsto} |\psi\rangle + e^{i\theta}|\phi\rangle.$$

As Λ preserves the purity of $(|00\rangle + e^{i\theta}|11\rangle)$, the state $|\psi\rangle + e^{i\theta}|\phi\rangle$ is product for all θ, with respect to $\mathcal{H}_{AB} \otimes \mathcal{H}_R$. Lemma 3.9 implies that $|\psi\rangle$ and $|\phi\rangle$ are both product, that is:

$$|00\rangle \otimes |R\rangle \overset{U}{\mapsto} |\psi_{00}\rangle \otimes |R_{00}\rangle \tag{3.8a}$$

$$|11\rangle \otimes |R\rangle \overset{U}{\mapsto} |\psi_{11}\rangle \otimes |R_{11}\rangle. \tag{3.8b}$$

Let $\mathfrak{B} = \{|\Psi_\pm\rangle, |\Phi_\pm\rangle\}$ be the Bell basis in $\mathcal{H}_{AB}$. The map Λ satisfies:

$$\mathbb{1} = \Lambda(\mathbb{1}) = \Lambda(|\Phi_+\rangle\langle\Phi_+| + |\Phi_-\rangle\langle\Phi_-| + |\Psi_+\rangle\langle\Psi_+| + |\Psi_-\rangle\langle\Psi_-|).$$

Since the images $\Lambda(|\Phi_\pm\rangle\langle\Phi_\pm|)$ and $\Lambda(|\Psi_\pm\rangle\langle\Psi_\pm|)$ are 4 unidimensional projectors (Λ preserves purity of maximally entangled states) that sum up to the identity, they must be mutually orthogonal.

Observe that the combinations $(|\psi_{00}\rangle \otimes |R_{00}\rangle) \pm (|\psi_{11}\rangle \otimes |R_{11}\rangle)$ must be product with respect to $\mathcal{H}_{AB} \otimes \mathcal{H}_R$, because they are images of $|\Phi_\pm\rangle \otimes |R\rangle$ under U. We state that

$$|R_{00}\rangle = e^{i\gamma}|R_{11}\rangle.$$

Otherwise, $|\psi_{00}\rangle \propto |\psi_{11}\rangle$, and then $\Lambda(|\Phi_+\rangle\langle\Phi_+|) = |\Psi_{00}\rangle\langle\Psi_{00}| = \Lambda(|\Phi_-\rangle\langle\Phi_-|)$ contradicting the fact that $\Lambda(|\Phi_\pm\rangle\langle\Phi_\pm|)$ are mutually orthogonal. Again, from

$$|01\rangle \otimes |R\rangle \overset{U}{\mapsto} |\psi_{01}\rangle \otimes |R_{01}\rangle,$$
$$|10\rangle \otimes |R\rangle \overset{U}{\mapsto} |\psi_{10}\rangle \otimes |R_{10}\rangle,$$

we derive that $|R_{01}\rangle = e^{i\delta}|R_{10}\rangle$. Now, define $|\xi\rangle = a|\Phi_+\rangle + b|\Phi_-\rangle + c|\Psi_+\rangle + d|\Psi_-\rangle$,

for a suitable choice of constants $a, b, c, d \neq 0$ such that $|\xi\rangle$ is maximally entangled. Therefore

$$U(|\xi\rangle \otimes |R\rangle) = (a|\psi_{00}\rangle + be^{-i\gamma}|\psi_{11}\rangle) \otimes |R_{00}\rangle + (c|\psi_{01}\rangle + de^{-i\delta}|\psi_{10}\rangle) \otimes |R_{01}\rangle,$$

and then $|R_{00}\rangle = e^{i\beta}|R_{01}\rangle$. We can define a unitary operator V, acting on $\mathcal{H}_{AB}$, given by:

$$|00\rangle \overset{V}{\mapsto} |\psi_{00}\rangle, \tag{3.12a}$$

$$|11\rangle \overset{V}{\mapsto} e^{-i\gamma}|\psi_{11}\rangle, \tag{3.12b}$$

$$|01\rangle \overset{V}{\mapsto} e^{i(\delta-\beta-\gamma)}|\psi_{01}\rangle, \tag{3.12c}$$

$$|10\rangle \overset{V}{\mapsto} e^{-i(\delta+\gamma)}|\psi_{10}\rangle. \tag{3.12d}$$

With this definition, we have $\Lambda(\cdot) = V(\cdot)V^*$. □

When $\mathcal{H}_A = \mathcal{H}_B$, we can define the so-called SWAP operator S, by $S(|\phi\rangle \otimes |\psi\rangle) = |\psi\rangle \otimes |\phi\rangle$. If the Hilbert spaces are not the same, but have the same dimension, we can take any isomorphism $\Psi : \mathcal{H}_A \to \mathcal{H}_B$ between them and define the operators $S_\Psi = (\Psi^{-1} \otimes I_B) \circ S \circ (\Psi \otimes I_B)$, where I_B is the identity operator on $\mathcal{H}_B$, *i.e*, $S_\Psi |\phi\rangle \otimes |\psi\rangle = \Psi^{-1}(|\psi\rangle) \otimes \Psi(|\phi\rangle)$ which we shall also denote by SWAP.

The theorem below characterizes unitary operations acting on composite Hilbert spaces that preserve product vectors:

Theorem 3.11. *Let U be a unitary operation acting on a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_{A(B)}$ has finite dimension $d_{A(B)} \geq 2$. Then U is product preserving if, and only if, it is a local unitary operation or, for the case* $\dim(\mathcal{H}_A) = \dim\ (\mathcal{H}_B)$ *, a composition of a local unitary operation with a SWAP operator.*

Proof. Consider an orthonormal basis in each space $\{|j\rangle_A\}_{j=0}^{\dim(\mathcal{H}_A)-1}$, $\{|k\rangle_B\}_{k=0}^{\dim(\mathcal{H}_B)-1}$. The unitary operation must map states $|j\rangle_A \otimes |k\rangle_B$ into elements $\left|\psi_{jk}\right\rangle_A \otimes \left|\phi_{jk}\right\rangle_B$, which are mutually orthogonal. Since the images of the product vectors $(|j\rangle_A + |j'\rangle_A) \otimes |k\rangle_B$, that is $\left|\psi_{jk}\right\rangle_A \otimes \left|\phi_{jk}\right\rangle_B + \left|\psi_{j'k}\right\rangle_A \otimes \left|\phi_{j'k}\right\rangle_B$ are also product vectors, we must have one of two options

$$\left|\psi_{jk}\right\rangle_A \perp \left|\psi_{j'k}\right\rangle_A \text{ and } \left|\phi_{jk}\right\rangle_B \propto \left|\phi_{j'k}\right\rangle_B, \tag{3.13a}$$

or

$$\left|\phi_{jk}\right\rangle_B \perp \left|\phi_{j'k}\right\rangle_B \text{ and } \left|\psi_{jk}\right\rangle_A \propto \left|\psi_{j'k}\right\rangle_A. \tag{3.13b}$$

For a fixed k, if one of the options is valid for a pair j and j', it must be valid for all such pairs. Indeed, suppose that the first option is valid for, say, $j = 0$ and $j' = 1$ and the second for $j = 0$ and $j' = 2$. The image of the product vector $(|1\rangle_A + |2\rangle_A) \otimes |k\rangle_B$, given by $|\psi_{1k}\rangle_A \otimes |\phi_{1k}\rangle_B + |\psi_{2k}\rangle_A \otimes |\phi_{2k}\rangle_B$ would be an entangled vector, since we would have $|\psi_{1k}\rangle_A \perp |\psi_{0k}\rangle_A, |\psi_{2k}\rangle_A \propto |\psi_{0k}\rangle_A$, $|\phi_{1k}\rangle_B \propto |\phi_{0k}\rangle_B$ and $|\phi_{2k}\rangle_B \perp |\phi_{0k}\rangle_B$. Therefore, $|\psi_{1k}\rangle_A \perp |\psi_{2k}\rangle$ and $|\phi_{1k}\rangle_B \perp |\phi_{2k}\rangle_B$.

i) Assume that (3.13a) is true. That means that the vectors $\left|\phi_{jk}\right\rangle_B$ are proportional to each other for fixed k, while the vectors $\left|\psi_{jk}\right\rangle_A$, also for fixed k, form an orthonormal basis. We can write then $U|j\rangle_A \otimes |k\rangle_B = e^{i\theta_{jk}} \left|\psi_{jk}\right\rangle_A \otimes |\phi_{0k}\rangle_B$.

If we consider the image of the vectors $|j\rangle_A \otimes (|k\rangle_B + |k'\rangle_B)$, we deduce that we have the following options

$$\left|\phi_{jk}\right\rangle_B \perp \left|\phi_{jk'}\right\rangle_B \text{ and } \left|\psi_{jk}\right\rangle_A \propto \left|\psi_{jk'}\right\rangle_A, \tag{3.14a}$$

or

$$\left|\psi_{jk}\right\rangle_A \perp \left|\psi_{jk'}\right\rangle_A \text{ and } \left|\phi_{jk}\right\rangle_B \propto \left|\phi_{jk'}\right\rangle_B. \tag{3.14b}$$

Again, similarly to what we have above, if one of the option is valid for a pair k and k', for fixed j, it must be valid for all such pairs. But given that (3.13a) is true, now only (3.14a) can also be. Indeed, if (3.14b) were true, we would have, for example, the subspace generated by the vectors $\{|j\rangle_A \otimes |0\rangle_B, |0\rangle_A \otimes |k\rangle_B\}$, of dimension $\dim(\mathcal{H}_A) + \dim(\mathcal{H}_B) - 1$, mapped to the subspace $\mathcal{H}_A \otimes |\phi_{00}\rangle$, of dimension $\dim(\mathcal{H}_A)$, contradicting the fact the U is unitary.

Since we have that (3.14a) is true, we can write $U|j\rangle_A \otimes |k\rangle_B = e^{i\theta_{jk}}|\psi_{j0}\rangle_A \otimes |\phi_{0k}\rangle_B$. Using this expression, and demanding that the states $(|j\rangle_A + |j'\rangle_A) \otimes (|k\rangle_B + |k'\rangle_B)$ are of the product form for all pairs j, j' and k, k', we obtain $e^{i(\theta_{jk}+\theta_{j'k'})} = e^{i(\theta_{jk'}+\theta_{j'k})}$. In particular, if $k' = j' = 0$, we get $\theta_{jk} = \theta_{j0} + \theta_{0k} (\mathrm{mod}\, 2\pi)$, since $\theta_{00} = 0$ by construction. Finally, we have $U = U_A \otimes U_B$ with $U_A|j\rangle_A = e^{i\theta_{j0}}|\psi_{j0}\rangle_A$ and $U_B|k\rangle_B = e^{i\theta_{0k}}|\phi_{0k}\rangle_B$.

ii) Assume that (3.13b) is true. Note firstly that it is necessary to have $\dim(\mathcal{H}_A) \geq \dim(\mathcal{H}_B)$ since, for fixed k, we are varying over $\dim(\mathcal{H}_A)$ orthonormal vectors on A, which therefore give rise to a set of orthonormal vectors $\left|\phi_{jk}\right\rangle_B$ in $\mathcal{H}_B$. So $U(|j\rangle_A \otimes |k\rangle_B) = e^{i\tilde{\theta}_{jk}}|\psi_{0k}\rangle_A \otimes \left|\phi_{jk}\right\rangle_B$. Now only the option (3.14b) can be true, so again we have $\dim(\mathcal{H}_B) \geq \dim(\mathcal{H}_A)$, and therefore $\dim\mathcal{H}_A = \dim\mathcal{H}_B$, which allows us to write $U(|j\rangle_A \otimes |k\rangle_B) = e^{i\tilde{\theta}_{jk}}|\psi_{0k}\rangle_A \otimes |\phi_{j0}\rangle_B$. Considering again that the image of the states $(|j\rangle_A + |j'\rangle_A) \otimes (|k\rangle_B + |k'\rangle_B)$ must be product vectors, we have $\tilde{\theta}_{jk} = \tilde{\theta}_{j0} + \tilde{\theta}_{0k} (\mathrm{mod}\, 2\pi)$. In other words $U = (U_A \otimes U_B) \circ S_\Psi$, where $U_A|j\rangle_A = e^{i\tilde{\theta}_{0j}}|\psi_{0j}\rangle$, $U_B = e^{i\tilde{\theta}_{k0}}|\phi_{k0}\rangle_B$ and $\Psi|k\rangle_A = |k\rangle_B$. □

Putting these results together we have the following:

Corollary 3.12. *If U is a unitary operator acting on a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_{A(B)}$ has finite dimension and preserves entangled states, then it is a local unitary operation or, for the case* $\dim(\mathcal{H}_A) = \dim(\mathcal{H}_B)$*, a composition of a local unitary operation with a SWAP operator.*

Proof. If U preserves entangled states, its inverse U^{-1} preserves product states. From Theorem 3.11, there are unitaries V_A and V_B acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, such that $U^{-1} = V_A \otimes V_B$ or $U^{-1} = S \circ V_A \otimes V_B$, therefore $U = U_A \otimes U_B$ or $U = U_A \otimes U_B \circ S$, with $U_A = V_A^{-1}$ and $U_B = V_B^{-1}$. □

Chapter 4

Conclusions, Discussions and Further Works: All Parts Together

Well, I think I can now assume once again an informal style of writing. After all these chapters and discussions it will be good to read a smooth text one more time.

So, I hope I have proved my point of view on how important for Quantum Physics the Tensor Product is . Yes, I know there is a lot of other instances in the literature, all well established, and some of them even more amazing than those that have been discussed here. Specially when the issue addressed is Entanglement. But I want to emphasize that our results are, so far as we know, original and reveal more than the beauty of Entanglement itself, they reveal how this purely algebraic structure could be useful and fruitful i) to study Foundations of Quantum Physics, as has been performed at Chapter 1; ii) to open a new class of protocols for Quantum Information, as performed and extensively analysed in Chapter 2; and iii) to study the universality of Sudden Death of Entanglement as in Chapter 3. Although outside the scope of this Thesis, we can also cite that we have proven that Entanglement Transformations, even at the presence of an extra entangled state, cannot act as a marker for quantum phase transitions [107], remaining yet as an open problem if Self-Catalysis cannot as well.

In fact, the first Chapter shows how we might use the tensor product, and the novel structure of Orthogonal Projective Representation related to it, in order to define a new graph invariant, called *Multigraph Lovász Number*, and shed some light onto foundations of Quantum Physics. We have shown that any Bell inequality can be associated to a specific type of edge-coloured multigraph (Sec. 1.2) and that the CSW graph-theoretical approach to quantum correlations can be adapted to NC inequalities with Bell-like constraints, including Bell Inequalities themselves. This allows us to, *e.g.*, calculate the actual maximum of quantum correlations XXXXXXXXXXXXx for Bell inequalities for which the CSW approach only gives an upper bound (Sec. 1.5). In this sense, our multigraph approach is a refinement of the graph approach introduced by CSW. Let us now examine some of the implications of this refinement for the problem of understanding quantum correlations from first principles.

There are two different approaches to this problem: (I) Finding the principles that limit the

quantum non-local correlations in any Bell inequality [76–79]. (II) Finding the principles that limit the quantum contextual correlations for the most general scenario described by a given exclusivity graph [80–84]. So far, none of the proposed principles has explained the entire set of quantum correlations for any Bell inequality. However, for some exclusivity graphs, the exclusivity principle [80–84] has succeeded in preventing sets of correlations larger than the set allowed by QT [34, 83]. The multigraph approach connects (I) and (II) and opens a new perspective (as, alternatively, does the hypergraph approach in Ref. [29]).

The fact that any conceivable CSW graph (G, w) corresponds to a physically realizable situation shows that there is a physically realizable layer of quantum correlations that can be put in correspondence with CSW graphs. The characterization of the possible correlations in this first layer is mathematically simple: The maximum is given by the Lovász number of (G, w) and can be calculated by a single SDP, and the set of quantum correlations, $Q^{\text{CSW}}(G)$, is equal to the GLS theta body of the exclusivity graph [27, 28]. Of course, $Q^{\text{CSW}}(G)$ is, in general, larger than the set of quantum correlations for a *specific* NC or Bell inequality whose exclusivity graph is (G, w).

In Ref. [45] we have shown that a specific type of edge-coloured multigraphs can be used to encode the extra constraints on quantum correlations that typically appear in some NC and Bell-inequality scenarios. The fact that any conceivable multigraph of the type considered in this thesis also corresponds to a physically realizable situation shows that there is a deeper layer in which extra constraints limit the values of the quantum correlations with respect to the ones corresponding to CSW graphs. For instance, notice that the set of quantum correlations corresponding to the CSW exclusivity graph for the CHSH Bell inequality, $Q^{\text{CSW}}(G)$, and the set of bipartite quantum correlations corresponding to the exclusivity multigraph in Fig. 1.1, $\hat{Q}(\mathsf{G})$, are distinct, although both give the same maximum for the CHSH inequality. This connects with the observation that the set of quantum correlations for Bell scenarios can be strictly contained in the theta body of the corresponding CSW graph [86, 87].

In this sense, the multigraphs introduced here can be embedded into this deeper layer, the multipartite quantum correlations in the set $\hat{Q}(\mathsf{G})$. The characterization of the possible correlations in this deeper layer leads to a more complex problem since the multigraph Lovász number is, in general, NP-hard to approximate, see Ref. [85] (in the context of non-local games).

It is worth noting that, given a multigraph G, there can be three different sets of quantum correlations associated to it. On the one hand, the set of probability assignments allowed by QT to the vertices of G *under the constraints imposed by the fact that one knows that* (G, w) *originates from a specific S associated to a specific NC or Bell inequality within a specific experimental scenario*. On the other hand, there are two sets of quantum correlations whose definition does not require to knowledge the experimental scenario that originates (G, w). These sets are $Q(\mathsf{G})$ and $Q^{\text{CSW}}(G)$. $Q(\mathsf{G})$ is the set of all probability assignments allowed by QT to the vertices of (G, w) consistent with the relationships of exclusivity in G and allows us to define the number $\theta(\mathsf{G}, w)$ introduced for the first time in Ref. [45]. $Q^{\text{CSW}}(G)$ is the set of all probability assignments allowed by QT to the vertices of (G, w) consistent with the relationships of exclusivity in G and leads to the original Lovász $\vartheta(G, w)$. Naturally, $Q(\mathsf{G}) \subset Q^{\text{CSW}}(G)$ and $\theta(\mathsf{G}, w) \leq \vartheta(G, w)$. The two sets defined solely

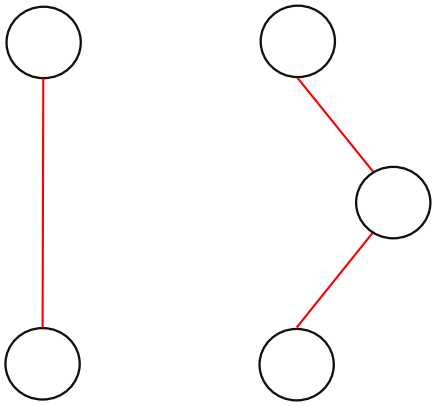


Figure 4.1: Schematic drawing of a break operation onto a graph.

from G are not immediately comparable to the set defined with the additional constraints imposed by a specific experimental scenario. There are two reasons for this, that are better discussed in the Appendix B: On the one hand, without the knowledge of the scenario, only subnormalization of probabilities must be applied (see condition (B.8)). On the the other hand, the labelling of vertices of G imposes additional restrictions on the possible probability assignments.

Certainly we could not forget that our graph invariant *is a graph invariant*, and as such, it belongs to Graph Theory. In that spirit, we believe our results also fits perfectly in that world, and they could be of the interest to a graph theorist as well. It is in this dual sense that we highlight some interesting open problems:

- Since, till today, we were only able to evaluate, for non-trivial graphs, the Multigraph Lovász Number numerically, finding some examples of graphs and colourings where θ can be analytically determined is extremely important. It can give insights not only of the invariant itself, but at the physical meaning behind it;

- In order to classify Bell Inequalities, or NC inequalities with Bell-type constraints, it is important to understand which types of coloured graphs can be associated with a valid Bell Inequality. Refining, or extending, therefore, previous classifications which are based on CSW graphs [93];

- It would be interesting to investigate the behaviour of θ under some (physically) meaningful (coloured) graph operations, for instance:

    1. The behaviour of θ when we *break* some edges (see Fig.4.1), adding new vertices into the graph. We have already noted that for some kinds of breaking procedures (see Fig.4.2), that operation adds $+1$ to the new Multigraph Lovász Number. So, after understood how one might associate a coloured-graph with a Bell Inequality, this graph operation of breaking an edge, is a machine to produce Bell Inequalities such that one has control of θ.

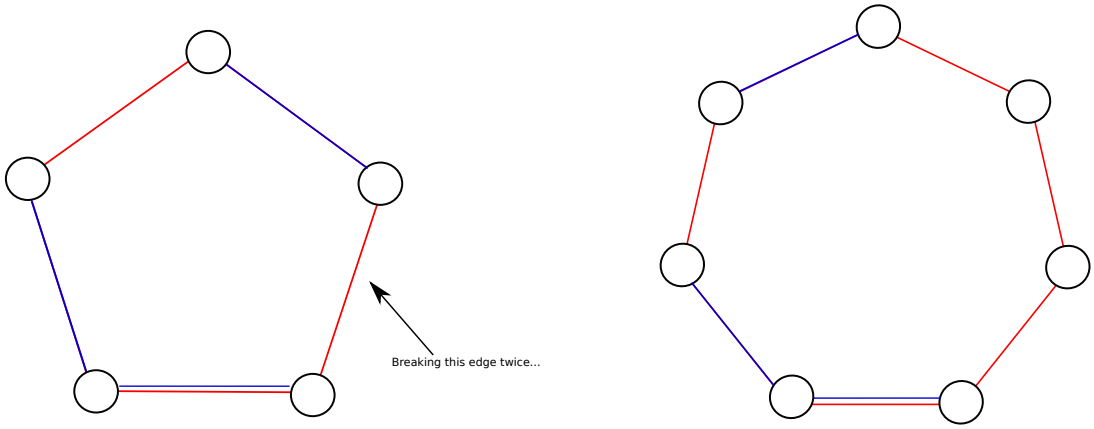


Figure 4.2: Tranforming a coloured C_5 into C_7 after breaking a specific edge.

2. Fixed a number of vertices, to add coloured edges. For this case, we are sure[1] that our θ is a monotonically non-increasing function. In fact a whole hierarchy for two-coloured C_7's has already been constructed[2] and we believe that, aside from the aesthetic beauty, Bell Scenarios holding those coloured graphs with 7 vertices could be understood under that hierarchy of graphs (see Fig. 4.3);

- To define and understand the mathematics and the physical meaning when we optimize θ over all possible colourings of a fixed graph. In fact, this new optimized invariant is upper bounded by the usual Lovász number, and lower bounded by the multigraph Lovász number of each colouring. Nevertheless the *when*, *how* and the *why* it is equal to the ordinary Lovász ϑ, remain unknown.

- The use of multigraphs also opens the door for solving some interesting problems. For example: Which is the simplest bipartite Bell inequality exhibiting full quantum non-locality? That is, the Bell inequality in which the maximum quantum value equals the maximum no-signalling value [88] as occurs with the Bell inequality in Ref. [89].

Additionally, inside the scope of Quantum Information Theory, our results also have revealed the phenomenon of Self-Catalysis conversion of pure entangled states. That is, the possibility to circumvent a non-possible transformation $|\alpha\rangle \nrightarrow |\beta\rangle$, using for that a copy of $|\alpha\rangle$:

$$|\alpha\rangle \otimes |\alpha\rangle \rightarrow |\beta\rangle \otimes |\alpha\rangle,$$

without using any other states that were not previously in the game. We have explored numerically, and by arguments of typicality, how frequent they are, and showing that the phenomenon is much more common in SLOCC case than the deterministic one. Even more, self-catalysis under SLOCC becomes more common as the systems sizes increase, whereas the direct self-catalysis decreases with the dimension. Moreover, we also investigated how the phenomenon may depend on the

[1] To add new edges is intuitively related to strengthen the constraints at (1.4). Therefore θ cannot increase. However a formal proof of this fact has never been performed so far.
[2] Thanks L. Guerini.

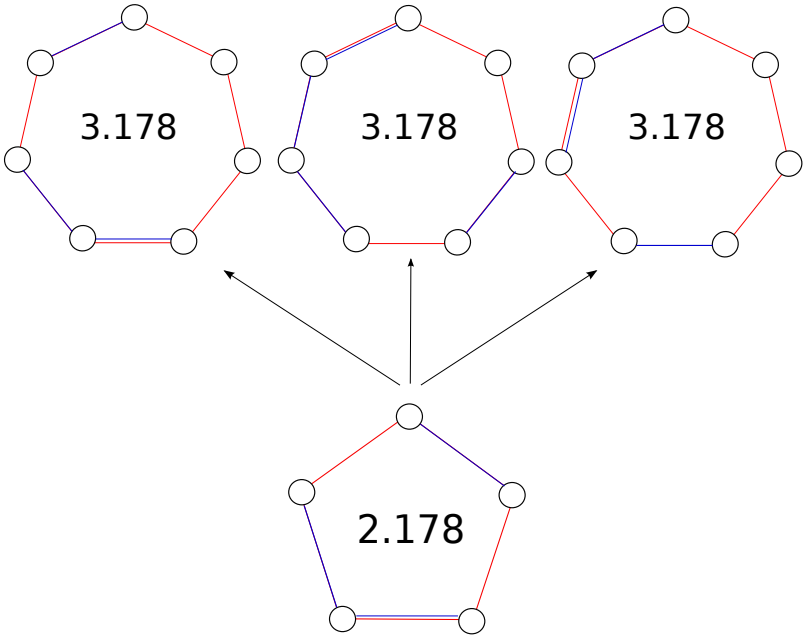


Figure 4.3: A piece from the cited graph hierarchy. Three coloured C_7's arising from the same coloured Pentagon (see Fig. 4.2) holding the same Multigraph Lovász Number.

number of copies used as catalyst, finding examples of different behaviours, running from cases where there is no gain in considering multiple copies, to cases where the conversion becomes deterministic for a finite number of copies. Since we rest on numerical, our techniques could not guarantee the existence of a transition where the probability of conversion asymptotically goes to 1. Finally, we computed the average gain in probability in the SLOCC case, showing that this gain, as in the LOCC case, has (apparently) a global maximum, and also decreases with larger systems sizes.

In answering the question about existence of self-catalysis, we obtained many results, not only on deterministic and probabilistic self-catalysis, but also on ordinary catalysis. About the typicality of self-catalysis, our data support two conjectures: under LOCC, the probability of finding a self-catalytic reaction increases monotonically attaining a local maximum for a dimension about 20. We believe that the origin of this overall non-monotonic behaviour is due the competition between the *sizes* of each Schmidt vectors and the measure *concentration* phenomenon. On the other hand, the data suggests that under SLOCC the probability of finding a self-catalytic reaction increases monotonically with the dimension.

In a sense, we estimated numerically the volumes of the sets of pairs of Schmidt vectors where the phenomena take place, but it was not possible to characterize completely the asymptotic behavior with the vectors sizes. In fact, some of our numerical results have a reasonable dependence on the way we sort the random Schmidt vectors. That is something to be explored elsewhere. Since we've touched at themes to be explored elsewhere, we should highlight that for this topic a lot of problems remain open (some of them are already being addressed):

- First of all, it is of great importance to analyse the geometrical content inherent to catalysis

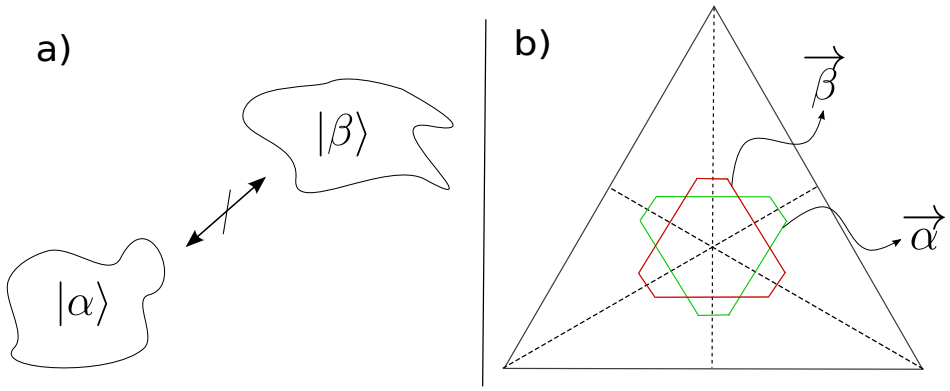


Figure 4.4: Whereas geometrically $|\alpha\rangle$ and $|\beta\rangle$ represent 2 unconnected regions, in the probability simplexes since neither $|\alpha\rangle$ access $|\beta\rangle$ nor $|\beta\rangle$ access $|\alpha\rangle$, then by the Birkhoff's neither $\boldsymbol{\alpha}$ lies in the convex hull of the orbit of $\boldsymbol{\beta}$ under the group of permutation matrices, nor $\boldsymbol{\beta}$ lies in the convex hull of the orbit of $\boldsymbol{\alpha}$ under action of the permutation group.

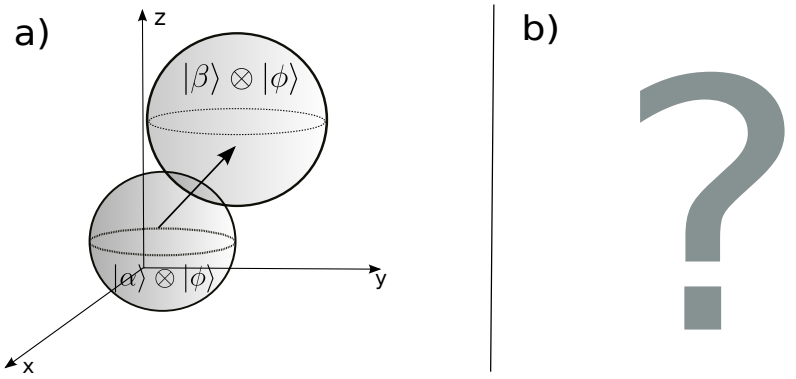


Figure 4.5: Using extra dimensions now it is geometrically possible cross the gap, but remains open what is the equivalent image for probability simplexes.

and self-catalysis. We really believe that the phenomenon could be better understood if one grasps that point. This geometrical content comes from the Birkhoff's Theorem [150] that says that if $\boldsymbol{\alpha} \prec \boldsymbol{\beta}$, then $\boldsymbol{\alpha} = D\boldsymbol{\beta}$ for some doubly stochastic matrix D. Therefore, since all doubly stochastic matrix is a convex combination of permutations, $\boldsymbol{\alpha}$ lies in the convex hull of the orbit of $\boldsymbol{\beta}$ under action of the permutation group (see Fig. 4.4). Thus, in that sense, we can trace an elucidative parallel: In the realm of probability simplexes the scenario where $|\alpha\rangle \nleftrightarrow |\beta\rangle$ corresponding to the part b) of the Fig. 4.4, has some resemblance with the geometrical situation where a gap, or a hole, separates two (unconnected) regions. No one can reach one region, having started from the other one, without falling into the hole. However when using extra dimensions, building a "bridge" between those 2 regions, could be possible now to circumvent that geometrical gap (see Fig. 4.5).

And the existence of a state $|\phi\rangle$ (equals to $|\alpha\rangle$ or not) allowing the transformation is somehow equivalent to use a smart higher dimensional "bridge" to cross the gap between those 2 states. The most important part here is that this extra-dimension, and this "bridge" should

be well adapted since neither all $|\phi\rangle$ is a catalyst for the initial transformation, nor every $|\alpha\rangle$ is self-catalytical[3];

- In order to fully understand the phenomenon of Self-Catalysis, we should generalize the typicality graphics for different dimensions of vectors. We emphasize that in Chapter 2 we have only worked with Schmidt vectors belonging to the same simplex $\mathbb{V}^d$.

- The theory of majorization and its variants, including thermomajorization [144], have been found to play a central role [156] in the formulation of many physical resource theories [145, 146, 151, 152], ranging from entanglement theory [147] to quantum thermodynamics [148, 154, 155, 157], going even through the Classical Thermodynamics [153]. And in this sense we have been found that our works fit, and moreover they could throw some light both in the context of these Resource Theories as in the context of Quantum Thermodynamics, much in the spirit of [144, 145, 155], where the phenomenon of Catalysis is studied and used to design laws and bounds in Quantum Thermodynamics.

By the last, we also have some words to say about the *Entanglement Sudden Death* or *Finite Time Disentanglement* (FTD) phenomenon, as treated at Chapter 3. There, aside from the technical details, the most important point/part is the Topology and Geometry induced by the tensor product structure. The requirement of finite dimensional Hilbert spaces seems to be essential. Indeed, that topological insight is based on the fact that the set of separable states has non-empty interior [131–133], which ceases to be true whenever one of the Hilbert spaces is of infinite dimension [126]. Of course, even in that case, where generically one does not expect FTD, many physically relevant dynamics actually can show it, such as those preserving Gaussian states [122]. There, what we have done, was to guarantee that in some instant $t_a > 0$ of time certain collections of dynamical mappings push, at least, one state towards (the interior of) $\mathcal{S}$. And since $\text{int}(\mathcal{S})$ is non-empty, that state shall remain there for a non-degenerate interval of time $[t_a, t_b]$, s.t. $t_a < t_b$. Although we were not able to prove Conjecture 3.2 in its full generality, we manage to do it for some large and important families of quantum dynamics. They include all possible dynamics for a bipartite closed system, whatever interaction the parts might have and whatever time variation their Hamiltonian may have. For qbits a much larger class of dynamics possibilities were considered, only requiring a technical condition (unitality) on CPTP maps describing the time evolution. Since the proof for qbits seems quite technical and the geometric ingredients are the same for other finite dimensions, the Conjecture that the only class of bipartite dynamics not to show FTD is the local unitaries must hold, but still demands a final proof.

Other situation where topology changes, and consequently entanglement dynamics changes, is when one restricts to pure states. There, the set of separable states (indeed, product states) has empty interior. For these systems, FTD can only happen if "hand tailored", *e.g.*: starting from an entangled state, some family of global unitaries is applied up to a time when the state is product, from this time on, only local unitaries are applied. This is clearly not generic in the set of dynamics.

[3] Thanks A. Baraviera for point out to us this characterization.

As a last commentary, it is natural to remember that for practical implementations of quantum information processing, it is important to fight against FTD. Our results about the genericity of FTD do not make this fight impossible. Even for dynamics where FTD does happen, is is natural to search for initial states where it can be avoided, or, at least, delayed [118, 119, 127, 128].

So, to summarize, much have been done. But there is a lot of thing to do yet. All works yielded fruits and more are (and certainly will) coming. I hope you (the Reader) have had fun in reading these lines, and in case you have comments or thoughts about these issues, I will be more than happy to discuss! ;)

Appendix A

A bit of qubits

A.1 Introduction

As we have said in introduction, this first appendix is a short road to learn the basic, the principles, that is, what is necessary (probably far away to be sufficient) from Quantum Mechanics to understand the core of the thesis. We will keep it simple, direct, rigorous, and for this, we will adopt a style quite similar to [129–131]. Other standard references in area are the excellent [15,132] and [133] for a more geometrical approach.

Indeed, all previous references, and even this Appendix, are influenced by the Quantum Information point of view, and therefore the classical quantum words as Compton Effect, Black Body Radiation, Hydrogen Atom, Potential Wells, Sum of Angular Momentum, Clebsch-Gordan Coefficients... will not appear here. For this kind of classic introduction to quantum subject, accounting for the historical point of view, we refer to [1–3, 13, 14, 16].

Here our intentions are to clarify, introducing and defining, those words and concepts that we judge to be outside from the ordinary readers' dictionary, whether he/she be a mathematician or a physicist. Do you really know what states, pure states, measurement, joint systems, entanglement, entangled states, quantum channels... mean? No? So, this first Appendix was designed for you.

A.2 Axioms and Definitions

Let us begin considering a physical system $\mathcal{S}$ described by Classical Mechanics [134]. Suppose that this system $\mathcal{S}$ is composed by a single particle with mass m, which is restricted to move in only one spatial dimension. Its spacial position $\boldsymbol{q}$ is completely described given one parameter $t \in \mathbb{R}^+$, and suppose that $V(\boldsymbol{q})$ represents its potential energy. The linear momentum, on the other hand, is $\boldsymbol{p} = m\boldsymbol{v}$, where $\boldsymbol{v}$ is the velocity of the single particle S. We should stress that the mere knowledge of the pair $(\boldsymbol{q}(t = t_0), \boldsymbol{p}(t = t_0))$, in $t = t_0$, has strong implications:

1. We can calculate the value obtained from the measurement of any relevant physical quantity in t_0, since almost all quantities are functions of $\boldsymbol{p}$ and $\boldsymbol{q}$. For instance, the kinetic energy

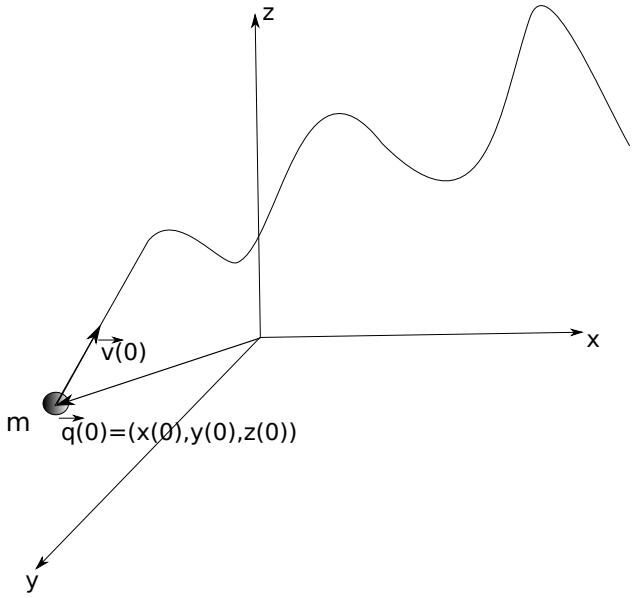


Figure A.1: Schematic draw of a particle moving on an 1-dimensional space. With $v(0)$ and $q(0)$ its velocity and position at $t = 0$.

$K(p) = \frac{\|p\|^2}{2m}$ or the total mechanical energy $E = K(p) + V(q)$.

2. We can also predict, using Newton's Laws, all pairs $(q(t), p(t)), \forall t \geq t_0$. Moreover, using the same reasoning of item 1, any other interesting physical quantity in any posterior instant t of time can be predicted.

The previous arguments guarantee that we may access generically all the information contained in $\mathcal{S}$. And for this reason we often call the pair $(q(t), p(t))$ as the **State** of the system at t. Obviously, the collection $\mathcal{D}(\mathcal{S})$ of all the states of $\mathcal{S}$ is called the **State Space** associated with $\mathcal{S}$. As we have mentioned above, the **Measurements** on $\mathcal{S}$ are described by smooth functions $f(q, p)$, while the **Dynamics** is determined using Newton's Laws. Finally, given two systems $\mathcal{S}, \mathcal{S}'$ with associated state spaces $\mathcal{D}(\mathcal{S}), \mathcal{D}(\mathcal{S}')$ the **Jointly State Space** $\mathcal{D}(\mathcal{S} + \mathcal{S}')$ is defined as $\mathcal{D}(\mathcal{S}) \times \mathcal{D}(\mathcal{S}')$, that is, it is enough to consider only the position and momentum of both particles. With these ideas in mind, now we can move our description to the Quantum side of Physics. So, let us start with the first...

Axiom A.1. *For each quantum system $\mathcal{S}$ there is a Hilbert Space $\mathcal{H}_\mathcal{S}$ associated with it. Each possible state of $\mathcal{S}$ is described by an operator $\rho : \mathcal{H}_\mathcal{S} \to \mathcal{H}_\mathcal{S}$ positive semi-definite with trace equals to 1, called density operator. The whole set of density operators, describing all the states of $\mathcal{S}$, is denoted by $\mathcal{D}(\mathcal{H}_\mathcal{S})$, and called the State Space of $\mathcal{S}$.*

So, now we do know how to describe a quantum system in laboratory, what can we do with it? Probably we want to know/describe it better, learning something about it, thus and in order to do that, we must extract information from it. In some way we shall ask to the system its

properties, interacting with or disturbing it. The axiom A.4 addresses this issue. But first, we need the following definition:

Definition A.2. *A Positive Operators Valued Measure, or POVM for short, is a triple* $(\Omega, \mathcal{H}, \Pi)$*, where* $\Omega = \{\omega_i\}_{i=1}^N$ *is a finite set,* $\mathcal{H}$ *is a Hilbert Space, and* $\Pi : \mathcal{P}(\Omega) \to \{A : \mathcal{H} \to \mathcal{H}; A \geq 0\}$*, s.t.:*

1. $\Pi(E) = \sum_{\omega_i \in E} \Pi(\{\omega_i\}),\ \forall\ E \subset \Omega$;
2. $\Pi(\Omega) = \mathbb{1}_{\mathcal{H}}$.

Remark A.3. *Given a POVM* $(\Omega = \{\omega_i\}_{i\in[N]}, \mathcal{H}, \Pi)$*, it is common to define* $\Pi_k = \Pi(\{\omega_k\}), \forall\ k \in [N]$*, and call each* Π_k *as a POVM element (with respect to* Π*).*

Axiom A.4. *A measurement on a quantum system* $\mathcal{S}$ *is described by a POVM* $(\Omega, \mathcal{H}_\mathcal{S}, \Pi)$*, where* $\Omega = \{\omega_1, ..., \omega_N\}$ *represents the potential outcomes from the measurement, and* $\mathcal{H}_\mathcal{S}$ *is the Hilbert Space associated with* $\mathcal{S}$*. Moreover, if a state of the system* $\mathcal{S}$ *is described by* $\rho \in \mathcal{D}(\mathcal{H}_\mathcal{S})$*, then the probability* $p(E)$ *of observing an event* $E \subset \Omega$ *is defined*[1] *as* $p(E) = Tr[\rho\Pi(E)]$.

Roughly speaking, we could interpret the axioms A.1 and A.4 in the following way: Suppose you can manipulate[2] a quantum system consisted by, we say, a single Hydrogen atom. Now, inside this simple picture, we are able to ask to this system questions like "if we measure the energy of this atom, which values, or outcomes, can we obtain?" and "What are the probabilities of obtain which one of them?". And the both axioms are readily used in order to answer the questions above. First of all, we must identify the Hilbert space $\mathcal{H}_\mathcal{S}$ associated with the system. Secondly, identify the $POVM$ $(\Omega, \mathcal{S}, \Pi)$ that describe the referred measurement(s)[3]. By the end, calculate each $P(E)$, where each $E \subset \Omega$ represents the possible outcomes in this idealized situation.

As we have seen, given two systems $\mathcal{S}, \mathcal{S}'$ described by Classical Mechanics, with associated state spaces $\mathcal{D}(\mathcal{S}), \mathcal{D}(\mathcal{S}')$, the composed system $\mathcal{S} + \mathcal{S}'$ has space state given by $\mathcal{D}(\mathcal{S} + \mathcal{S}') = \mathcal{D}(\mathcal{S}) \times \mathcal{D}(\mathcal{S}')$. On the other hand:

Axiom A.5. *Given two quantum systems* $\mathcal{A}$ *and* $\mathcal{B}$*, with associated Hilbert spaces* $\mathcal{H}_\mathcal{A}, \mathcal{H}_\mathcal{B}$ *respectively, the Hilbert Space associated with the composed system* $\mathcal{AB}$ *is* $\mathcal{H}_{\mathcal{AB}} = \mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$.

Remark A.6. *Whereas in Classical Mechanics, the composition rule is dictated by "*$\times$*", in Quantum Mechanics the composition rule says we must take "*$\otimes$*" in order to compose two quantum systems. Thus, while in classical physics the dimensionality of the spaces grows with the sum, here in quantum physics, it grows with the product*[4].

[1] Note that:

- $\Pi(\Omega) = \mathbb{1} \implies p(\Omega) = 1$; and
- $\Pi : \mathcal{P}(\Omega) \to \{A : \mathcal{H} \to \mathcal{H}; A \geq 0\} \implies 0 \leq p(E) \leq 1,\ \forall\ E \subset \Omega$.

[2] Or suppose you know someone that can do it.

[3] In fact, in this simple situation, we can change the toolbox, for an equivalent one, and instead to use a $POVM$, we could use a Hermitian Operator $M : \mathcal{H}_\mathcal{S} \longrightarrow \mathcal{H}_\mathcal{S}$ representing the required measurement. The spectrum $\mathcal{S}(M)$ of M, consisted by real numbers, corresponds to the outcomes, and the probability of each $m_i \in \mathcal{S}(M)$ is $p(m_i) = Tr(\rho P_i)$, where $M = \sum_{i=1}^N m_i P_i$ is the spectral decomposition for M.

[4] Since $\dim(\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}) = \dim(\mathcal{H}_\mathcal{A}) \times \dim(\mathcal{H}_\mathcal{B})$.

Since we know how to combine two, or more, quantum systems, now we can write a few words about a striking kind of correlation displayed by quantum mechanics, without any correlate counterpart in classical physics. In fact, there is a entire world of discussions, applications, implications, characterizations, on this subject, and for that we suggest [99–101]. Here, in appendix, we are just focusing on the standard definition:

Definition A.7. *Let $\mathcal{S} = \mathcal{AB}$ be a bipartite system, and let $\rho \in \mathcal{D}(\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B})$ a state of $\mathcal{S}$. Within this tensor product structure, ρ is separable when there exist $\{\rho_i^\mathcal{A}\}_{i\in[N]} \subset \mathcal{D}(\mathcal{H}_\mathcal{A}), \{\rho_i^\mathcal{B}\}_{i\in[N]} \subset \mathcal{D}(\mathcal{H}_\mathcal{B})$, and a probability distribution $(p_1, ..., p_N)$, s.t. $\rho = \sum_{i=1}^N p_i \rho_i^\mathcal{A} \otimes \rho_i^\mathcal{B}$. Otherwise it is entangled.*

Before discussing how the evolution of quantum systems could be described, we need the following definitions:

Definition A.8. *Let $\Lambda : \mathcal{L}(\mathcal{H}) \longrightarrow \mathcal{L}(\mathcal{H})$ be a linear map, with $\mathcal{L}(\mathcal{H})$ is the set of all linear operators acting on $\mathcal{H}$. We say that Λ is Completely Positive, or CP, when there exists a set $\{K_i\}_{i=1}^N \subset \mathcal{L}(\mathcal{H})$ s.t. $\Lambda(\sigma) = \sum_{i=1}^N K_i \sigma K_i^*$, $\forall\, \sigma \in \mathcal{L}(\mathcal{H})$.*

Definition A.9. *Let $\Lambda : \mathcal{L}(\mathcal{H}) \longrightarrow \mathcal{L}(\mathcal{H})$ be a linear map. We say that Λ is a Quantum Channel when:*

- *Λ is CP;*
- *$Tr[\Lambda(\sigma)] = Tr(\sigma)$, $\forall\, \sigma \in \mathcal{L}(\mathcal{H})$.*

Roughly speaking, a quantum channel represents an idealized situation, very common in information theory, where the map Λ acts like a real channel[5], sending quantum states (inputs) to quantum states (outputs). For this reason we have imposed both CP and trace preserving constraints.

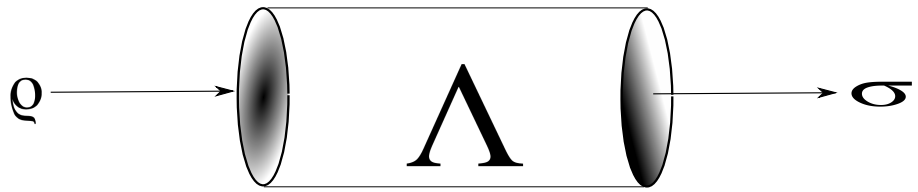


Figure A.2: Schematic drawing of a Quantum Channel

For other characterizations, equivalences, and examples of completely positive maps and quantum channels, we suggest [15, 131, 132]. So, now we have all necessary toolbox for:

Axiom A.10. *Given a quantum system $\mathcal{S}$ and its Hilbert space $\mathcal{H}_\mathcal{S}$, a dynamical mapping of $\mathcal{S}$ is given by a one-parameter family of quantum channels $\{\Lambda_t\}_{t\in\mathcal{I}}$ from $\mathcal{L}(\mathcal{H}_\mathcal{S})$ into itself, where $\mathcal{I}$ is some ordered subset of $[0, \infty)$, each mapping Λ_t modelling the evolution of $\mathcal{S}$ from the initial time $t_0 \in \mathcal{I}$, to later times $t \geq t_0$. When $|\mathcal{I}| = card(\mathbb{N})$ the dynamics is called Discrete Dynamics, and it is a Continuous Dynamics when $|\mathcal{I}| = card(\mathbb{R})$.*

[5] An antenna, an wire, a telephone...

A.2.1 Pure States, Projectors, 1 and 2 Qubits, and all that

It is very common, at least at modern books of Quantum Information, that the authors start their discussions with Pure States representing states and Projectors playing the role of Measurements. Always exploring the Quantum Bit (Qubit) as a good prototype. This point of view, is didactically well suited for beginners, since the level of mathematics involved, as we are going to see, is quite simple. In fact it is the simplest possible. However, to reach the axioms A.1 and A.4 starting from this simple picture is not a simple task. Since our readers are more mature, we have decided begin at full generality, and now to describe these simple, but very important, particular cases in a easier way. Let us start with the following...

Definition A.11. *Let $\mathcal{S}$ be a quantum system, and let $\mathcal{H}_{\mathcal{S}}$ be the Hilbert Space associated with $\mathcal{S}$. When the state of the system is described by a density operator $\rho \in \mathcal{D}(\mathcal{H}_{\mathcal{S}})$ s.t. $rank(\rho) = 1$, the state of the system is called a Pure State.*

Remark A.12. *There exists a mnemonic notation due Dirac [13], commonly used in physics[6]. The idea is to represent a vector contained in $\mathcal{H}_{\mathcal{S}}$ as $|\psi\rangle$, read* ket psi*, and the associated linear functional: "do inner product with $|\psi\rangle$", as $\langle\psi|$, read* bra psi*. Therefore, using Dirac's Notation:*

$$\langle |\phi\rangle, |\psi\rangle \rangle = \langle \phi | (|\psi\rangle) = \langle \phi | \psi \rangle.$$

Getting back to Definition A.11, when $rank(\rho) = 1$, we can decompose, via Spectral Decomposition, ρ as an unidimensional projector $|\psi\rangle\langle\psi|$, and then to represent the pure state of the system using the vector $|\psi\rangle$, since it contains all necessary informations about the state. To summarize, without lost of generality, pure states could be described by vectors $|\psi\rangle \in \mathcal{H}_{\mathcal{S}}$.

In fact, the most impressive aspect[7] of Quantum Information Theory, that has even influenced other areas, relies on the fact that all protocols; algorithms; or experiments, in a broad and general sense; are performed with finite dimension, *i.e.* the Hilbert Space $\mathcal{H}_{\mathcal{S}}$ associated with each system is, in general, such that $\dim(\mathcal{H}_{\mathcal{S}}) < \infty$. And it is superb, since it is possible to design faster algorithms, better strategies, and foundational experiments using only ordinary Linear Algebra. In this sense, the most important piece of Quantum Information Theory is, probably, the concept of *Qubit*, *i.e.* the simplest quantum system that could be prepared in laboratory. Whereas a Classical Bit can be mathematically represented using a random variable X taking values on $\{0, 1\}$, and thus assuming either 0, or 1, on the other hand a Quantum Bit, or Qubit, is represented by a vector $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \in \mathcal{H}_2 \simeq \mathbb{C}^2$. Therefore, and here resides the entire mystery, a Qubit *is* in a superposition state [15, 129, 130], neither $|0\rangle$, nor $|1\rangle$, but a superposition of both. Any (quantum) two-level system in laboratory can be used as a qubit: photons, electrons, atoms, quantum dots [135], and so on... The same idea is replicated, and d-level systems, represented by vectors $|\phi\rangle = \sum_{i=1}^{d} \alpha_i |i\rangle \in \mathcal{H}_d$ is called a Qu*d*it.

[6] Articles, introductory and advanced textbooks, classes, and so on. However there exist good references that, justifiably, avoid it. For instance [16, 131]

[7] And beauty.

When we are allowed to play with two, or more, systems, even 2-qubits[8] already display the strong behaviour of treating with composed system in quantum information. Among these, two pairs should be highlighted:

$$|\phi^{\pm}\rangle = \frac{|00\rangle \pm |11\rangle}{\sqrt{2}} \tag{A.1}$$

$$|\psi^{\pm}\rangle = \frac{|01\rangle \pm |10\rangle}{\sqrt{2}} \tag{A.2}$$

They are the so famous Bell States, and their use are extremely common, important, and sometimes fundamental in many protocols of quantum information[9]. In fact, these pairs play essential role in some experiments concerned on Violations[10] of Bell Inequalities [23, 136–138].

The two pairs of pure states shown in the Eqs. (A.1) and (A.2) above can be extended, in a certain sense, when we are considering instead 2 (bipartite) parts, a number $N \in \mathbb{N}$ of (bipartite) parts [15, 109]:

$$|GHZ\rangle = \frac{|0\rangle^{\otimes N} + |1\rangle^{\otimes N}}{\sqrt{N}} \tag{A.3}$$

$$|W\rangle = \frac{|100...0\rangle + |010...0\rangle + ... + |000...1\rangle}{\sqrt{N}} \tag{A.4}$$

Now, just to keep the things simple enough, let us fix our discussion at[11] bipartite systems that have Hilbert space given by $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$. For these, we can pick out, for instance, three different states as below:

$$|\psi\rangle = |00\rangle \tag{A.5}$$

$$|\alpha, \beta\rangle = \alpha|00\rangle + \beta|11\rangle, \text{ with } |\alpha|^2 + |\beta|^2 = 1 \text{ and } \alpha \neq \beta \tag{A.6}$$

$$|\phi^{+}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \tag{A.7}$$

and anyone will agree that albeit different, they are somehow *substantially* different. That one in Eq. (A.5) is in a product form $|\psi\rangle = |0\rangle \otimes |1\rangle$, whereas those in Eqs. (A.6) and (A.7) cannot be settled in such a form, since theirs Schmidt Rank [15, 132] are greater than 1. Furthermore, $|\alpha, \beta\rangle$ and $|\phi^{+}\rangle$ are different each other, for while the former is "unbalanced", the last is "completely balanced".

The more alert Reader could imagine that the concept hidden into the last paragraphs, which is central in Quantum Information Theory [15, 99, 139–141], is that of Entanglement. Remembering Axiom A.7:

A system $\mathcal{S}$ with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, in a state represented by $\rho \in \mathcal{D}(\mathcal{H})$, is separable when there exists $\{\rho_i^A\}_{i=1}^N \in \mathcal{D}(\mathcal{H}_A)$, $\{\rho_i^B\}_{i=1}^N \in \mathcal{D}(\mathcal{H}_B)$ and a probability distribution $(p_1, ..., p_N)$ such that

$$\rho = \sum_{i=1}^{N} p_i \rho_i^A \otimes \rho_i^B. \tag{A.8}$$

Otherwise $\mathcal{S}$ is entangled.

[8] By convenience we will write $|ab\rangle$ for $|a\rangle \otimes |b\rangle$.
[9] Despite the fact that sometimes they are completely useless for Quantum Information Protocols: see Chapter 2.
[10] See Appendix C and the discussion at the introductory section of the main text.
[11] Two qubits.

Remark A.13. *The Axiom. A.7 was made for bipartite systems, but it can be straightforwardly generalized for more general cases.*

Given a mixed state $\rho \in \mathcal{D}(\mathcal{H}_A) \otimes \mathcal{D}(\mathcal{H}_B)$, to check whether is possible, or is not, write it in a separable form is a hard task[12], however the thing changes of figure for bipartite pure states:

Theorem A.14 (Schmidt Theorem [15])**.** *Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be two finite Hilbert spaces, such that $dim(\mathcal{H}_A) = n \leq m = dim(\mathcal{H}_B)$. For all $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ there exist orthonormal basis $\{|a_1\rangle, ..., |a_n\rangle\} \subset \mathcal{H}_A$, $\{|b_1\rangle, ..., |b_m\rangle\} \subset \mathcal{H}_B$, and a non-negative vector $(p_1, ..., p_m)$ such that:*

$$|\psi\rangle = \sum_{i=1}^{m} p_i |a_i b_i\rangle \tag{A.9}$$

and $\sum_{i=1}^{m} p_i^2 = 1$.

Remark A.15. *The expression in A.9 is called the Schmidt Decomposition for $|\psi\rangle$. Except by indexes permutations it is unique for each vector in $\mathcal{H}_A \otimes \mathcal{H}_B$. For this reason, the number $Srank(|\psi\rangle) = |\{i \in [m];\ p_i \neq 0\}|$ is called the* Schmidt Rank *of $|\psi\rangle$.*

Theorem A.16. *A bipartite pure system represented by $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is separable if, and only if, $Srank(|\psi\rangle) = 1$.*

It is clear that for the states in Eqs. (A.5), (A.6), and (A.7) we have $Srank(|\psi\rangle) = 1$ and $Srank(|\alpha, \beta\rangle) = 2 = Srank(|\phi^+\rangle)$, *i.e.* the former is separable whereas the last two are entangled. But remains to say why $|\alpha, \beta\rangle$ and $|\phi^+\rangle$ are also different each other, despite the fact that both are entangled.

Entanglement has been now seen as resource [15, 145–147], therefore to measure how useful it is for some tasks[13] turns out to be of extreme importance. Actually, there are a bunch of entanglement measures, each of them with an interpretation [99, 142, 143]. But, since Bell states (are the only entangled states that) can be transformed into any other via *Local Operations with Classical Communication* (*LOCC*)[14], it is reasonable to set them up as maximally entangled. Moreover as pure product states do not reach anyone, it is also natural one sets them as zero-entangled. In fact, any reasonable entanglement measure has to be maximum for those states that behaviour themselves like Bell States[15], and somehow it shall differentiate them from other entangled states and, of course, being zero for all separable states.

[12] See [99, 132] and references therein

[13] For instance: Superdense Coding, Teleportation, SWAP [99, 129, 130] and *LOCC* protocols.

[14] See [15, 98, 132, 149] and references therein.

[15] For instance, the $|GHZ\rangle$ and $|W\rangle$. They are maximally entangled, since they attain sets of other states that do not reach both of them. However via *LOCC* they are non-interconvertible and therefore constitute different classes of maximally entanglement

Appendix B

Bounding $\theta(\mathsf{G}, w)$

In this Appendix we review the NPA method and give some details of the SDPs used to estimate the multigraph Lovász number $\theta(\mathsf{G}, w)$. Our account of the NPA method does not intend to be complete; for further details, consult Refs. [48, 49]. For simplicity, we will consider bipartite scenarios, but extensions to more parties are straightforward.

As discussed in Sec. 1.4, the Lovász number of a two-colour edge-coloured multigraph (G, w) can be written as

$$\theta(\mathsf{G}, w) = \sup_{\mathbf{P} \in Q(\mathsf{G})} \sum_{i \in V} w_i P(i, i), \tag{B.1}$$

where V is the vertex set of (G, w) and $Q(\mathsf{G})$ denotes the set of multipartite quantum behaviours (see Appendix C) of G, that is, the set of all behaviours whose elements are of the form

$$P(a, b) = \langle \psi | \Pi_a^A \otimes \Pi_b^B | \psi \rangle, \quad \forall\, a, b \in V, \tag{B.2}$$

for orthogonal projective representations on Hilbert spaces of arbitrary dimension $\{\Pi_a^A : a \in V\}$ and $\{\Pi_b^B : b \in V\}$ of $\overline{G_A}$ and $\overline{G_B}$, respectively, assuming that the multigraph (G, w) is composed of exclusivity factors (G_A, w) and (G_B, w), and pure states $|\psi\rangle$ in the Hilbert space in which the projectors act on.

In finite dimensional Hilbert spaces, the set $Q(\mathsf{G})$, as defined above, is known to be the same as a set $\overline{Q}(\mathsf{G})$ of quantum behaviours similarly defined, though where, in the latter, the elements are of the form

$$P(a, b) = \langle \psi | \Pi_a^A \Pi_b^B | \psi \rangle, \quad \forall\, a, b \in V, \tag{B.3}$$

where $[\Pi_a^A, \Pi_b^B] = 0$ for all a and b. The problem of whether or not the equality between $Q(\mathsf{G})$ and $\overline{Q}(\mathsf{G})$ holds in infinite dimensional Hilbert spaces has been known as *Tsirelson's problem* [94, 95]. From now on this latter definition will be assumed, and hence we may use sets $Q(\mathsf{G})$ and $\overline{Q}(\mathsf{G})$ indistinctively. Note that, in the worst-case scenario in which the maximum quantum violation of some inequality is reached only for infinite dimensional systems and assuming $Q(\mathsf{G}) \neq \overline{Q}(\mathsf{G})$, maximization over $\overline{Q}(\mathsf{G})$ will, nonetheless, give an upper bound to such maximum.

Define the sets $\mathcal{P}_A = \{\Pi_a^A : a \in V\}$ and $\mathcal{P}_B = \{\Pi_b^B : b \in V\}$, and let $\mathcal{P} = \mathcal{P}_A \cup \mathcal{P}_B$, assuming, as in the definition above, that $[\Pi_a^A, \Pi_b^B] = 0$ for all a and b. Define a sequence of $\mathcal{P}$ as a product

of elements in $\mathcal{P}$; the length k of a sequence is defined as the minimum number of elements of $\mathcal{P}$ needed to generate it. Let us remark that some sequences may correspond to the null operator, for instance, $\Pi_a^A \Pi_{a'}^A$, if a and a' are connected vertices in the graph (G_A, w). Let S_k denote the set of non-null sequences of length not larger than k, assuming the identity operator $\mathbb{1}$ to be a sequence of length 0. Thus,

$$\begin{aligned} S_0 &= \{\mathbb{1}\}, \\ S_1 &= S_0 \cup \{\Pi_a^A\} \cup \{\Pi_b^B\}, \\ S_2 &= S_1 \cup \{\Pi_a^A \Pi_{a'}^A\} \cup \{\Pi_b^B \Pi_{b'}^B\} \cup \{\Pi_a^A \Pi_b^B\}, \\ S_3 &= S_2 \cup \dots \end{aligned}$$

For a set S_k, define a matrix Γ^k in the following way. For every two elements of S_k, say, O_i and O_j, take the product $O_i^\dagger O_j$. If this sequence results in a product of compatible operators of $\mathcal{P}$, for instance, $\Pi_a^A \Pi_b^B$, then assign the joint probability $P(a, b)$ to the entry $\Gamma_{i,j}^k$. If, however, the sequence results in a product of operators of $\mathcal{P}$ which are not compatible, say, $\Pi_a^A \Pi_{a'}^A$, then, to the entry $\Gamma_{i,j}^k$ assign a variable $x(a, a')$, indexed by the labels a and a', if the vertices a and a' are not connected in the graph (G_A, w), or assign the value 0 if the vertices are connected.

If the behaviour $\mathbf{P}$ is quantum, then real numbers can be assigned to the variables x such that the matrix Γ^k is positive semi-definite. This holds because if $\mathbf{P}$ is quantum all entries of Γ^k can be defined to be of the form $\Gamma_{i,j}^k = \langle\psi|O_i^\dagger O_j|\psi\rangle$. Then, positive semi-definiteness follows:

$$\begin{aligned} v^\dagger \Gamma^k v &= \sum_{i,j} v_i^\dagger \Gamma_{i,j}^k v_j \\ &= \langle\psi| \left(\sum_i v_i^\dagger O_i^\dagger \right) \left(\sum_j O_j v_j \right) |\psi\rangle \\ &= \langle\psi| V^\dagger V |\psi\rangle \geq 0, \end{aligned} \tag{B.4}$$

where $V = Ov$ and this holds for every vector v since any operator of the form $V^\dagger V$ is positive semi-definite. The set of behaviours that lead to a positive semi-definite Γ^k is denoted Q_k, and, as proven above, contains the set of quantum behaviours Q. Since the sets of sequences S_k are ordered as a hierarchy where $S_1 \subseteq S_2 \subseteq \dots$, the sets Q_k are also hierarchically structured as $Q_1 \supseteq Q_2 \supseteq \cdots \supseteq Q$. According to NPA, the set Q_k converges to the set of quantum behaviours Q in the limit of k going to infinity, $\lim_{k\to\infty} Q_k = Q$.

It is important to remark that intermediate sets of behaviours can be defined between two sets Q_k and Q_{k+1}. This can be done by defining a set of sequences S which strictly contains the set S_k but is strictly contained in the set S_{k+1}, and defining a matrix Γ as above. An important example was introduced by NPA as the set denoted Q_{1+AB}. The corresponding set for the multigraph G is given by

$$S_{1+AB} = S_1 \cup \{\Pi_a^A \Pi_b^B : a, b \in V\}. \tag{B.5}$$

In some of the cases we study in this thesis, even the set $Q_{1+AB}(\mathsf{G})$ is too resource demanding to deal with. It is necessary, then, to introduce intermediate sets between $Q_1(\mathsf{G})$ and $Q_{1+AB}(\mathsf{G})$, sets

that we denote as $Q_{1.x}(\mathsf{G})$, defined by means of the set of sequences

$$S_{1.x} = S_1 \cup \{\Pi_a^A \Pi_b^B : a, b \in V_x\}, \tag{B.6}$$

where V_x is a subset of V with x elements. Notice that different choices of V_x can lead to different sets $S_{1.x}$. We adopt this notation, assuming that the set V_x is the set of vertices which allows for the most restrictive value for $\theta(\mathsf{G}, w)$.

Optimisation of linear functions of behaviours over the sets $Q_k(\mathsf{G})$ can be implemented as a SDP. Semi-definite programming is a subfield of convex optimisation concerned with problems of the type

$$\begin{aligned} &\max \operatorname{tr}(FX), \\ &\text{subject to } \operatorname{tr}(C_i X) \leq d_i, \quad i = 1, \ldots, p, \\ &X \geq 0. \end{aligned}$$

The problem variable is the matrix X, and the parameters of the problem are the matrices F and C_i, the scalars d_i, and the number of constraints p.

In our case, the problem variable is the matrix Γ^k, and the parameters can be read from the multigraph alone. First, notice that the multigraph Lovász number can be written, in the limit $k \to \infty$, as $\operatorname{tr}(F\Gamma^k)$, where F is a matrix that selects in Γ^k the entries associated to the probabilities $P(i,i)$, with $i \in V$, and assign the correct weights w_i to each one of them. This can be easily implemented if the elements of the set S_1 are labelled from 1 to $2|V|+1$, where $O_1 = \mathbb{1}$, $O_{1+a} = \Pi_a^A$, for $a \in V$, and $O_{1+|V|+b} = \Pi_b^B$, for $b \in V$, and assuming this order is kept for higher order S_k. Then, the probabilities $P(i,j)$ are always assigned to the same entries of Γ^k. They are

$$P(i,j) = \Gamma^k_{1+i,1+|V|+j}, \quad \forall\, i,j \in V, \tag{B.7}$$

regardless of the degree k.

In the NPA method it is assumed that the sets of measurement operators of each party are partitioned in subsets in which the elements of each are assumed to be associated with the different outcomes of the same measurement. Because of this assumption, the operators in each of these subsets are said to be *complete*, in the sense that they form a resolution of the identity. On the one hand, this assumption allows the definition of marginal probabilities that also respect the no-signalling conditions present in a Bell scenario. On the other hand, it introduces redundancies in the sets of measurement operators and constraints in the joint probability distributions. To get rid of these constraints, NPA redefine the sets of measurement operators and the set of quantum behaviours. This way, all the probabilities present in the matrix Γ^k are independent and no relations of the type $\operatorname{tr}(C_i X) \leq d_i$ are necessary.

In our method, though, this notion of completeness is not directly defined and this has a consequence in the definition of the marginal probabilities. Marginal probabilities appear as entries in the matrix Γ^k and, in our case, they are not fully independent of the joint probabilities associated to the vertices of the multigraph. It is important to note that in our definition of multipartite quantum behaviour we assume the measurement operators to be projectors, and it

follows as a property that the local projectors of, e.g., party A associated to vertices that compose a clique K_A of the exclusivity factor (G_A, w) project onto complementary subspaces of the Hilbert space, and thus must sum to, at most, the identity operator,

$$\sum_{i \in K_A} \Pi_i^A \leq \mathbb{1}, \tag{B.8}$$

for all cliques K_A in (G_A, w). This property implies that the marginal probabilities associated to all vertices of an exclusivity factor of B must satisfy

$$\sum_{i \in K_A} P(i,j) \leq P_B(j), \quad \forall\, j \in V, \tag{B.9}$$

where $P_B(j)$ is the marginal probability associated to vertex j of party B. Analogous relations follow for cliques K_B in (G_B, w). These restrictions must be inserted as constraints of the SDP. It is easy to note that they are of the form $\mathrm{tr}(C_i \Gamma^k) \leq d_i$, since both the joint probabilities $P(i,j)$ and the marginal probabilities $P_B(j)$ are present as entries of Γ^k.

Notice that one could replace restriction (B.8) by the stronger condition of saturating this inequality. Imposing the later is equivalent to assuming that the size of the clique coincides with the number of possible outcomes for such observable, while imposing the former is equivalent to assuming that this is only a lower bound. Imposing subnormalization (i.e., (B.8)) is more appropriate, since in actual experiments some of the prepared particles are not detected. Naturally, correlation sets obtained imposing subnormalization are, in general, larger than those obtained assuming normalization. However, this simply follows from defining differently what is meant by a measurement to have a number of outcomes. We have performed simulations using both the strong normalization constraint and the subnormalization constraint, and we obtained the same upper bounds for the multigraph Lovász number for all the multigraphs studied in this text. An interesting open problem is whether there are cases where a Lovász optimum projective representation does not saturate some of the conditions (B.8).

Additionally, it is worth noting that, in the case of exclusivity multigraphs that represent specific NC or Bell inequalities, our method does not take into account the labels $a \ldots c|x \ldots z$ of the events associated to the vertices of the multigraph. If labels were considered, then it would be possible to identify, in the factor of a particular party, different vertices that represent the same party's part of the event, and the program would converge faster, since a reduced number of measurement operators would be considered. This would be essentially equivalent to using the NPA method as described in Refs. [48, 49]. The novel point in our approach is that, even though we do not add this constraint, we observe that the optimal results obtained are consistent with it, in the sense that if two vertices i and j are supposed to represent the same local event $a|x$ of party A, then, in the optimal results obtained, $P_A(i) = P_A(j)$ and $P(i,k) = P(j,k)$, for all $k \in V$ [1]. This

[1] Let i and j be two vertices of a factor G_A of a multigraph (G, w), and let $\mathcal{N}_i$ and $\mathcal{N}_j$ be the sets of neighbours of i and j (i.e., the sets of vertices in G_A which are connected by an edge to i and j, respectively). For i and j to be associated to the same projector Π, it is necessary that $\mathcal{N}_i = \mathcal{N}_j = \mathcal{N}$, so let us assume that this is the case. Let $R(\mathcal{N})$ be the union of the ranges of all projectors associated to the vertices in $\mathcal{N}$. Then, the ranges of both Π_i and Π_j are contained in the subspace complementary to $R(\mathcal{N})$; denote it as $R^\perp(\mathcal{N})$. Since this is the only restriction on the projectors Π_i and Π_j, we can see that the multigraph Lovász number is obtained when $\Pi = \Pi_i = \Pi_j$ and the range of this projector is equal to $R^\perp(\mathcal{N})$.

implies that our method cannot perform better than NPA's when the Bell scenario is given, and the bounds obtained are necessarily greater than or equal to the bounds of NPA for the same level in the hierarchies.

The program we used to implement our version of the NPA method was written in MATLAB and made use of the packages `YALMIP` [96], `SeDuMi` [63] and `SDPT3` [64]. The inputs are the multigraph (G, w), given in terms of the adjacency matrices of its exclusivity factors, and the degree k of the hierarchy to be considered. It is interesting to note that the only challenge is to create the matrix Γ^k and to identify the entries that correspond to the same variables and whether they are probabilities or not.

The first routine creates a $(2|V|+1)$-dimensional structure R^1 in which each entry stores the label of one of the symbolic elements of S_1. As mentioned above, we assume the elements of S_1 to be labelled from 1 to $2|V|+1$, where R^1_1 is assigned to $\mathbb{1}$, R^1_{1+a} is assigned to Π^A_a, for $a \in V$, and $R^1_{1+|V|+b}$ is assigned to Π^B_b, for $b \in V$. Then, a structure R^k, associated to S_k, is constructed recursively. Each entry stores the product of the labels of the elements of S_1 —i.e., the labels stored in R^1— that compose each sequence in S_k. As an example, for the sequence $\Pi^A_a \Pi^B_b$ the corresponding entry in, e.g., R^2, will be $(1+a, 1+|V|+b)$, since these are the labels assigned to these projectors in R^1. In this step, the information in the multigraph is relevant: If a sequence, e.g., $\Pi^A_a \Pi^A_{a'}$, is such that there is an edge between vertices a and a' in (G_A, w), then the operators are associated to locally exclusive events and their product is the null operator, resulting in a null sequence. Only non-null sequences are considered.

We consider levels which are between $Q_1(\mathsf{G})$ and $Q_{1+AB}(\mathsf{G})$, levels which we denote as $Q_{1.x}(\mathsf{G})$. Specifically, to construct the structure $R^{1.x}$, we randomly pick x elements among the $|V|$ associated to the projectors of party A and x elements among the $|V|$ associated to the projectors of party B. We repeat this process several times and the described results are the best obtained in the sample.

After the structure R^k is built, a routine checks whether there are redundant entries and, if this is the case, removes them. Then, matrix Γ^k is built based on the information of labels present in R^k. It is a $|R^k| \times |R^k|$ symmetric structure in which entry (i, j) stores the composition of the labels stored in entries $R^{k\dagger}_i$ and R^k_j; the $\dagger$ is to remind that the labels should be composed in reverse order, since, in the definition of Γ^k, the entry (i, j) should be associated to the product $O^\dagger_i O_j$. Again, in the composition, it should be checked whether there is a product of locally exclusive events in the result; if this is the case, then the value 0 is assigned to the corresponding entry.

In the next step, after the construction of Γ^k, a routine identifies which entries are supposed to represent probabilities and which represent undetermined variables. A non-negativity constraint is imposed to the probabilities if the level considered is lower than $Q_{1+AB}(\mathsf{G})$. As remarked by NPA, in such cases it is not guaranteed that the behaviours will be non-negative. Then the routine searches for equal elements in the matrix and identifies them. A last routine searches for the cliques in the exclusivity factors of (G, w) and implements the constraints (B.9). The solver is invoked to solve the SDP.

Appendix C

Non-Locality in a Nutshell

In order to make the present Thesis as self contained as possible, we are providing to the reader unfamiliar with Non-Locality a brief introduction to this subject. The idea of this appendix is to give only the necessary definitions to follow those points that may have caused confusion, or that could be misunderstood in the core of the text. For more extensive accounts on this theme, we strongly suggest the Refs. [7–10] and mainly [34].

C.1 Test and Preparations: Exclusivity Relation

In both Introduction and Chapter 1 we discussed the idea of events being objects like $ab...c|xy...z$, where $xy...z$ represents a list of jointly measurable observables, and $ab...c$ are the outcomes for x, and y,..., and z respectively. Moreover we indiscriminately talked about *preparations*, *tests*, and *jointly measurable observables* without defining them properly. The idea of this present Section is to develop that concepts into more formal terms, helping the unfamiliar reader, or clarifying points which may have become obscured in the core of the thesis. Certainly the approach of *Operational Theories* adopted here is not new, and we refer to [40, 159] for an extensive explanation, and [34] for a deep and precise mathematical account on the subject.

Let us begin assuming the following three primitive notions [158]:

- *A Preparation:* motivated by, and associated with the idea of a sequence of unambiguous and reproducible experimental procedures;
- *An Outcome:* linked with the idea of a macroscopically perceptible result, arising from the interaction with a system;
- *A Test:* connected with the a notion of a scheme of preparation followed by a step in which outcome information is supplied to an observer. The set of all outcomes associated with a test T is denoted by $\sigma(T)$;

A theory that specifies probabilities $p(X|T,P)$ for each possible outcome X of each possible test T given a preparation P is called an *Operational Theory*.

Definition 1. *Two preparations P and P' are (operationally)* equivalent *when for all test T, $p(X|T,P) = p(X|T,P')$, $\forall\ X$. Each equivalence class of preparations is called a* state. *We denote by $\rho(P)$, or simply ρ when the preparation is implicit, the class $[P] = \{P';\ p(X|T,P) = p(X|T,P'),\ \forall\ X\}$.*

Definition 2. *Two tests T and T' are (operationally)* equivalent *when for all preparation P, $p(X|T,P) = p(X|T',P)$, $\forall\ X$. Each equivalence class of tests is called an* observable. *We denote by $\mu(T)$, or simply μ when the test is implicit, the class $[T] = \{p(X|T,P) = p(X|T',P),\ \forall\ X\}$*

Now it is possible to talk about Jointly Measurable Observables, Events and Exclusive Events.

Definition 3. *Given two observables μ_1 and μ_2, we say they are* jointly measurable *when there is an observable μ such that:*

1. *the outcome set of μ is $\sigma(\mu) = \{(X_i, X_j);\ X_i \in \sigma(\mu_1)$ and $X_j \in \sigma(\mu_2)\}$;*
2. *for all states ρ:*

$$p(X_i|\mu_1,\rho) = \sum_{X_j \in \sigma(\mu_2)} p((X_i,X_j)|\mu,\rho),\ \forall\ X_i \in \sigma(\mu_1) \tag{C.1a}$$

$$p(X_j|\mu_2,\rho) = \sum_{X_i \in \sigma(\mu_1)} p((X_i,X_j)|\mu,\rho),\ \forall\ X_j \in \sigma(\mu_j) \tag{C.1b}$$

Remark C.1. *The equations (C.1a) and (C.1b) are saying that for all states, the outcome probability distributions for jointly measurable observables are recovered as marginals of the outcome probability distribution of (a third, and higher observable) μ.*

The idea of an event[1] is related to a special kind of preparation. We will focus on preparations, denoted by $P_{M,X,T}$, which can be operationally view as a result from a test T, with outcome X, subject to another specific preparation P. We call these particular preparations as *Event Preparations*

Definition 4. *Two event preparations P_{T_1,X_1,P_1} and P_{T_2,X_2,P_2} are (operationally) equivalent when for all subsequent test T' we have: $p(X'|T', P_{T_1,X_1,P_1}) = p(X'|T', P_{T_2,X_2,P_2})$, $\forall\ X'$. Each one of these equivalence classes are called an* event.

By the last:

Definition 5. *Two events e_1 and e_2 are* Mutually Exclusive *when there is an observable μ associated with other two jointly measurable observables μ_1 and μ_2, s.t. there are $X_1 \in \sigma(\mu_1)$ and $X_2 \in \sigma(\mu_2)$, with $X_1 \neq X_2$, and $p(X_1|\mu,e_1) = 1 = p(X_2|\mu,e_2)$.*

Albeit confusing at a first look, the Definition 5 captures the naive notion of exclusive events from Chapter 1.

Of course, these definitions could be more and more elaborated, making links with Topos and Category Theory. For that, we suggest to the interested reader the outstanding references [34, 35].

[1] Or Measurement Event [34].

C.2 Local, Quantum and Non-Signalling Sets

At the previous Section C.1 we have defined[2] an event e as an equivalence class of a specific kind of preparations, *i.e.* those preparations $P_{X,T,P}$ which can be seen arising after that an outcome X is obtained for a test T, provided a preparation P. It is clear that in such a manner, the event e formalizes the naive notion of event as defined at Chapter 1, *i.e.* an object like $ab...c|xy...z$, meaning that *the outcomes $a, b, ...c$ were obtained respectively when the (jointly measurable) questions $x, y, ..., z$ were asked on each part of the system*. However, we will maintain, and use, this last notation. It is more clear and appealing, since the role of each part is crystal clear.

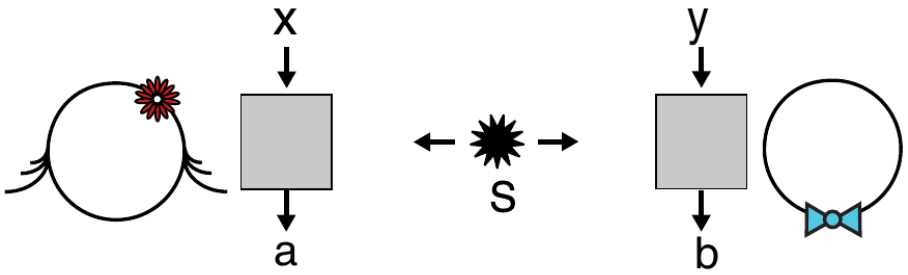


Figure C.1: Alice and Bob sharing a physical system enclosed in 2 black-boxes.

We are considering just two causally disjoint observers, Alice and Bob[3], performing measurements on a shared physical system[4] (see Fig. C.2). Each observer can perform m different measurements (or questions), and each measurement has d (classically) possible outcomes. We will label the measurements by x, y and outcomes by a, b. Moreover, since we are considering only *Operational Theories* (see Section C.1), for each event $ab|xy$ it is associated a probability $p(ab|xy)$, denoting the probability to obtain the output a, b given the (jointly measurable) inputs[5] x, y. Therefore, in this sense, the whole scenario[6] can be characterized specifying all $(dm)^2$ such jointly probabilities. Each

$$\boldsymbol{p} = \left(p(ab|xy)\right)_{\substack{a,b\in[d]\\ x,y\in[m]}} \in \mathbb{R}^{d^2m^2}, \tag{C.2}$$

which characterizes a black-box scenario, is called a *Behaviour*. Of course, due the normalization and positiveness constraints, each behaviour $\boldsymbol{p}$ belongs to a smaller subset

$$\mathcal{P} = \{\boldsymbol{p} \in \mathbb{R}^{d^2m^2}; \boldsymbol{p} \geq 0 \text{ and } \sum_{a,b\in[d]} p(ab|xy) = 1,\ \forall\ x, y \in [m]\}. \tag{C.3}$$

Beyond these two straightforwardly constraints, one may be interested in to investigate those behaviours that allow for a well-definition of marginal probabilities:

[2] Our approach in this Section is quite similar to that which may be found in the Refs. [9] and [7].
[3] Generalizations are possible, but we will fix the simplest scenarios.
[4] Again, we are considering the device-independent, or black-box, point of view.
[5] Implicitly assuming here the black-box point of view.
[6] Called a Bell Scenario.

Definition 6. *A behaviour $\boldsymbol{p} \in \mathcal{P}$ is called a non-signalling behaviour when:*

$$\sum_{b\in[d]} p(ab|xy) = p(a|x) = \sum_{b\in[d]} p(ab|xy'),\ \forall\ a \in [d] \text{ and } x, y, y' \in [m], \tag{C.4}$$

$$\sum_{a\in[d]} p(ab|xy) = p(b|y) = \sum_{a\in[d]} p(ab|x'y),\ \forall\ b \in [d] \text{ and } x, x', y \in [m]. \tag{C.5}$$

The set $\mathcal{NS}$ of all non-signalling behaviours is called Non-Signalling *set.*

Remark C.2. *In particular, in our pre-specified scenario, where Alice and Bob are causally disjoint, equations (C.4) and (C.5) prevent instantaneous signalling of information between Alice and Bob's boxes.*

We will admit without proofs, referring to [55] for that, the following proposition:

Proposition 7. *The set $\mathcal{NS}$ is an convex set of $\mathbb{R}^{d^2m^2}$ with convex dimension [51, 54] equals to $2(d-1)m + (d-1)^2m^2$.*

Now, remembering the discussion that we have shown at Introduction, we define a subset of $\mathcal{P}$ enclosing more restrictive constraints:

Definition 8. *A behaviour $\boldsymbol{p} \in \mathcal{P}$ is called a local behaviour, when there are a measurable space (Λ, Σ, μ) and a measurable function $q : \Lambda \longrightarrow [0, 1]$ s.t.:*

$$p(ab|xy) = \int_\Lambda q(\lambda)p(a|x,\lambda)p(b|y,\lambda)d\mu(\lambda),\ \forall\ a, b \in [d] \text{ and } \forall\ x, y \in [m]. \tag{C.6}$$

The set $\mathcal{L}$ of all behaviours obeying Eq. (C.6) is called Local set.

Indeed, Eq. (C.6) operationally means that Alice and Bob divide a sort of *shared randomness*, represented by the variable λ. Furthermore, it is clear that $\mathcal{L} \subset \mathcal{NL}$, but the converse is not true [76]:

$$P(a, b|x, y) = \begin{cases} \frac{1}{2}, & \text{if } a \oplus b = xy \\ 0, & \text{otherwise} \end{cases}, \tag{C.7}$$

where $a, b, x, y \in \{0, 1\}$.

Once again, we will assume without proofs the following:

Proposition 9 ([7]). *The set $\mathcal{L}$ of local behaviours is a convex hull of d^{2m} points.*

Proceeding to the Quantum World, we have shown Introduction that there is a particular quantum Bell Scenario, with two parts, two measurements per part, and two outcomes for each measurement, whose behaviour (there without using this name) **do not** respect Eq. (C.6), despite the fact that our introductory example **respects** Eqs. (C.4) and (C.5). To obtain this, it is clear that we have taken a specific quantum example, showing how further can Quantum Theory go when one compares it with its Classical counterpart. But in analogy to $\mathcal{L}$ and $\mathcal{NS}$ we may define the collection $\mathcal{Q}$ consisting of all quantum behaviours, *i.e.* the behaviours obtainable using quantum theory, such as:

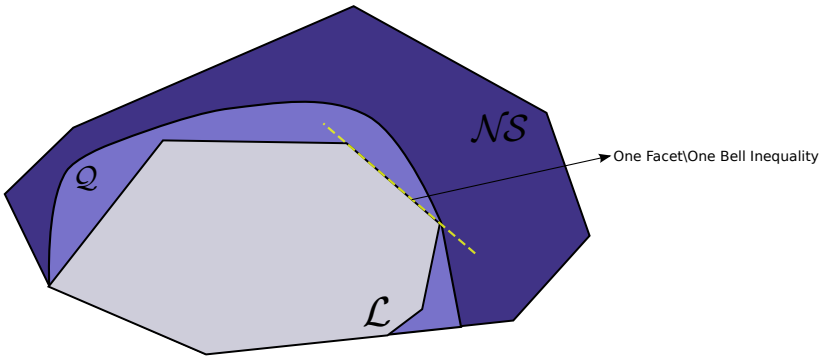


Figure C.2: Schematic drawing of the Local, Quantum, and Non-Signalling sets. Beyond the geometry of each one, it is also represented the strict inclusions $\mathcal{L} \subset \mathcal{Q} \subset \mathcal{NS}$. In yellow we are highlighting the separating hyperplane defining the facet and the corresponding Bell Inequality.

Definition 10. *A behaviour $\boldsymbol{p} \in \mathcal{P}$ is called Quantum, when there are a bipartite system $\mathcal{S}_{AB}$ with associated Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, a state represented by $\rho_{AB} \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$, a POVM $\{M_{a|x}\}_{\substack{a\in[d]\\x\in[m]}}$ on Alice's side, and a POVM $\{M_{b|y}\}_{\substack{b\in[d]\\y\in[m]}}$ on Bob's side s.t.:*

$$p(ab|xy) = tr(\rho_{AB} M_{a|x} \otimes M_{b|y}),\ \forall\ a,b \in [d] \text{ and } \forall\ x,y \in [d]. \tag{C.8}$$

The set $\mathcal{Q}$ of all quantum behaviours is named Quantum set.

Remark C.3. *As we are not upper bounding the Hilbert space's dimensionality, we are able to purify [15, 132] the state ρ_{AB} and instead POVM's, working only with projective measurements (see Appendix A). In this sense, if Eq. (C.8) is valid, one can rewrite it in the following form:*

$$p(ab|xy) = \langle\psi|\Pi_{a|x} \otimes \Pi_{b|y}|\psi\rangle,\ \forall\ a,b \in [d] \text{ and } \forall\ x,y \in [d]. \tag{C.9}$$

where $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is a pure state shared by Alice and Bob, $\{\Pi_{a|x}\}_{\substack{a\in[d]\\x\in[m]}}$ is a projective measurement on Alice's side, and analogously $\{\Pi_{b|y}\}_{\substack{b\in[d]\\y\in[m]}}$ for Bob. Therefore $\boldsymbol{p} \in \mathcal{Q}$ if, and only if, Eq. (C.9) is valid.

It is clear that every quantum behaviour is non-signalling, and all local behaviours are quantum. Moreover, the example depicted at Eq. (C.7) can be used to show that there is a non-signalling behaviour that does not obey Eq. (C.9), *i.e.* it is not quantum. Therefore (see Fig. C.2):

$$\mathcal{L} \subset \mathcal{Q} \subset \mathcal{NS}. \tag{C.10}$$

In fact a lot of works in foundations of quantum theory could be exclusively rephrased in geometrical (see Fig C.2) terms[7]. Then, to close this Appendix, and to reinforce the role played by the tensor product itself, a bit of geometry and topology seems necessary, and cannot be hidden.

We summarize the simplest, and even then beautiful, results below[8]:

Proposition 11. *Given a Bell Scenario with 2 parts, $m \in \mathbb{N}$ measurements per part, and $d \in \mathbb{N}$ outcomes for each measurement, the following statements are true:*

[7] Or Algebraic Geometrical terms, since some quantum bounds are related to the Grothendick's constants [7–11, 34].
[8] We suggest [7] and [8, 9, 34] for the proofs.

1. *The local set $\mathcal{L}$ is a closed, bounded and convex polytope;*
2. *The quantum set $\mathcal{Q}$ is a closed, bounded and convex set;*
3. *The non-signalling set $\mathcal{NS}$ is a closed, bounded and convex polytope*

Remark C.4. *We call the reader's attention (see Fig. C.2) to the fact that $\mathcal{Q}$ is not, in general, a polytope! Even more, since $\mathcal{L}$ is a polytope, then it can be characterized by its extremal points,* i.e. *each point inside of it is a convex combination of those vertices. On the other hand, equivalently it may be completely described by its faces, meaning that each point inside $\mathcal{L}$ satisfies a given number of inequalities. Faces $F = \{\boldsymbol{p} \in \mathcal{L};\ \boldsymbol{s} \cdot \boldsymbol{p} = b\}$ of $\mathcal{L}$ such that $dim(F) = dim(\mathcal{L}) - 1$ are called facets of $\mathcal{L}$, and the correspondent inequalities defining it are known as* Bell Inequalities. *Therefore, in this sense, to violate a Bell Inequality meaning to be Non-Local.*

Appendix D

Graphs and Its Invariants

Since in this text, in many places, various words belonging to Graph Theory have appeared (Cliques, Theta Body, Lovász Number, Multigraph, Colourings...) and were indiscriminately used, and keeping on mind that anybody is not obligated to know them by heart, we will dedicate this Appendix to try to make all them clear. For those readers which are interested in a deeper approach to this subject, or are somehow curious in Graphs, we suggest [56–58] for accounts in Graph Theory itself, and [34, 36–39, 41] for outstanding approaches on Graphs Invariants and Combinatorial Optimization.

D.1 A bit of Graph Theory

Let us start with the following...

Definition 1. *A Graph G is a triple (E, V, φ) where $E \neq \emptyset$ is the set of edges, $V \neq \emptyset$ is vertex set, and*

$$\varphi : E \longrightarrow V \cup \binom{V}{2} \cup \binom{V}{3} ... \cup \binom{V}{|V|} \tag{D.1}$$

is the assignment function. Each element $e \in E$ is called an edge, and each $v \in V$ is called a vertex.

Remark D.1. *Note that our definition sets edges and vertices on the same foot. Everything might be and edge, and analogously everything might be a vertex. Connections among vertices by means of the edges is ruled by the assignment function φ.*

Our definition of a graph $G = (E, V, \varphi)$ it is not standard, since it encompass:

- loops: $e \in E,$ s.t. $\varphi(e) = v \in V$;
- ordinary edges: $e \in E,$ s.t. $\varphi(e) = \{u, v\} \in \binom{V}{2}$;
- multiple-edges between two vertices $u, v \in V$: $e, e' \in E,$ s.t. $\varphi(e) = \{u, v\} = \varphi(e')$;
- hyperedges: $e \in E,$ s.t. $\varphi(e) = \{u_1, u_2, ..., u_k\} \in \binom{V}{k}$.

And albeit that, we believe that it is the best option to prepare the way to talk about simple graphs, multi and hypergraphs all together. We would like to remember the reader that all of

them have nowadays appeared constantly in Foundations of Quantum Mechanics: for instance, see [27–29, 45].

Definition 2. *A graph $G = (E, V, \varphi)$ is called to be a Simple Graph when:*

1. *φ is injective, and*
2. *$\varphi(E) \subset \binom{V}{2}$.*

Remark D.2. *Saying in other words, a Simple Graph has not either loops, or multi-edges, or hyperedges. Since in a simple graph there is a injective function between E and $\binom{V}{2}$, it is tacitly understood that an edge* is *a unordered pair of vertices, therefore the assignment φ is never mentioned and the graph is identified with the pair a $G = (E', V)$ where $E' \subset \binom{V}{2}$. We will adopt this convention when there is no risk of misunderstood.*

Definition 3. *A graph G is called to be a Multigraph when there exist at least one multiple-edges between a pair of vertices. Analogously, G is a Hypergraph when there is at least one hyperedge among the vertices of G.*

Now it is time to talk about *cliques* in G, but first we must define the central concept of adjacency between (or among) vertices:

Definition 4. *Given a graph $G = (E, V, \varphi)$, one says that $v, u \in V$ are adjacent, or are connected, when there is $e \in E$ s.t. $\{u, v\} \subset \varphi(e)$. The set $N(v) = \{u \in V;\ u \text{ is adjacent to } v\}$ is called the neighbourhood of v.*

Remark D.3. *When $i, j \in V$ are adjacent, we write $i \sim j$.*

Definition 5. *Given a graph $G = (E, V, \varphi)$, one says that a subset $X \subset V$ is a clique when all pair $u, v \in X$ are adjacent.*

On the other hand:

Definition 6. *Given a graph $G = (E, V, \varphi)$, one says that a subset $A \in V$ is an independent set when all pair $u, v \in A$ are non-adjacent.*

Remark D.4. *A Clique is a set where everybody is connected with everybody, and an Independent set is a set where every member is not connected each other.*

In the light of the observation above, a Clique and an Independent set are instances of two extreme structures arising from graph theory. Intermediate constructions, which are present at the core of the thesis, are the following [56]:

Definition 7. *A path $P = (E, V)$ is a simple graph whose vertices can be arranged in a linear sequence such a way that two vertices are adjacent if, and only if, they are consecutive in that sequence.*

Definition 8. *A cycle $C = (E, V)$ is a simple graph, with $|V| \geq 3$, whose vertices can be arranged in a cyclic sequence in a such way that two vertices are adjacent if, and only if, they are consecutive in the sequence.*

Other important concept is that of (induced) Subgraph. Roughly speaking, a subgraph is a graph inside another graph, whereas an induced subgraph is a graph S that can be obtained from G removing some vertices or some edges. In order to turn these statements more precise, we need some graph operations first:

Definition 9. *Given a graph $G = (E, V, \varphi)$ and an edge $e \in E$, the graph (F, V, ψ) with the same vertex set V, defined putting:*

- $F = E - \{e\}$;
- $\psi = \varphi|_F$

is denoted by $G - e$, and we say that the edge e was removed from G. $G - e$ is called an edge-deleted subgraph.

Definition 10. *Given a graph $G = (E, V, \varphi)$ and a vertex $v \in V$, the graph (F, W, ψ) defined setting:*

- $W = V - \{v\}$;
- $F = \{e \in E;\ \varphi(e) \cap \{v\} = \emptyset\}$;
- $\psi = \varphi|_F$,

is denoted by $G - v$, and we say that the vertex v was removed from G. $G - v$ is called a vertex-deleted subgraph.

Remark D.5. *Note that when a vertex is removed from a Graph, every edge that touch that vertex is removed as well.*

In general:

Definition 11. *Given a graph $G = (E(G), V(G), \varphi)$, we say that $H = (E(H), V(H), \psi)$ is a subgraph of G when:*

- $V(H) \subset V(G)$;
- $E(H) \subset E(G)$;
- $\psi = \varphi|_{E(H)}$.

When H is a subgraph of G we write $H \subset G$.

As we have said before, two concepts deserve contrast:

Definition 12. *A subgraph obtaied by vertex deletions only is called an induced subgraph, whereas a subgraph obtained by edge deletions only is called a spanning subgraph.*

By the last, we formalize the central of colourings:

Definition 13. *Given a graph $G = (E, V, \varphi)$, a colouring with M colours for the edges of G is a function*

$$C : E \longrightarrow [M] \tag{D.2}$$

such that $C(E) = [M]$. Furthermore, we say that C is a proper colouring for the edges of G when:

$$C(e) \neq C(e'),\ \forall\ e, e' \in E\ s.t.\ \varphi(e) \cap \varphi(e') \neq \emptyset. \tag{D.3}$$

D.2 Some Invariants

Once again, we stress that here we only focus on that invariants which appear in the main text of the present work, or those that were implicitly used/discussed and could have raised a couple of questions and misunderstood. If the reader has a deeper interest on Graphs Invariants in general, and in their relationship with Optimization and Complexity, we strongly suggest [36, 38]. The reference [34] shows brightly how to applying some of them on foundations of quantum theory, and accordingly might be of the interest of some of the readers. So, let us begin with the following...

Definition 14. *Given a simple graph $G = (V, E)$, the independence number [56] of G is defined by:*

$$\alpha(G) = \max\{|A|;\ A \subset V \text{ is an independent set of } G\}. \tag{D.4}$$

Remark D.6. *When G is a simple graph together with a weight function $\omega : V \longrightarrow [0, 1]$, then one can change the above definition to bear that new information. All one has to do is to perform the optimization above, but now seeking for the independent set whose the sum of weights is as large as possible.*

Definition 15. *Given a simple graph $G = (V, E)$, the fractional packing [34, 36] number of G, denoted by $\alpha^*(G)$, is defined by:*

$$\alpha^*(G) = max\left\{\sum_{i=1}^{|V|} x_i\right\} \tag{D.5}$$

where the maximum is taken over all assignments $x : V \longrightarrow \mathbb{R}$ such that $x \geq 0$ and $\sum_{v \in K} x(v) \leq 1$ for all cliques $K \subset V$ (see Def. 17 below).

Now, among various different definitions to the same invariant, (see [36, 41]) we pick out that one which fits better in our purposes:

Definition 16. *Given a simple graph $G = (V, E)$, the Lovász number of G, denoted by $\vartheta(G)$, is defined by:*

$$\vartheta(G) = \max\left\{\sum_{i=1}^{|V|} (\boldsymbol{d} \cdot \boldsymbol{x_i})^2\right\}, \tag{D.6}$$

where the maximum extends over all normalized vectors $\boldsymbol{d}$, and all assignments $x : V \longrightarrow \mathbb{R}^n$ such that $\|\boldsymbol{x_i}\| = 1$ and:

$$\boldsymbol{x_i} \cdot \boldsymbol{x_j} = 0,\ \text{whenever } i \text{ is adjacent to } j. \tag{D.7}$$

Remark D.7. *We would like to remark two points:*

1. *Given a graph G, assignments such as those presented in Eq. (D.7) are called orthonormal representations of $\bar{G}$. And the idea behind these representations for a graph*[1] *G, which born with Lovász in 1979, is to codify a graph inside of a vector space, and using orthogonal subspaces to distinguish vertices that cannot be confused each other. Indeed, Lovász's original idea was to find an upper bound (in polynomial time) the Shannon Capacity of a Graph [41].*

2. *Using the Dirac's notation, we may rewrite (D.6):*

$$\vartheta(G) = \max\left\{\sum_{i=1}^{|V|}\langle d|\Pi_i|d\rangle\right\} \tag{D.8}$$

where each $\Pi = |v_i\rangle\langle v_i|$. Therefore, $\vartheta(G)$ can be somehow seen as the best association of quantum probabilities descriptions for the graph G. It will be good keep this idea on mind.

We could also take other route to reach the same end. See:

Definition 17. *Given a simple graph $G = (V, E)$, an assignment $x : V \longrightarrow \mathbb{R}$ is a real labelling of G. When:*

- *is given a subset $U \subset V$, and x satisfies*

$$x(v) = \begin{cases} 1 \text{ if } v \in U; \\ 0 \text{ if } v \notin U; \end{cases} \tag{D.9}$$

  x is called a characteristic labelling for U;

- *x is a characteristic labelling for a independent set $A \subset V$, then x is called a stable labelling;*

- *x is a characteristic labelling for a clique $K \subset V$, then x is called a clique labelling.*

Definition 18. *Given a simple graph G we define:*

- $STAB(G) = convhull(\{x; x \text{ is a stable labelling of } G\})$;

- $QSTAB(G) = \{x \geq 0;\ \sum_{v\in K} x(v) \leq 1 \text{ for all cliques } K \subset V\ \}$;

- $TH(G) = \left\{x \geq 0;\ \sum_{v\in V} \frac{a(v)_1^2}{\|a(v)\|^2} x(v) \geq 1 \text{ for all orthogonal representations of } G\right\}$.

Remark D.8. *$QSTAB$ was first defined by Shannon [46], and the first study of $STAB$ was performed in [47]. The theta body of a graph $TH(G)$ was first defined by Grötschel, Lovász and Schrijver in [42].*

After these definitions, we are able to formulate the sandwich theorem:

Proposition 19 ([36]). *Given a simple graph G, then $TH(G)$ is sandwiched between $STAB(G)$ and $QSTAB(G)$:*

$$STAB(G) \subset TH(G) \subset QSTAB(G). \tag{D.10}$$

Now, following this path, it is time to reach the same end, *i.e.* the same invariants as shown at Defs. 14, 15, and 16:

[1] Not its complement $\bar{G}$.

Definition 20. *Given a simple graph $G = (V, E)$ and a weight function $\omega : V \longrightarrow [0, 1]$ we define:*

$\widetilde{\vartheta}(G, \omega) = \max\{\sum_{v \in V} x(v)\omega(v);\ x \in TH(G)\}$;

$\widetilde{\alpha}(G, \omega) = \max\{\sum_{v \in V} x(v)\omega(v);\ x \in STAB(G)\}$;

$\widetilde{\alpha^*}(G, \omega) = \max\{\sum_{v \in V} x(v)\omega(v);\ x \in QSTAB(G)\}$.

Remark D.9. *When $\omega(v) = 1$, for all $v \in V$, we write $\widetilde{\vartheta}(G, \omega) = \widetilde{\vartheta}(G)$, and analogously to $\widetilde{\alpha}(G, \omega)$ and $\widetilde{\alpha^*}(G, \omega)$.*

As the reader can imagine, we can drop the $\sim$ symbol over the invariants:

Proposition 21. *Given a simple graph $G = (V, E)$, then:*

$$\widetilde{\vartheta}(G) = \vartheta(G) \qquad \widetilde{\alpha}(G) = \alpha(G) \qquad \widetilde{\alpha^*}(G) = \alpha^*(G). \tag{D.11}$$

Furthermore, the Proposition 19 guarantees that:

$$\alpha(G) \leq \vartheta(G) \leq \alpha^*(G). \tag{D.12}$$

We close this Appendix enunciating a version of a theorem, proposed by Cabello-Severini-Winter [27, 28], connecting Graph Theory (and its invariants) with Foundations of Operational Theories:

Theorem 22. *Given S corresponding to a Bell or Non-Contextual Inequality, the maximum value of S for classical (LHV and NCHV) theories, Quantum Theories (QT), and More General Probabilistic Theories satisfying the Exclusivity Principle (EP)[2] is give by:*

$$S \overset{LHV,\ NCHV}{\leq} \alpha(G, \omega) \overset{Q}{\leq} \vartheta(G, \omega) \overset{EP}{\leq} \alpha^*(G, \omega), \tag{D.13}$$

where (G, ω) is the weighted exclusivity (simple) graph (see Chap 1) associated with the inequality S.

[2] The idea behind this principle is the following: the sum of the probabilities for exclusive events cannot surpass 1. See [27–29, 34].

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