Universitat Autònoma de Barcelona

Entanglement, non-locality and quantum maps in systems of indistinguishable particles

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Entanglement, non-locality and quantum maps in systems of indistinguishable particles

by
Carlo Marconi

under the supervision of

Prof. Anna Sanpera Trigueros

A thesis submitted in partial fulfillment for the degree of
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A mia madre, a mia sorella, a Nicola.
A tutte le persone che sono casa.

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Resum

L'entrellaçament quàntic i la no localitat representen dos dels fenòmens més sorprenents de la física quàntica, la importància dels quals es reconeix no només des d'un punt de vista conceptual, sinó també a la llum de les seves aplicacions en diversos protocols d'informació quàntica. Per aquesta raó, trobar criteris per a la caracterització d'aquests fenòmens en sistemes de molts cossos és una qüestió molt important. Malauradament, ja en el cas de sistemes de baixa dimensió, aquesta tasca sol ser extremadament difícil de resoldre i, de fet, s'ha demostrat que la seva solució és NP-difícil (NP-hard) en el cas general. Una estratègia típica per simplificar el problema és considerar sistemes dotats de simetries en què sembla raonable esperar que un grau d'ordre més gran pugui resultar en una reducció de la complexitat del problema original. En aquesta tesi, investiguem la caracterització de l'entrellaçament i de les correlacions no locals en sistemes de partícules indistingibles, els estats dels quals, anomenats simètrics, són invariants sota qualsevol intercanvi de les parts.

En primer lloc, en el context de la detecció d'entrellaçament, establim una dualitat formal entre el problema de separabilitat per a estats simètrics de dos qudits en dimensió arbitrària i la teoria de matrius copositives. Aquesta correspondència és particularment valuosa per detectar estats entrellaçats que són positius sota transposició parcial (PPTES) i per relacionar les propietats dels entanglement witnesses (testimoni d'entrellaçament) que els detecten amb les de les matrius copositives associades. La dualitat entre aquests conceptes permet generar famílies d'estats simètrics PPTES entrellaçats en dimensió arbitrària i pot ser explotada a més utilitzant tècniques de semidefinit programming per generar exemples de matrius copositives excepcionals, la caracterització de les quals sol ser molt difícil.

En segon lloc, investiguem la robustesa de la no localitat en sistemes simètrics

de molts cossos que interactuen amb un entorn extern. Utilitzant desigualtats de Bell, demostrem que les correlacions no locals no només sobreviuen en presència de soroll tèrmic, sinó també en el cas d'estats estacionaris de no-equilibri. A més, inspeccionem un escenari on el sistema de molts cossos se sotmet a mesures repetides, demostrant que, fins i tot en aquest cas, la no-localitat sobreviu a l'efecte de la dissipació durant un temps curt, encara que significatiu.
Finalment, la darrera part d'aquesta tesi ha estat dedicada a l'anàlisi de les xarxes neuronals quàntiques del tipus atractor (aQNNs). En aquest cas, atesa la complexitat del model, les simetries són fortament desitjables per reduir la intrincació original del problema. Sota aquestes hipòtesis, demostrem que el rendiment de les aQNNs es pot estudiar utilitzant eines de la teoria de recursos de la coherència, les quals proporcionen el marc idoni per analitzar les propietats dels mapes quàntics que descriuen l' evolució de les aQNNS.

Resumen

El entrelazamiento y la no localidad representan dos de los fenómenos más sorprendentes de la física cuántica, cuya importancia se reconoce no sólo desde un punto de vista conceptual, sino también a la luz de sus aplicaciones en diversos protocolos de información cuántica. Por esta razón, encontrar criterios para la caracterización de dichos fenómenos en sistemas de muchos cuerpos es una cuestión de suma importancia. Tipicamente, ya incluso para sistemas de baja dimensión, esta tarea suele ser extremadamente difícil de resolver y, de hecho, se ha demostrado que determinar si un sistema es entrelazado es NP-difícil en el caso general. Una estrategia típica para simplificar este problema es considerar sistemas dotados de simetrías en los que parece razonable esperar que un mayor grado de orden pueda resultar en una reducción de la complejidad del problema original. En esta tesis, investigamos la caracterización del entrelazamiento y de las correlaciones no locales en sistemas de partículas indistinguibles, cuyos estados, denominados *simétricos*, son invariantes bajo cualquier intercambio de las partes.

En primer lugar, en el contexto de la detección de entrelazamiento, establecemos una dualidad formal entre el problema de separabilidad para estados simétricos bipartitos en dimensión arbitraria y la teoría de matrices copositivas. Dicha correspondencia es particularmente valiosa para detectar estados entrelazados que son positivos bajo transposición parcial (PPTES) y para relacionar las propiedades de los entanglement witnesses (testigos de entrelazamiento) que los detectan con las de las matrices copositivas asociadas. La dualidad entre estos conceptos permite generar familias de estados simétricos bipartitos PPTES en dimensión arbitraria, y permite utitzando técnicas de semidefinite programming generar ejemplos de matrices copositivas excepcionales, cuya caracterización suele ser muy difícil.

En segundo lugar, investigamos la robustez de la no localidad en sistemas simétricos

de muchos cuerpos que interactúan con un entorno externo. Utilizando desigualdades de Bell, demostramos que las correlaciones no locales sobreviven no sólo en presencia de ruido térmico, sino también en el caso de estados estacionarios de no-equilibrio. Además, inspeccionamos un escenario en el que el sistema de muchos cuerpos se somete a medidas repetidas, demostrando que, incluso en este caso, la no-localidad sobrevive al efecto de la disipación durante un tiempo corto, aunque significativo.
Finalmente, la última parte de esta tesis ha sido dedicado al análisis de las redes neuronales cuánticas llamadas atractoras (aQNNs). En este caso, dada la complejidad del modelo, las simetrías son fuertemente deseadas para reducir la intrincación original del problema. Bajo estas hipótesis, demostramos que el rendimiento de las aQNNs puede estudiarse utilizando herramientas de la teoría de recursos de la coherencia, que proporciona un marco conveniente para analizar las propiedades de los mapas cuánticos que describen la evolución de las aQNNS.

Abstract

Entanglement and non-locality represent two of the most striking phenomena of quantum physics whose importance is acknowledged not only from a conceptual point of view but also in light of their applications in a variety of quantum information protocols. For this reason, finding criteria for their characterisation in many-body systems, is a question of uttermost importance. Unfortunately, already in the case of low dimensional systems, this task is usually extremely difficult to solve and indeed, its solution has been proven to be NP-hard in the general scenario. A typical strategy to circumvent this drawback is to consider systems endowed with symmetries where it seems natural to expect that a higher degree of order might result in a reduced complexity of the original problem. In this thesis, we investigate the characterisation of entanglement and non-local correlations in systems of indistinguishable particles, whose states, dubbed *symmetric*, are invariant under any exchange of the parties.

First, in the context of entanglement detection, we establish a formal duality between the separability problem for two-qudit symmetric states in arbitrary dimension and the theory of copositive matrices. Such correspondence is particularly valuable to detect entangled states which are positive under partial transposition (PPTES) and to relate the properties of the entanglement witnesses that detect them with those of the associated copositive matrices. The duality between these concepts allows to generate families of two-qudit symmetric PPTES states in arbitrary dimension and can be further exploited with semidefinite programming techniques to generate examples of exceptional copositive matrices, which are typically hard to characterise.

Second, we investigate the robustness of non-locality in symmetric many-body systems which interact with an external environment. Using Bell inequalities we

show that non-local correlations survive not only in the presence of thermal noise, but also in the case of non-equilibrium stationary states. Moreover, we inspect a scenario where the many-body system undergoes repeated measurements, showing that, also in this case, non-locality survives the effect of the dissipation for a short, although significant, time.
Finally, the last part of this thesis has been devoted to the analysis of the so-called attractor quantum neural networks (aQNNs). In this case, given the complexity of the model, symmetries are strongly desired to reduce the original intricacy of the problem. With this assumptions, we show that the performance of aQNNs can be studied using tools of the resource theory of coherence, which provides a convenient framework to inspect the properties of the quantum maps that describe the evolution of aQNNS.

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Declaration

I declare that this thesis has been composed by myself and that this work has not been submitted for any other degree or professional qualification. I confirm that the work submitted is my own, except where work which has formed part of jointly-authored publications has been included. My contribution and those of the other authors to this work have been explicitly indicated below. I confirm that appropriate credit has been given within this thesis where reference has been made to the work of others.

List of Publications

[MAT+21] C. Marconi, A. Aloy, J. Tura, and A. Sanpera, "Entangled symmetric states and copositive matrices", Quantum **5**, 561 (2021).

[MRS+22] C. Marconi, A. Riera-Campeny, A. Sanpera, and A. Aloy, "Robustness of nonlocality in many-body open quantum systems", Phys. Rev. A **105**, arXiv:2202.12079, L060201 (2022).

[MSD+22] C. Marconi, P. C. Saus, M. G. Díaz, and A. Sanpera, "The role of coherence theory in attractor quantum neural networks", Quantum **6**, 794 (2022).

In preparation:

C. Marconi, A. Sanpera and J. Tura, "Generating exceptional copositive matrices via semidefinite programming".

C. Marconi, J. Tura and A. Sanpera, "Symmetric PPT bound entangled states of two qudits in $d < 5$".

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Acknowledgments

When I think about the word Ph.D. the first thing that comes to my mind is that it might be an acronym for pretty much anything except “Philosophiae Doctor”. It certainly starts being an acronym for a Ph.ysicist’s D.ream: everything shines the light of new beginnings, your head is filled up with words you did not even know could possibly exist and you start wondering how you will be able to keep up with the amount of information that you receive every day. But it does not matter: Ph.ysics D.emands commitment, and you are eager to obey. So you begin to move your first steps in this world, desperately looking for a balance between the heap of work on your desk (Ph.ysics D.ictates) and your social life (Ph.ysicists D.rink). After your first and a half year, you have already realised that you are likely to be remembered more for your language learning skills (Ph.ilology D.eserved a chance) than for the results of your research. After all, no surprises: Ph.ysics D.isappoints. You have accumulated so much frustration that resentment is your only engine. You feel betrayed: Ph.ysics D.eserted you, there is nothing else left to do. For quite some time I thought that this would be the only possible ending for this story, a tragedy in three acts titled: “Ph.D., a tale of Ph.ysical D.eterioration”. But then something changed, so abruptly that before I even had the time to figure it out, all the discouragement piled up over the years had been replaced by that curiosity which is probably the most human of our instincts. I thought it was the thrill of my first publication. I was wrong. It was thanks to the constant support of many people that the word Ph.D. has finally turned into a much nicer acronym, something like Ph.ysics D.elights (or, if nothing else, Ph.ew, I D.id it).

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Contents

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Introduction

Vi arriva il poeta
e poi torna alla luce con i suoi canti
e li disperde.
Di questa poesia
mi resta
quel nulla
di inesauribile segreto.

Giuseppe Ungaretti

Among all human features, curiosity is arguably the noblest. Long before the first examples of civilisations, humans have always been fascinated by the surrounding world and, to some extent, our existence is nothing but a constant attempt to explain what we feel or what we see. It is often argued that poetry, music and Art in general should be concerned only with emotions, while physics, mathematics and Science should deal exclusively with empirical observation. To some extent, this remark is undoubtedly true: after all, applying logical reasoning to feelings would have little result if not to convert mankind into an insensitive army of robots. However, drawing such a neat line between these disciplines, seems to suggest that certain features, that are typically associated with the world of Humanities, cannot be shared by the realm of Science, conventionally depicted as an exciting,

although intrinsically arid, field. Nevertheless, it should be stressed that physics is not less concerned about beauty than what Art is, and indeed, the elegance of a mathematical proof is often regarded as an additional confirmation of the correctness of a result. Even more important is the role played by symmetry. In the same way as ancient Greeks regarded certain proportions as perfect, physicists know that symmetries are a hint of some interesting underlying features. Clearly, being physics a scientific discipline, symmetries are also envisaged as a mathematical tool to reduce the intrinsic complexity of certain problems and intuitively, it seems a reasonable assumption that systems displaying a certain degree of order would be, *a priori*, easier to treat. This is particularly evident in quantum physics, where the characterisation of some phenomena, such as entanglement and non-local correlations, is often a hard task already for simple systems, and dealing with symmetric systems typically yields a great advantage. It is in this spirit that the present thesis should be understood: symmetry is not only an elegant way that allows for a nicer mathematical treatment of certain problems, but is often a necessary assumption to be able to deal with the inherent complexity of quantum phenomena.
In the following, we present the structure of this thesis. We provide a general overview of the state of the art of the topics we cover, namely, entanglement characterisation, non-locality detection and quantum neural networks, along with a concise presentation of our results for each section.

1.1 The separability problem

1.1.1 State of the art

By the time of its first appearance in 1935 [EPR35; Sch35], the phenomenon of *entanglement* was initially regarded as a problem related to an incompleteness of quantum theory. The impossibility to describe the state of a quantum particle independently of the ones of other subsystems strongly clashed with the ideas of classical physics, where the knowledge of a composite system as a whole implies complete information about its constituents. Quoting E. Schrödinger, one of the fathers of quantum mechanics, "best possible knowledge of a whole does not include best possible knowledge of its parts — and this is what keeps coming back to haunt us" [Sch35]. It was only half a century later, with the advent of the new field of quantum information theory, that the central role of entanglement was acknowledged in a plethora of applications ranging from quantum cryptography [Eke91; GRT+02] and quantum teleportation [BBC+93] to entanglement swapping [ZZH+93] or measurement-based quantum computation [RB01], just to name a few. Thanks to the recent progress in quantum control, entangled states have been achieved not only for systems of few particles [LKS+05; HHR+05; LZG+07] but also for many-body systems [HSS+99; MGW+03; AFO+08; MZH+15] and, recently, even for "macroscopic" objects [LSS+11; KPS+21]. For this reason, the so-called *separability problem*, that is, deciding whether a given quantum state is separable or entangled, is a relevant question not only due to its theoretical implications but also in light of its experimental applications. Over the years, it has become clear that entanglement characterisation is a challenging task [HHH+09]. Moreover, it cannot be quantified by a unique measure. The exception lies in (bipartite) pure entangled states where it is trivial to determine if the state is entangled and, being in this case all entanglement measures equivalent, entanglement entropy is the only measure needed [NC10; BZ06]. Interestingly, in the asymptotic limit, for a sufficient number of copies of the system, the entanglement entropy measures the resource interconversion capacity between different pure states, within the paradigm of local operations and classical communication [BBP+96a]. However, already in the case of bipartite mixed states, two such measures are needed to quantify this interconversion rate: the entanglement of formation and the entanglement of distillation.

A closely related, although inherently different, approach is the characterisation of entangled states independently of any measure or of their usefulness for a specific task. In this context, the characterisation of entangled states has been proven to be NP-hard, in the general case [Gur03]. However, partial characterisation has been achieved employing criteria that provide necessary, but not sufficient, conditions to determine if a given state is entangled or not. The most powerful of such criteria, formulated in terms of linear positive maps, is the positivity under partial transposition (PPT) [Per96], which is the paradigmatic example of a positive, but not completely positive map [Cho75; Wor76]. States that do not fulfil the PPT criterion are entangled but the converse is not true, except for low dimensional cases [HHH96]. In this regard, quantum maps and their associated entanglement witnesses (EWs), provide the strongest criteria for entanglement characterisation: a quantum state is entangled if, and only if, there exists an EW that detects it [TV00; LKC+00; CS14]. Crucially, in order to characterise entanglement in states that do not break the PPT criterion, dubbed *PPT-entangled* states (PPTES), it is necessary to construct non-decomposable EWs [LKH+01]. Interestingly, EWs have been shown to provide also a measure of entanglement which is upper and lower bounded by other entanglement measures [Bra05].

Another possible approach is the method proposed in [DPS02; DPS04], based on the construction of PPT-symmetric extensions, which allows recasting the separability problem in terms of a semidefinite program (SDP). Remarkably, this technique provides numerical solutions in the case of relatively small systems, although it becomes computationally demanding when the dimension of the system under investigation grows. Moreover, it cannot be used to characterise families of entangled states, but only to check the separability of specific instances of quantum states.

Nowadays, it is still unclear whether, in general, the problem of entanglement characterisation remains equally hard for systems displaying some symmetries [VW01; TG10; TV00; EW01; CK07; Yu16; QRS17; TAQ+18; MAT+21]. A possible approach in this direction is to investigate if, and how, symmetries can help to construct EWs for such systems. A natural choice in this sense is to consider permutationally invariant systems and, more specifically, a subclass of them whose states, dubbed *symmetric*, are invariant under any permutation of the parties. Such states have a clear physical meaning since they provide a natural description for sets of indistinguishable particles, i.e., bosons. The first entanglement characterisation for symmetric states of two qudits was given in [Yu16], where it was discussed the case of particularly simple symmetric states, said *diagonal symmetric* (DS), that correspond to mixtures of projectors on symmetric states. The analysis performed in [TAQ+18] is also particularly valuable for at least two reasons: i) it shows that the separability property of a two-qudit DS state ρ_{DS}, represented by a $d^2 \times d^2$ matrix, can be recast in terms of an associated $d \times d$ matrix $M(\rho_{DS})$, thus confirming the role of symmetry in simplifying the complexity of the original problem; ii) it proves that there exists a class of matrices, known as copositive, which act as entanglement witnesses for DS states. As a consequence, the separability problem for a state ρ_{DS} can be recast as the equivalent problem of checking the membership of its related matrix $M(\rho_{DS})$ to the cone of the so-called completely positive matrices. Notice that checking the membership to this latter cone is still an NP-hard problem, an observation which is consistent with the result provided in [Gur03]. Nevertheless, the reduced dimension of the matrix $M(\rho_{DS})$ offers a great simplification for numerical calculations, thus reducing the computational cost of the original task.

1.1.2 Main results

In chapter 3 we study the separability problem for two qudits of arbitrary dimension in the symmetric subspace. Our analysis is articulated in two steps. First, we complement the analysis tackled in [TAQ+18], further exploring the possibility to use copositive matrices as EWs for DS states. To this end, we first introduce the basic notions regarding the theory of copositive matrices and provide an explicit method to derive an EW, starting from a matrix of this class. Moreover, we establish a link between the properties of the copositive cone and the features of the related EWs. Specifically, we prove that: i) copositive matrices that can be decomposed as the sum of a positive semidefinite and a non-negative matrix, lead to decomposable EWs; ii) copositive matrices that do not admit such decomposition, dubbed *exceptional*, correspond to non-decomposable EWs, and iii) *extreme* copositive matrices, i.e., those that are extremal in the copositive cone, lead to optimal EWs. This analysis further extends the previous work regarding the entanglement characterisation for DS states, offering valuable insights about the properties that a copositive matrix must satisfy in order to define a valid EW.

Second, we investigate the existence of two-qudit PPT-entangled states in the symmetric subspace, focusing on the first non-trivial case, i.e., $d = 3$. Making use of both analytical and numerical techniques, we provide a new family of two-qutrit PPT-entangled states, along with the expression of the non-decomposable EW that is able to detect it. We conjecture that any symmetric PPT-entangled state of two qutrits must belong to such family, a conjecture which is strongly supported by numerical evidence. It is important to remark that, to the best of our knowledge, there are no known examples of non-decomposable EWs for generic symmetric states, with the sole exception of few examples [TG10], which have been found numerically using weaker entanglement criteria [LKH+01; SBL01; Cla06; KO12; CĐ11; MMO10]. For this reason, our work offers a complementary approach to the characterisation of the entanglement in the symmetric subspace of two qudits. These results are part of the published paper [MAT+21] which is a joint collaboration with Albert Aloy, Jordi Tura and Anna Sanpera. Finally, in Appendix A, we present a method, based on the technique proposed in [DPS02], to recast the search for exceptional copositive matrices as an SDP problem. Since the characterisation of such matrices is, in general, an NP-hard problem, our method provides an alternative tool to find new examples of exceptional copositive matrices of order d for $d \geq 5$.

1.2 Non-locality in open quantum systems

1.2.1 State of the art

Strictly related to entanglement, the concept of *non-locality* represents one of the most intriguing phenomena of Nature, in which local measurements on a shared resource lead to correlations that cannot be explained by any local realistic theory [Bel64]. Such correlations, dubbed as *non-local*, are of uttermost importance not

only from a foundational point of view but also as a resource for technological applications, ranging from device-independent quantum key distribution [Eke91; BHK05; SGB+06] and shared randomness generation [CR12] to quantum communication protocols [SGB21]. Operationally, this resource is assessed by means of Bell inequalities [BCP+14] whose violation signals unequivocally the presence of non-local correlations.
Entanglement and non-locality are known to be related but non-equivalent resources for any number of parties [BGS05; VB14; ADT+15; FVM+19]: while every non-local state is entangled, the converse is not necessarily true if the state is mixed, and it still remains unclear the intimate nature of such connection. In the last two decades, following the development of quantum platforms that allow for the control and manipulation of large systems of particles, the study of entanglement in many-body systems has become a major trend in modern physics. While on the one hand, this has led to seminal insights into the physics of condensed matter and material science, on the other, the role of non-local correlations in many-body systems has remained widely unexplored, with the sole exception of few significant advances [TAS+14; LSA12; TDA+17]. The reasons behind this gap are several. First, the characterisation of non-locality in many-body systems typically requires the construction of N-body correlators [ŻB02; WW01], which in general poses an unrealistic task within the current technological capabilities. Second, the complexity of this task grows with the dimension of the system, resulting in an NP-complete problem in the general case [BFL91]. Nevertheless, recent progress has been achieved by constructing many-body Bell inequalities that are constrained by symmetries and involve only one- and two-body correlators [TAS+14; TAS+15; ATB+19; PAL+19], an advance that has led to the experimental detection of Bell correlations in some many-body quantum systems [SBA+16; EKH+17; SLS+21].

All the above examples, typically refer to ground states or excited states of isolated many-body systems. For this reason, a natural question is whether the interaction with an environment results in a decay or an enhancement of non-local correlations. Besides its theoretical implications, an answer to this question would bring key insights at an operational level, especially in view of the recent idea to use non-locality as a resource in the so-called Device-Independent (DI) framework. The DI framework exploits the operational assessment of non-locality in order to perform quantum information processing tasks without the need to require trust in their implementation. At first sight, the features of the DI framework make non-locality the ideal tool for the certification of genuinely quantum properties in noisy environments such as the emergent quantum technological platforms [AM16; ABG+07]. However, given the fragile nature of quantum correlations, one is tempted to believe that non-locality is lost when the quantum system is allowed to interact with an external environment with many degrees of freedom. In this thesis, we prove that this is not the case and show that non-locality can be detected also in many-body open quantum systems (OQS).

1.2.2 Main results

In chapter 4, we investigate the presence of non-local correlations in open quantum systems. The standard setting for an OQS [BP+02] consists of a quantum system coupled to an external environment, typically acting as a bath/reservoir at inverse temperature $\beta = 1/\kappa_B T$. Of particular interest, especially in the context of quantum thermodynamics, is to consider a scenario that may give rise to non-equilibrium steady states. Our analysis is structured as follows. First, we introduce a class of Bell inequalities, originally designed in [TAS+15] for symmetric many-body systems, which is the main tool that we use for non-locality detection. Then, we present the physical model that describes the many-body OQS under exam and inspect how the presence of the environment affects non-local correlations. In particular, we discuss the coupling with a thermal bath, as well as the case of non-thermal noise. Using quantum master equation methods, we inspect the presence of non-local correlations in the stationary states as well as in the dynamical regime, that is during the evolution that leads to the aforementioned stationary states. In both cases, we show that non-local correlations are present and can be detected by means of Bell inequalities involving only one- and two-body correlators. Finally, we investigate an adversarial scenario in which the principal system undergoes a series of repeated measurements. Also in this case, starting from a non-local state, we show that non-local correlations are robust under the presence of noise for a short, although significant, time. This result is particularly interesting in light of its potential application in the field of quantum cryptography. Indeed, the action of repeatedly measuring a system can be seen as the attempt of an eavesdropper to extract information, while remaining hidden. It is important to remark that, to the best of our knowledge, this is the first example of non-locality detection in open quantum systems, an observation which makes our analysis particularly valuable. These results are part of the published paper [MRS+22] which is a joint collaboration with Andreu Riera-Campeny, Anna Sanpera and Albert Aloy.

1.3 Quantum neural networks & quantum maps

1.3.1 State of the art

Modelled on the structure of the nervous system in animals, a neural network consists of n computational units, usually dubbed (artificial) neurons, interconnected between them. Analogously to the case of real biological systems, the computational power of artificial neural networks relies on the connections between neurons, a feature that makes them the ideal candidates in a variety of fields, such as pattern recognition [BBK10; CQ18], stock market predictions [GKD11; SSC14] as well as medical diagnosis [Kon01; SAL+03; ALP+13], just to name a few. Among the different types of artificial neural networks, an interesting class is represented by attractor neural networks (aNNs), where a collection of n Ising spins with binary states $s_i \in \{\pm 1\}$, dynamically evolve towards one of the states of minimal energy of the system [Ami89]. Such states are called *attractors* or *patterns*. Attractor neural networks display an exciting feature known as associative memory, that is, the capability to retrieve, out of a set of stored patterns, the state which is the closest to a noisy input according to the Hamming distance. Clearly, the larger the number of attractors, the greater the associative memory, i.e., the storage capacity of the network. When considering the quantum analogue of aNNs, called attractor quantum neural networks (aQNNs), classical bits are replaced by qubits which evolve under the action of a completely positive and trace-preserving (CPTP) map. The storage capacity of an aQNN then corresponds to the maximum number of stationary states of such a map. Adding quantum features like correlations, entanglement and superposition to the parallel processing properties of classical neural networks is expected to result in an enhancement of their performances [RDR+17; CCC+19; LAT21]. Indeed, an exponential increase in the storage memory of an aQNN, with respect to its classical counterpart, was already shown in [VM98] by means of quantum search algorithms. Also, in [RBW+18], the same result was recovered by using a feed-forward interpretation of the quantum Hopfield neural networks (for recent development of this model see [MNP20; CGA17]). More recently, in [LGR+21], the explicit form of the CPTP maps possessing the maximal number of stationary states was derived. Interestingly, such CPTP maps correspond to non-coherence-generating operations. Such observation motivates our choice of addressing aQNNs from a coherence-theoretic approach.

1.3.2 Main results

Within this framework, in chapter 5, we investigate the relation between the quantum maps that describe aQNNs and the resource theory of coherence. In particular, starting from the case of error-free aQNNs with maximal number of stationary states, we show that the related quantum maps correspond to genuinely incoherent operations (GIOs) and provide the expression for the unitary operators that allow for their physical implementation. Furthermore, we show that the equivalent of the Hamming distance in the quantum case is represented by the relative entropy between the input state and its closest attractor. Hence, we introduce the concept of the *depth* of the network, that is, the number of times the map has to be applied to retrieve faithfully the state which is the closest to the initial input, and show that is related to the decohering power of the corresponding map. Making use of this quantity, we provide some no-go results about the performances of error-free aQNNs. Finally, we tackle the above issues also in the realistic scenario of faulty aQNNs, i.e., when some error in the realisation of the network is taken into account. In this case, we prove that the corresponding quantum maps are described by either strictly incoherent operations (SIOs) or maximally incoherent operations (MIOs), a result which opens the possibility, in the latter case, for an enhancement of the performance of the network using coherence as an external resource. These results are part of the published paper [MSD+22] which is a joint collaboration with Pau Colomer Saus, María García Díaz and Anna Sanpera.

2

Preliminaries

Ho provato a parlare.
Forse, ignoro la lingua.
Tutte frasi sbagliate.
Le risposte: sassate.
Giorgio Caproni

In this chapter we introduce the main tools that we use in this thesis. In section 2.1, we provide a general overview of the formalism of quantum mechanics regarding the state of closed systems, their composition and their evolution. Moreover, we introduce quantum maps and their representations, a tool that we use extensively throughout this thesis. Section 2.2 is devoted to the theory of open quantum systems, i.e., the mathematical description of systems that are interacting with an external environment. The next two sections are dedicated to two of the most remarkable features of quantum theory, which also represent the main themes of this thesis: in section 2.3 we introduce the phenomenon of quantum entanglement, while section 2.4 deals with the related concept of non-locality. Finally, in section 2.5, we present the mathematical tools required to describe symmetric states, i.e., the states of systems of indistinguishable particles, which represent the general framework of this thesis.

2.1 Quantum states & quantum maps

2.1.1 Pure and mixed states

The first postulate of quantum mechanics asserts that every physical system S is associated to a complex Hilbert space $\mathcal{H}_S$. Hence, the state of S is represented by a unit vector $|\psi_S\rangle \in \mathcal{H}_S$, i.e., $\langle\psi_S|\psi_S\rangle = 1$. States of this kind are called *pure*, since they encode complete knowledge of the properties of the system S.
An equivalent description for the state of a quantum system S is provided by the *density operator* ρ_S, i.e., a positive semidefinite operator ($\rho_S \succeq 0$) with unit trace ($\mathrm{Tr}[\rho_S] = 1$) acting on $\mathcal{H}_S$. This formalism is particularly useful when dealing with quantum systems whose state is not completely known. For instance, one could imagine the case where a system might be found with probability p_k in some pure state $|\psi_k\rangle \in \mathcal{H}_S$. Hence, given the ensemble $\{p_k, \{|\psi_k\rangle\}\}_k$, the density operator ρ_S is defined as

$$\rho_S = \sum_k p_k |\psi_k\rangle\langle\psi_k| \, , \tag{2.1}$$

where the coefficients p_k satisfy $\sum_k p_k = 1, p_k \geq 0 \; \forall k$.
The state of a system described by Eq.(2.1) is called *mixed*. In the particular case when there is only one non-zero coefficient $p_k = 1$ in the sum, ρ_S reduces to a rank-one projector onto the pure state $|\psi_k\rangle$, i.e., $\rho_S = |\psi_k\rangle\langle\psi_k|$. It is a well known result that ρ_S corresponds to a pure state if and only if $\mathrm{Tr}[\rho_S^2] = 1$. Notice that the decomposition of Eq.(2.1) is not unique and different ensembles of pure states $\{p_k, \{|\psi_k\rangle\}\}_k$ may correspond to the same quantum state ρ_S.
If we denote as $\mathcal{B}(\mathcal{H}_S)$ the space of bounded linear operators over $\mathcal{H}_S$, the space of the density operators is defined as $\mathcal{D}(\mathcal{H}_S) = \{\rho_S \in \mathcal{B}(\mathcal{H}_S) \mid \rho_S \succeq 0, \mathrm{Tr}[\rho_S] = 1\}$. As a consequence of Eq.(2.1), any mixed state can be expressed as a convex combination of pure states. This result is particularly relevant because it implies that $\mathcal{D}(\mathcal{H}_S)$ is a convex set, meaning that for any $\rho_1, \rho_2 \in \mathcal{D}(\mathcal{H}_S)$ and any $\lambda \in [0, 1]$, it follows that $\lambda\rho_1 + (1-\lambda)\rho_2 \in \mathcal{D}(\mathcal{H}_S)$. Notice that not every state in $\mathcal{D}(\mathcal{H}_S)$ can be expressed as a linear combination of the other elements: those states that stand out for their impossibility to be decomposed are usually referred to as the *extreme* points of a convex set. Hence, from Eq.(2.1) we deduce that pure states, i.e., rank one projectors, are extreme points in the set of density operators.

2.1.2 Quantum measurements

The most general approach to describe measurements in quantum mechanics is by means of a collection of operators $\{M_m\}$, where $M_m : \mathcal{H} \to \mathcal{H}'$ is a so-called *measurement operator*, with associated outcome m. Measuring the state $|\psi_S\rangle$ with an operator M_m yields the outcome m with probability $p_m = \langle\psi_S|M_m^\dagger M_m|\psi_S\rangle$ and leaves the system in the state $|\psi_S^{(m)}\rangle$, given by

$$|\psi_S^{(m)}\rangle = \frac{M_m\,|\psi_S\rangle}{\langle\psi_S|M_m^\dagger M_m|\psi_S\rangle}\ . \tag{2.2}$$

Since $\sum_m p_m = 1$, the operators $\{M_m\}$ satisfy the completeness relation, i.e.,

$$\sum_m M_m^\dagger M_m = \mathbb{1}_S\ , \tag{2.3}$$

but they are not necessarily orthogonal. Eq.(2.2) can be easily generalised to density operators. In this case, assuming that a measurement M_m is performed on a density matrix ρ_S, the outcome m is obtained with probability $p_m = \mathrm{Tr}[M_m\rho_S]$, and the post-measurement state $\rho_S^{(m)}$ is given by

$$\rho_S^{(m)} = \frac{M_m\rho_S M_m^\dagger}{\mathrm{Tr}[M_m^\dagger M_m\rho_S]}\ . \tag{2.4}$$

If we are only interested in the outcome probabilities and not in the post-measurement state, quantum measurements can be described by means of positive operator-valued measurements (POVMs), defined as a collection $\{E_m, m\}$, where $\{E_m\}$ is a set of positive operators, i.e., $E_m \succeq 0$, fulfilling $\sum_m E_m = \mathbb{1}$. Notice that a POVM is not unique since there exists, in general, different collections of measurements operators $\{M_m\}$ such that $E_m = M_m^\dagger M_m \succeq 0$. As a consequence, while a POVM allows to compute unambiguously the probability p_m related to a certain outcome m, i.e., $p_m = \langle\psi_S|E_m|\psi_S\rangle$, the expression of the post-measurement state depends on the explicit choice of the measurements operators $\{M_m\}$ that implement the POVM.

2.1.3 Composite systems

The composition of quantum systems is described by means of the tensor product postulate, which states that, given two physical systems, A and B, the Hilbert space $\mathcal{H}_{AB}$ associated to the composite system $A + B$ is given by the tensor product of the Hilbert spaces of each subsystem, i.e., $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. As a consequence, if $\{|\psi_A^{(i)}\rangle\}, \{|\psi_B^{(i)}\rangle\}$ are orthonormal basis for the Hilbert spaces $\mathcal{H}_A, \mathcal{H}_B$, respectively, then the state of $A + B$ can be represented as

$$|\Psi_{AB}\rangle = \sum_{ij} c_{ij} |\psi_A^{(i)}\rangle \otimes |\psi_B^{(j)}\rangle \ , \tag{2.5}$$

where the coefficients $c_{ij} \in \mathbb{C}$ sastify the normalisation condition $\sum_{ij} |c_{ij}|^2 = 1$. In the particular case where there is only one coefficient, i.e., $c_{ij} \equiv c = 1$, Eq.(2.5) reduces to $|\Psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$. Equivalently, in the case of mixed states, the expression for the density operator $\rho_{AB} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ reads

$$\rho_{AB} = \sum_i p_m |\Psi_{AB}^{(m)}\rangle\langle\Psi_{AB}^{(m)}| \ , \tag{2.6}$$

where $\sum_m p_m = 1$ and $|\Psi_{AB}^{(m)}\rangle = \sum_{ij} c_{ij}^{(m)} |\psi_A^{(i,m)}\rangle |\psi_B^{(j,m)}\rangle$. If the systems A and B are uncorrelated, then Eq.(2.6) takes the simpler form

$$\rho_{AB} = \rho_A \otimes \rho_B \ , \tag{2.7}$$

where ρ_A, ρ_B are the density operators for the systems A, B, respectively.
Finally, the state of the subsystem A can be obtained from ρ_{AB} performing the *partial trace* over B, i.e.,

$$\rho_A = \mathrm{Tr}_B[\rho_{AB}] \ , \tag{2.8}$$

and similarly for the subsystem B. As we will see in the next section, Eq.(2.8) has several applications both in the context of entanglement certification as well as in the case of open quantum systems.

2.1.4 Evolution of quantum states

The evolution of a pure state $|\psi_S\rangle \in \mathcal{H}_S$ is ruled by the Schrödinger's equation, i.e.,

$$\frac{d}{dt} |\psi_S(t)\rangle = -\frac{i}{\hbar} H(t) |\psi_S(t)\rangle \ , \tag{2.9}$$

where the Hermitian operator $H(t)$ is the (time-dependent) Hamiltonian of the system and $\hbar$ is the Planck's constant, which in the following of this thesis will be set equal to 1. Due to the linearity of Eq.(2.9), its solution can be cast as

$$|\psi_S(t)\rangle = U(t, t_0) |\psi_S(t_0)\rangle \ , \tag{2.10}$$

where $U(t, t_0)$ is a unitary operator $(U(t, t_0)^\dagger = U(t, t_0)^{-1})$ fulfilling $U(t_0, t_0) = \mathbb{1}_S$. In the case of closed systems, an explicit expression for $U(t, t_0)$ can be found. First, let us cast the Hamiltonian $H(t)$ as

$$H(t) = H_0 + V(t) \ , \tag{2.11}$$

where we have distinguished between the time-dependent term, $V(t)$, and the "free" term, H_0. Then, let us consider the *interaction picture* where the representation $A_I(t)$ of a generic operator A evolves with H_0 according to

$$A_I(t) = e^{iH_0(t-t_0)} A(t) e^{-iH_0(t-t_0)} \ . \tag{2.12}$$

As a consequence, the representation of the Hamiltonian of Eq.(2.11) in the interaction picture is given by

$$H_I(t) = e^{iH_0(t-t_0)} V(t) e^{-iH_0(t-t_0)} \ . \tag{2.13}$$

Hence, the expression for $U(t, t_0)$ is given by [Dys49]

$$U(t, t_0) = \mathcal{T}\left[e^{-i\int_{t_0}^{t} dt' H_I(t')}\right] \ , \tag{2.14}$$

where $\mathcal{T}$ is the time-ordering operator which, in the case of two operators, is defined as

$$\mathcal{T}\left[H_I(\tau_1)H_I(\tau_2)\right] = \theta(\tau_1 - \tau_2)H_I(\tau_1)H_I(\tau_2) + \theta(\tau_2 - \tau_1)H_I(\tau_2)H_I(\tau_1) \ , \tag{2.15}$$

where $\theta(\tau)$ is the Heaviside function.
In the particular case where $H(t)$ is time-independent, i.e., $H_I(t) \equiv H$, Eq.(2.14) takes the simpler form

$$U(t, t_0) = e^{-iH(t-t_0)} \ . \tag{2.16}$$

Similarly to the case of a pure state, quantum theory also provides a method to describe the dynamics of a system S whose state is represented by a density operator ρ_S. In this case, the time evolution of the operator ρ_S can be deduced by applying the Schrödinger's equation to the collection of pure states $\{|\psi_k\rangle\}$ of its associated ensemble. In fact, let us suppose that at time t_0 the system of interest is described by a density operator $\rho_S(t_0)$ of the form

$$\rho_S(t_0) = \sum_k p_k |\psi_k(t_0)\rangle\langle\psi_k(t_0)|. \tag{2.17}$$

Then, acting with the evolution operator $U(t,t_0)$ on the left and with the adjoint operator $U^\dagger(t,t_0)$ on the right of Eq.(2.17), we find

$$\rho_S(t) \equiv U(t,t_0)\rho_S(t_0)U(t,t_0)^\dagger = \sum_k p_k U(t,t_0)|\psi_k(t_0)\rangle\langle\psi_k(t_0)|U(t,t_0)^\dagger \ . \quad (2.18)$$

Finally, deriving Eq.(2.18) with respect to t, we arrive to an expression for the evolution of the density matrix $\rho_S(t)$, i.e.,

$$\frac{d}{dt}\rho_S(t) = -i[H(t), \rho_S(t)] \ , \quad (2.19)$$

where the symbol $[\cdot,\cdot]$ denotes the commutator between two operators.
Eq.(2.19) can be recast as

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\left[\rho_S(t)\right]] \ , \quad (2.20)$$

where $\mathcal{L}$ is the Liouville operator, acting on $\rho_S(t)$, whose expression, in the case of unitary dynamics, reduces to

$$\mathcal{L}\left[\rho_S(t)\right] = -i[H(t), \rho_S(t)]. \quad (2.21)$$

Objects like $\mathcal{L}$ of Eq.(2.21) are examples of *superoperators*, that will be discussed thoroughly in the next section.

2.1.5 Quantum maps

Transformations of quantum states are described by *quantum maps*, i.e., superoperators $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ that satisfy the following properties:

- Linearity: $\mathcal{E}(\alpha O_1 + \beta O_2) = \alpha\mathcal{E}(O_1) + \beta\mathcal{E}(O_2) \ , \quad \forall O_1, O_2 \in \mathcal{B}(\mathcal{H}_A) \ ,$ $\forall \alpha, \beta \in \mathbb{C} \ ,$
- Hermiticity: $\mathcal{E}(O^\dagger) = \mathcal{E}(O)^\dagger \ , \quad \forall O \in \mathcal{B}(\mathcal{H}_A) \ .$

Further constraints derive from the fact that $\mathcal{E}$ has to preserve the positivity of a state as well as its unitality. Formally, we have the following definitions:

Definition 2.1. *A linear map $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ is said positive if*

$$\forall O \in \mathcal{B}(\mathcal{H}_A), \ O \succeq 0 \implies \mathcal{E}(O) \succeq 0 \ . \quad (2.22)$$

Definition 2.2. *A linear, self-adjoint map $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ is said trace preserving if*

$$\mathrm{Tr}[\mathcal{E}(O)] = \mathrm{Tr}[O] \ , \quad \forall O \in \mathcal{B}(\mathcal{H}_A) \ . \tag{2.23}$$

Notice that, in general, the positivity property of a quantum map does not extend trivially to composite system. For this reason, we need to impose that $\mathcal{E}$ remains positive also when one takes into account the composition with a larger system. Formally, this is expressed by the notion of complete positivity:

Definition 2.3. *A positive map $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ is said completely positive if for every extension $\mathcal{E}' = \mathbb{1}_{A'} \otimes \mathcal{E}$, the map $\mathcal{E}'$ is positive, i.e., $(\mathbb{1}_{A'} \otimes \mathcal{E})[O] \succeq 0$ for every positive operator $O \in \mathcal{B}(\mathcal{H}_{A'} \otimes \mathcal{H}_A)$, where $\mathbb{1}_{A'}$ denotes the identity map on $\mathcal{B}(\mathcal{H}_{A'})$.*

Finally, quantum maps that meet all the above requirement are said CPTP maps, and represent the set of the allowed physical transformations of a quantum state.

Definition 2.4. *Physical operations on quantum states are described by quantum channels, i.e., linear maps that are completely positive and trace preserving.*

Let us conclude this section with the definition of a decomposable map, whose importance will become clearer in the following of this thesis.

Definition 2.5. *A positive map $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ is said decomposable if and only if it can be written as*

$$\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2 \circ T \ , \tag{2.24}$$

where $\mathcal{E}_1, \mathcal{E}_2$ are completely positive maps and T is the transposition map.

2.1.6 Representations of quantum maps

In this section we present some useful techniques to represent quantum maps. In particular, focusing on the class of CPTP maps, we show that such representations provide a way to relate the properties of a quantum channel in terms of those of some associated operators.

Choi-Jamiołkowski-Sudarshan isomorphism

The Choi-Jamiołkowski-Sudarshan (CJS) isomorphism [Cho75; Jam72; SMR61] provides a way to relate a quantum map $\mathcal{E}$ with an associated operator $J_{\mathcal{E}}$. Formally, we have the following result:

Theorem 2.1 ([Cho75; Jam72; SMR61]). *Given an operator $J_\mathcal{E} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ there exists an associated map $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ defined as*

$$\mathcal{E}(\rho) = \sum_{k,k'} \sum_{l,l'} \langle k, l | J_\mathcal{E} | k', l' \rangle \langle k | \rho | k' \rangle |l\rangle\langle l'| = \mathrm{Tr}_\mathrm{A}[J_\mathcal{E} \rho^T] \,, \tag{2.25}$$

with $\rho \in \mathcal{B}(\mathcal{H}_A)$. Conversely, given a map $\mathcal{E} : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_B)$ there exists an associated operator $J_\mathcal{E} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ defined as

$$J_\mathcal{E} = (\mathbb{1}_{A'} \otimes \mathcal{E})[|\Psi^+\rangle\langle\Psi^+|] \,. \tag{2.26}$$

where $|\Psi^+\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |ii\rangle$ is the maximal entangled state in $\mathcal{H}_{A'} \otimes \mathcal{H}_A$, where $d = \dim \mathcal{H}_{A'} = \dim \mathcal{H}_A$.

The operator $J_\mathcal{E}$ is usually called the *Choi matrix* (or Choi state) of the quantum map $\mathcal{E}$. The importance of the CJS isomorphism stems from the fact that it allows to recast the properties of a quantum map in terms of those of its Choi state, and vice versa, a result which is expressed by the following theorem:

Theorem 2.2 ([Cho75; Jam72; SMR61]). *Given an operator $J_\mathcal{E}$ and its associated map $\mathcal{E}$ through the CJS isomporphism, the following relations hold:*

- *$\mathcal{E}$ is completely positive $\iff J_\mathcal{E} \succeq 0$,*
- *$\mathcal{E}$ is trace preserving $\iff \mathrm{Tr}[J_\mathcal{E}] = 1$.*

As a consequence, checking if $\mathcal{E}$ is a CPTP map is equivalent to inspect whether its associated Choi state $J_\mathcal{E}$ defines a valid density operator. This result is particularly valuable in quantum information as it expresses an equivalence between quantum channels and quantum states and, for this reason, it is sometimes referred to as the *channel-state duality*.

Kraus representation

Another way to describe a quantum channel is provided by its *Kraus representation*, defined by the following theorem:

Theorem 2.3 ([Kra71; KBD+83]). *Let $\rho \in \mathcal{B}(\mathcal{H})$ be a quantum state. A map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is a CPTP map iff it admits a representation of the form*

$$\mathcal{E}(\rho) = \sum_{i=1}^r K_i \rho K_i^\dagger \,, \tag{2.27}$$

where the Kraus operators $\{K_i\} \in \mathcal{B}(\mathcal{H})$ *fulfil*

$$\sum_i K_i^\dagger K_i = \mathbb{1} \ , \tag{2.28}$$

and $r \leq \dim(\mathcal{H})^2$.

Remarkably, given a quantum map $\mathcal{E}$, it can be shown that the set of associated Kraus operators can be found diagonalising the Choi state $J_\mathcal{E}$ [JP18]. To see this, let us first introduce the operation, denoted as mat($|\lambda\rangle$), that transforms the $d^2 \times 1$ vector $|\lambda\rangle = (\lambda_{00}, \ldots, \lambda_{d-1,d-1})^T$ into a $d \times d$ matrix by stacking the entries of $|\lambda\rangle$ row by row, i.e.,

$$\text{mat}(|\lambda\rangle) = \begin{pmatrix} \lambda_{00} & \cdots & \lambda_{0,d-1} \\ \vdots & \ddots & \vdots \\ \lambda_{d-1,0} & \cdots & \lambda_{d-1,d-1} \end{pmatrix} . \tag{2.29}$$

Hence, the Kraus operator K_i is given by

$$K_i = \sqrt{\lambda^{(i)}}\text{mat}(|\lambda^{(i)}\rangle) \ , \tag{2.30}$$

where mat($|\lambda^{(i)}\rangle$) is the matrix corresponding to the eigenvector $|\lambda^{(i)}\rangle$ of $J_\mathcal{E}$, and $\lambda^{(i)}$ its associated eigenvalue.

Let us observe that the decomposition in Eq.(2.27) is by no means unique and different sets of Kraus operators may lead to the same CPTP map. Indeed, we have the following corollary:

Corollary 2.3.1. *Given two sets of Kraus operators,* $\{K_i\}$ *and* $\{\tilde{K}_i\}$*, they represent the same quantum map* $\mathcal{E}$ *iff there exists a unitary operator* U *such that*

$$\tilde{K}_i = \sum_j U_{ij} K_j \ . \tag{2.31}$$

Let us conclude by observing that, in general, Kraus operators are not necessarily orthogonal. Nevertheless, it can be shown [Wol12] that, given a CPTP map, there always exists a Kraus representation with r orthogonal Kraus operators , i.e., $\text{Tr}[K_i K_j^\dagger] = \delta_{ij}$.

Stinespring representation

A different, although related, representation of a quantum map, is given by the so-called *Stinespring representation* [Sti55]. In this picture, the action of a map over a system S is described by a process in which S is first coupled to an *ancillary system* A, then a unitary transformation is applied to the composite system $S + A$ and finally, the partial trace over A is performed. More formally, we have:

Theorem 2.4 ([Sti55]). *Let $\mathcal{E}(\rho) : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a CPTP map. Then there exist a Hilbert space $\mathcal{H}_A$ and a unitary operation $U \in \mathcal{B}(\mathcal{H} \otimes \mathcal{A})$ such that*

$$\mathcal{E}(\rho) = \mathrm{Tr}_A[U(\rho \otimes |0\rangle\langle 0|)U^\dagger] , \tag{2.32}$$

for every density operator $\rho \in \mathcal{B}(\mathcal{H})$.

Eq.(2.32) defines the Stinespring representation (or Stinespring dilation) of the CPTP map $\mathcal{E}$. Analogously to the case of Kraus operators, it can be shown that the dimension of the ancillary Hilbert space can always be chosen such that $\dim(\mathcal{A}) \leq \dim(\mathcal{H})^2$. This connection is by no means casual and indeed the two representations are related. In fact, given the set $\{K_i\}_{i=1}^{d^2}$ of Kraus operators for the quantum channel $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ and a Hilbert space $\mathcal{A}$ with orthonormal basis $\{|i\rangle\}_{i=1}^{d^2}$, it is possible to define a unitary operator $U \in \mathcal{B}(\mathcal{H} \otimes \mathcal{A})$ such that

$$U(|\phi\rangle \otimes |0\rangle) \equiv \sum_{i=1}^{d^2} K_i |\phi\rangle \otimes |i\rangle \ , \tag{2.33}$$

with $|\phi\rangle \in \mathcal{H}$. Conversely, expanding Eq.(2.32), we have

$$\mathcal{E}(\rho) = \sum_i (\mathbb{1}_\mathcal{H} \otimes \langle i|)U(\rho \otimes |0\rangle\langle 0|)U^\dagger(\mathbb{1}_\mathcal{H} \otimes |i\rangle) \tag{2.34}$$

$$= \sum_i (\mathbb{1}_\mathcal{H} \otimes \langle i|)U(\mathbb{1}_\mathcal{H} \otimes |0\rangle)\rho(\mathbb{1}_\mathcal{H} \otimes \langle 0|)U^\dagger(\mathbb{1}_\mathcal{H} \otimes |i\rangle) \equiv \sum_i K_i \rho K_i^\dagger \ , \tag{2.35}$$

where we have defined

$$K_i \equiv (\mathbb{1}_\mathcal{H} \otimes \langle i|)U(\mathbb{1}_\mathcal{H} \otimes |0\rangle) \ . \tag{2.36}$$

Let us conclude this section with the following remark: the Stinespring theorem implies the possibility to describe a CPTP map acting on a system S, as the result of a unitary evolution of a larger system, $S + A$, where the ancillary system A is eventually discarded. As we will see in the next section, this description becomes particularly natural when dealing with *open quantum systems*, i.e., those physical systems whose interaction with an external environment cannot be neglected.

2.2 Open quantum systems

In section 2.1 we have described the evolution of a quantum system S in terms of a unitary operator that depends on the Hamiltonian H_S of the system. Nevertheless, such approach can be defined only in the approximation of a closed system, i.e., when S is regarded as isolated from any other quantum systems. Although in the case of weakly interacting systems this assumption seems quite reasonable, in general no quantum system can be considered as perfectly isolated. For this reason, in the formalism of *open* quantum systems (OQS), the properties of a quantum system S are investigated, assuming an interaction with an external *environment*, E. Due to such interaction, although the evolution of the composite system $S + E$ is still unitary (being isolated), the same is no longer true for the dynamics of the open system S. Hence, the necessity of a new formalism that characterises correctly the behaviour of S in the presence of the dissipation introduced by the environment. Ever since its formulation in the '70s, the importance of the theory of OQS has been widely recognised, especially due the fact that it has led to great advances in the description of phenomena related to irreversible dynamics such as the decay of quantum coherences or the relaxation towards a non-equilibrium steady state, just name few [DD76; AL07; BP+02; RH12]. The typical approach in dealing with OQS dynamics is to describe the evolution of the open system by means of a differential equation, known as master equation, whose explicit form depends on the microscopical details between system and environment. In the following, we provide some examples of such master equations.

2.2.1 The GKSL master equation

When dealing with a composite system $S + E$, the tensor product postulate prescribes that the Hilbert space H_{SE} for the whole system is given by the tensor product of the Hilbert spaces of the subsystems, i.e., $\mathcal{H}_{SE} = \mathcal{H}_S \otimes \mathcal{H}_E$. Hence, the Hamiltonian H that rules the dynamics of $S + E$ takes the form

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_{SE} \; , \tag{2.37}$$

where H_S, H_E are the Hamiltonian for the systems S, E, respectively, and $H_{SE} \in \mathcal{H}_S \otimes \mathcal{H}_E$ models the interaction between the open system and the environment. Let us assume that, at t_0, system and environment are uncorrelated, so that the initial state for the composite system is described by

$$\rho(t_0) = \rho_S(t_0) \otimes \rho_E(t_0) \; . \tag{2.38}$$

Hence, the total state at time t is given by

$$\rho(t) = U(t, t_0)\rho(t_0)U(t, t_0)^\dagger \; , \tag{2.39}$$

where we have used the fact that, since the system $S+E$ is closed, its evolution is governed by the total unitary operator $U(t,t_0)$.

Recalling Eq.(2.8), the dynamics of S can be recovered by tracing out the environment, i.e.,

$$\rho_S(t) = \mathrm{Tr}_E[U(t,t_0)\rho(t_0)U(t,t_0)^\dagger] \ , \tag{2.40}$$

which can be cast equivalently as

$$\rho_S(t) = \mathcal{E}(t)[\rho_S(t_0)] \ , \tag{2.41}$$

where we have introduced a CPTP map $\mathcal{E}(t) : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$, known as *dynamical map*, that describes the evolution of the open system from the initial state $\rho_S(t_0)$ to a final state $\rho_S(t)$.

In almost any practical case, the exact characterisation of $\mathcal{E}(t)$ is extremely hard. For this reason, it is customary to introduce some approximation to reduce the original complexity of the problem. A typical requirement is to ask that the correlations between the main system and the environment decay over a time scale that is much smaller as compared to the time scale over which the system evolves. As a consequence, when considering the reduced dynamics of the system S, it is legitimate to neglect the memory effects, i.e., the future history of the system does not depend on the state of the system at previous times. Such condition can be formally expressed by the condition

$$\mathcal{E}(t_1+t_2) = \mathcal{E}(t_1)\circ\mathcal{E}(t_2) \ , \tag{2.42}$$

a relation known as the *semigroup* property. Hence, given a dynamical map that satisfies Eq.(2.42), it is possible to show that there exists an associated linear map $\mathcal{L}$ such that $\mathcal{E}(t)$ admits the following representation, i.e.,

$$\mathcal{E}(t) = e^{\mathcal{L}t} \ . \tag{2.43}$$

Recalling Eq.(2.41), one immediately finds the so-called Markov quantum master equation, i.e.,

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t) \ , \tag{2.44}$$

where $\mathcal{L}$ is the Liouville superoperator of Eq.(2.21).

Quantum master equations (QMEs) represent a way to approximate the exact dynamics described by Eq.(2.39) and obtain a linear differential equation for the state $\rho_S(t)$. It can be shown [BP+02] that the most general expression for $\mathcal{L}$ is given by the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation [Kos72; GKS76; Lin76], i.e.,

$$\mathcal{L}[\rho_{\rm S}] = -i[H, \rho_S] + \sum_k \gamma_k \left(\mathcal{J}_k \rho_S \mathcal{J}_k^\dagger - \frac{1}{2}\{\mathcal{J}_k^\dagger \mathcal{J}_k, \rho_S\} \right) , \tag{2.45}$$

where $\{\cdot, \cdot\}$ represents the anti-commutator between two operators. The operators $\mathcal{J}_k$ are referred to as Lindblad (or jump) operators and $\gamma_k \geq 0$ are dubbed dissipation rates.

Let us observe that the commutator in Eq.(2.45) represents the unitary evolution governed by the Hamiltonian H while the latter term takes into account the effect of the dissipation introduced by the environment. For this reason, the quantity

$$\mathcal{D}[\rho_S] \equiv \sum_k \gamma_k \left(\mathcal{J}_k \rho_S \mathcal{J}_k^\dagger - \frac{1}{2}\{\mathcal{J}_k^\dagger \mathcal{J}_k, \rho_S\} \right) , \tag{2.46}$$

is sometimes called *dissipator*, and Eq.(2.45) takes the form

$$\mathcal{L}[\rho_S] = -i[H, \rho_S] + \mathcal{D}[\rho_S] \; . \tag{2.47}$$

2.2.2 The Redfield master equation

Despite being completely general, Eq.(2.45) does not provide any information about the shape of the jump operators $\{\mathcal{J}_k\}$ nor about the corresponding rates $\{\gamma_k\}$, whose expressions can be recovered under some approximations. For reasons that will become clearer in the following, the validity of such approximations is based on the assumption that the environment is composed of a large number of degrees of freedom. To this end, let us consider the case where a system S interacts with a *bath* B, i.e., an environment which displays an infinite number of degrees of freedom. B can be conceived as a macroscopic object in thermal equilibrium, so that a temperature T can be assigned to describe its state. In analogy with Eq.(2.37), let us assume that the Hamiltonian for the system $S + B$ is given by $H = H_S + H_B + H_{SB}$. The derivation of a master equation for the open quantum system becomes easier in the interaction picture where, recalling Eq.(2.13), H_{SB} can be expressed as

$$H_I(t) = e^{iH_0(t-t_0)} H_{SB} e^{-iH_0(t-t_0)} \; , \tag{2.48}$$

with $H_0 \equiv H_S + H_B$. Hence, the evolution of the state of the total system, is given by

$$\frac{d}{dt}\rho_I(t) = -i[H_I(t), \rho_I(t)] \; , \tag{2.49}$$

where $\rho_I(t) = e^{iH_0(t-t_0)}\rho(t)e^{-iH_0(t-t_0)}$ is the representation of $\rho(t)$ in the interaction picture. Integrating Eq.(2.49) over time yields

$$\rho_I(t) = \rho_I(t_0) - i\int_{t_0}^{t} dt'[H_I(t'), \rho_I(t')] \, . \tag{2.50}$$

Substituting the above expression in Eq.(2.49) and tracing over the degrees of freedom of the bath, we can obtain the evolution of S, i.e.,

$$\frac{d}{dt}\rho_S(t) = -\int_{t_0}^{t} dt'\mathrm{Tr}_B\{[H_I(t), [H_I(t'), \rho_I(t')]]\} \, . \tag{2.51}$$

Notice that, in writing Eq.(2.51), we have assumed that $\mathrm{Tr}_B\left\{[H_I(t), \rho_I(t_0)]\right\} = 0$, a requirement which corresponds to neglect the effect of any first-order dynamics in the initial state of the system.

A closer look at Eq.(2.51) reveals that the right-hand term still depends on $\rho_I(t')$, a fact which makes this expression extremely hard to compute since the dynamics of S depends on the state of the total system at all previous times. A simpler expression is obtained introducing the so-called *Born approximation*, which consists in assuming a weak coupling between S and B, so that it is legitimate to neglect the back-action of the principal system on the state of the bath, i.e., $\rho_I(t) = \rho_S(t) \otimes \rho_B$. With this assumption, Eq.(2.51) becomes

$$\frac{d}{dt}\rho_S(t) = -\int_{t_0}^{t} dt'\mathrm{Tr}_B\{[H_I(t), [H_I(t'), \rho_S(t') \otimes \rho_B]]\} \, . \tag{2.52}$$

Observe that, if we perform the change of variables $t' \to t - t'$ in the above integral, the extremes of integration do not change, i.e.,

$$\frac{d}{dt}\rho_S(t) = -\int_{t_0}^{t} dt'\mathrm{Tr}_B\{[H_I(t), [H_I(t-t'), \rho_S(t') \otimes \rho_B]]\} \, . \tag{2.53}$$

Eq.(2.53) still depends on the dynamics of ρ_S at times $t' < t$, but can be converted into a time-local master equation by resorting to a second assumption, known as the *Markov approximation*. If we denote by τ_R the relaxation time of the S, i.e., the time scale over which the main system returns to equilibrium after the interaction with the bath, then the Markov approximation requires that $\tau_R \gg \tau_B$, where τ_B represents the time scale of bath correlations. This is equivalent to disregard the memory effects over times greater than τ_B, so that the upper bound of the integral in Eq.(2.53) can be sent to infinity committing a negligible error. The resulting equation is known as the Redfield master equation and takes the form

$$\frac{d}{dt}\rho_S(t) = -\int_{t_0}^{\infty} dt' \mathrm{Tr}_B\{[H_I(t), [H_I(t-t'), \rho_S(t') \otimes \rho_B]]\} \ . \tag{2.54}$$

Despite the two assumptions that we have considered, known as Born-Markov approximations, the Redfield master equation does not guarantee, in general, the positivity of $\rho_S(t)$ at all times. In order to avoid this problem we introduce a third assumption, known as *secular* approximation, which leads to a master equation of the same form of Eq.(2.45).

2.2.3 The Born-Markov secular master equation

We have already seen in the previous section that the expression of an operator in the interaction picture becomes time-dependent (see, e.g., Eq.(2.48)). The secular approximation consists in neglecting the rapidly oscillating contributions in the expression of the master equation, hence allowing to retrieve a positive density operator $\rho_S(t)$ for all times. In order to clarify this statement, let us consider an open quantum systems described by a total Hamiltonian $H = H_S + H_B + H_{SB}$. Without loss of generality, the interacting term H_{SB} can be written as

$$H_{SB} = \sum_k S_k \otimes B_k \ , \tag{2.55}$$

where $\{S_k\}, \{B_k\}$ are hermitian operators acting on the Hilbert spaces $\mathcal{H}_S, \mathcal{H}_B$ of the systems S, B, respectively. As for the system and the bath Hamiltonian, their spectral decomposition yields, respectively,

$$H_S = \sum_m E_m |E_m\rangle\langle E_m| \ , \tag{2.56}$$

$$H_B = \sum_n \epsilon_n |\epsilon_n\rangle\langle \epsilon_n| \ , \tag{2.57}$$

where $\{E_m\}, \{\epsilon_n\}$ are the eigenvalues of H_S, H_B, with corresponding eigenvectors $\{|E_m\rangle\}, \{|\epsilon_n\rangle\}$. Hence, we can define the operator $S_k(\omega)$ as

$$S_k(\omega) = \sum_{m,n} \delta(E_m - E_n - \omega)(S_k)_{m,n} |E_m\rangle\langle E_n| \ , \tag{2.58}$$

where $(S_k)_{m,n} = \langle E_m|S_k|E_n\rangle$ and ω is a fixed energy difference. Obviously, summing over ω, we recover S_k, i.e.,

$$S_k = \sum_\omega S_k(\omega) = \sum_\omega S_k^\dagger(\omega) \ . \tag{2.59}$$

The decomposition of Eq.(2.58) is particularly useful when moving to the interaction picture, where, recalling Eq.(2.48), the expression of the interacting Hamiltonian H_{SB} becomes

$$H_I(t) = \sum_k \sum_\omega e^{iH_S t} S_k(\omega) e^{-iH_S t} \otimes e^{iH_B t} B_k e^{-iH_B t} \ . \tag{2.60}$$

Notice that, due to the fact that the eigenprojectors $\{|E_m\rangle\langle E_m|\}$ commute with H_S, we have

$$[H_S, S_k(\omega)] = -\omega S_k(\omega) \ , \tag{2.61}$$

so that the following identity holds, i.e.,

$$e^{iH_S t} S_k(\omega) e^{-iH_S t} = e^{-i\omega t} S_k(\omega) \ . \tag{2.62}$$

It follows that Eq.(2.60) takes the simpler expression

$$H_I(t) = \sum_k \sum_\omega e^{-i\omega t} S_k(\omega) \otimes B_k(t) \ , \tag{2.63}$$

where $B_k(t)$ is the representation of the bosonic operator B_k in the interaction picture, i.e.,

$$B_k(t) = e^{iH_B t} B_k e^{-iH_B t} \ . \tag{2.64}$$

Getting back to the Redfield master equation of Eq.(2.54), we can substitute the expression for $H_I(t)$ given by Eq.(2.63), to find

$$\frac{d}{dt}\rho_S(t) = \sum_{k,k'} \sum_{\omega,\omega'} e^{i(\omega-\omega')t} C_{k,k'}(\omega) \left(S_{k'}(\omega)\rho_S(t) S_k^\dagger(\omega') - S_k^\dagger(\omega') S_{k'}(\omega)\rho_S(t) \right) + \text{h.c.} \ , \tag{2.65}$$

where we have defined the one-sided Fourier transform of the bath correlation functions, i.e.,

$$C_{k,k'}(\omega) = \int_{t_0}^{\infty} dt' e^{i\omega t'} \mathrm{Tr}_B\{B_k^\dagger(t) B_k(t-t')\} \ . \tag{2.66}$$

Notice that when ρ_B is an eigenstate of H_B, i.e., $[H_B, \rho_B] = 0$, the correlation functions $C_{k,k'}(\omega)$ become time-independent.

Looking at Eq.(2.65) we can now understand the meaning of the secular approximation, which simply consists in discarding all the terms such that $\omega \neq \omega'$. The inverse of the difference $|\omega - \omega'|$ for $\omega \neq \omega'$ gives the typical timescale τ_S over which the system S evolves, i.e., $\tau_S \approx |\omega - \omega'|^{-1}$. Hence, denoting by τ_R the typical relaxation time for the open quantum system, the secular approximation is valid whenever $\tau_S \ll \tau_R$, that is when the oscillating terms in Eq.(2.65) change rapidly during the time over which the evolution of the system becomes appreciable. In this limit, Eq.(2.65) takes the simpler form

$$\frac{d}{dt}\rho_S(t) = \sum_{k,k'}\sum_{\omega} C_{k,k'}(\omega)\left(S_{k'}(\omega)\rho_S(t)S_k^\dagger(\omega') - S_k^\dagger(\omega')S_{k'}(\omega)\rho_S(t)\right) + \text{h.c.}\ , \tag{2.67}$$

known as the *Born-Markov secular* master equation. Eq.(2.67) can be cast in the Linblad form by decomposing $C_{k,k'}(\omega)$ into its real and imaginary parts as

$$C_{k,k'}(\omega) = \frac{1}{2}\gamma_{k,k'}(\omega) + i\kappa_{k,k'}(\omega)\ , \tag{2.68}$$

where it can be shown that the real part $\gamma_{k,k'}(\omega) = C_{k,k'}(\omega) + C^*_{k',k}(\omega)$ defines a positive matrix. Finally, introducing the so-called Lamb-shift Hamiltonian H_{LS}, given by

$$H_{LS} = \sum_{k,k'}\sum_{\omega} \kappa_{k,k'}(\omega)S_k^\dagger(\omega)S_k(\omega)\ , \tag{2.69}$$

we get to the expression

$$\frac{d}{dt}\rho_S(t) = -i[H_{LS}, \rho_S(t)] + \mathcal{D}(\rho_S(t))\ , \tag{2.70}$$

where the dissipator $\mathcal{D}(\rho_S)$ takes the form

$$\mathcal{D}(\rho_S) = \sum_{k,k'}\sum_{\omega} \gamma_{k,k'}(\omega)\left(S_{k'}(\omega)\rho_S S_k^\dagger(\omega) - \frac{1}{2}\{S_k^\dagger(\omega)S_{k'}(\omega), \rho_S\}\right)\ . \tag{2.71}$$

2.3 Entanglement

Quantum superposition is a consequence of the first postulate of quantum mechanics. More specifically, the requirement that the state of a system S is described by a vector $|\psi_S\rangle \in \mathcal{H}_S$, implies that, by the linearity of Hilbert spaces, (normalised) linear combinations of vectors in $\mathcal{H}_S$ are also admissible states for S. In a similar fashion, entanglement stems from the tensor product postulate of quantum mechanics. In fact, let us consider the simple case of two qubits. One possible quantum state for the composite system $A + B$ could be $|\Psi_{AB}\rangle = |0_A\rangle |0_B\rangle$, or, analogously, $|\Psi_{AB}\rangle = |1_A\rangle |1_B\rangle$, where the labels A, B, remind that each ket is a vector in the corresponding Hilbert space $\mathcal{H}_A, \mathcal{H}_B$, respectively. Obviously, the superposition

$$|\Psi_{AB}\rangle = \frac{|0_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle}{\sqrt{2}} , \tag{2.72}$$

also defines a valid state for the composite system. However, the problem arises when one asks the following question: given a composite system whose state is described by the vector $|\Psi_{AB}\rangle$ of Eq.(2.72), what is the state of each subsystem? In fact, while the state of $A + B$ can be defined without ambiguity, the same is no longer true for the individual subsystems. A state such that of Eq.(2.72) is said to be *entangled*, because it cannot be written as the tensor product of the states of the subsystems. Similarly to the case of quantum superposition, also entanglement is a very fragile property and the generation of entangled states is one of the main challenges from an experimental point of view. Due to its many applications in quantum information tasks, it is crucial to derive criteria to decide whether a quantum state is entangled or not. Such problem is referred to as the *separability problem*, and it will be the central topic of the following sections.

2.3.1 Entanglement of pure states

In the case of pure states, entanglement can be defined as follows:

Definition 2.6. *Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be the Hilbert spaces of two physical systems A and B, respectively. A pure state $|\Psi_{AB}\rangle \in \mathcal{H}_{AB} \equiv \mathcal{H}_A \otimes \mathcal{H}_B$ is said separable or, equivalently, a product state, iff it can be written as*

$$|\Psi_{AB}\rangle = |\psi_A\rangle |\psi_B\rangle , \tag{2.73}$$

where $|\psi_A\rangle , |\psi_A\rangle$ are pure states in $\mathcal{H}_A, \mathcal{H}_B$, respectively. If such decomposition does not exist, the state $|\Psi_{AB}\rangle$ is said to be entangled.

Product states possess an operational interpretation since they correspond to those states that can be prepared by two distant parties, say Alice and Bob, acting on the systems A and B, respectively. On the contrary, the generation of an entangled state always requires an interaction between the two subsystems or, as in the case of entanglement swapping [ZZH+93], with an ancillary system that acts as a mediator of the interaction.

2.3.2 Entanglement of mixed states

In the case of mixed states, the definition of entanglement needs to be modified as follows:

Definition 2.7. *Let $\rho_{AB} \in \mathcal{B}(\mathcal{H}_{AB})$, with $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. We say that ρ_{AB} is a product state if it can be written as $\rho_{AB} = \rho^A \otimes \rho^B$. If ρ_{AB} can be cast as*

$$\rho_{AB} = \sum_k p_k \rho_k^A \otimes \rho_k^B \ , \quad \sum_k p_k = 1, \ p_k \geq 0 \ \forall k \ , \tag{2.74}$$

then it is said separable. Otherwise, it is called entangled.

As we have seen in the case of pure states, product states correspond to uncorrelated states, i.e., states that can be obtained by two parties, Alice and Bob, acting locally on their share of the quantum state ρ_{AB}. Differently, separable states can be prepared only when the two parties share classical correlations. Indeed, it is possible to show that the state of Eq.(2.74) is the most general state that Alice and Bob can create using local operations and classical communication (LOCC). An LOCC scenario can be thought as follows:

- Alice and Bob possess their share of the state ρ_{AB}.
- Alice performs a local quantum operation on her state, described in terms of a set of operators $\{A_i^1\}$ such that $\sum_i (A_i^1)^\dagger A_i^1 = \mathbb{1}_A$, where $\mathbb{1}_A$ is the identity operator on $\mathcal{H}_A$. Eventually, she measures her share and sends the result to Bob using a classical channel of communication (e.g., a phone).
- Depending on the outcome of Alice's measurement, Bob performs a local quantum operation on his state. Again, such quantum operator can be described in terms of some operators $\{B_{ij}^1\}$ such that $\sum_j (B_{ij}^1)^\dagger B_{ij}^1 = \mathbb{1}_B$.
- Bob sends the result of his measurement to Alice and the protocol goes on in this way until required.

Hence, let us suppose that Alice and Bob are given the states $|a_0\rangle$ and $|b_0\rangle$, respectively, so that the state of the composite system is described by the density operator $\rho_{AB} = |a_0\rangle\langle a_0| \otimes |b_0\rangle\langle b_0|$. Now, imagine that, following the aforementioned LOCC protocol, Alice prepares the state $|a_k\rangle$, with probability p_k, and then sends the result to Bob who prepares the state $|b_k\rangle$, depending on the outcome he receives. Thus, the final state for the composite system is given by

$$\rho_{AB} = \sum_k p_k |a_k\rangle\langle a_k| \otimes |b_k\rangle\langle b_k| \ , \tag{2.75}$$

which is of the same form of Eq.(2.74). As a consequence, LOCC is not sufficient to generate an entangled state, confirming the genuinely quantum feature of this phenomenon.

2.3.3 Separability criteria

Deciding whether a quantum state is separable or not is a task known as the separability problem. Despite its apparent simplicity, it has been proven that, in the general case, the separability problem is NP-hard [Gur03] and even in the bipartite case a complete solution is still missing. However, in some cases, there exist criteria that allow to assess the presence of entanglement in a given quantum state. In the next section we present some separability criteria, with special attention to those we will use explicitly in this thesis. Notice that, even though the definition of entanglement can be extended to the multipartite case, in what follows we will consider only bipartite states.

Schmidt decomposition

When dealing with pure bipartite states, Schmidt decomposition is a particular representation which turns out to be useful for the characterisation of entanglement.

Definition 2.8. *Let $|\Psi_{AB}\rangle$ be the state of a composite system in $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. Then there exist two orthonormal basis $\{|\alpha_i\rangle\}, \{|\beta_i\rangle\}$ for $\mathcal{H}_A, \mathcal{H}_B$, respectively, such that $|\Psi_{AB}\rangle$ can be decomposed as*

$$|\Psi_{AB}\rangle = \sum_{i=1}^{M} \lambda_i |\alpha_i\rangle |\beta_i\rangle \ , \tag{2.76}$$

where the positive, real coefficients λ_i satisfy $\sum_{i=1}^{M} \lambda_i^2 = 1$. Eq.(2.76) is said the Schmidt decomposition of the state $|\Psi_{AB}\rangle$ and $M \leq \min\{d_A, d_B\}$ is called Schmidt rank .

It can be shown that pure product states correspond to states that possess a Schmidt decomposition with rank one, i.e., with only one non-zero coefficient λ_i, while all entangled states have Schmidt rank $M > 1$. This condition can be easily computed by noticing that the square root of the Schmidt coefficients correspond to the eigenvalues of the reduced matrices ρ_A and ρ_B of Eq.(2.8). Hence, we can rephrase the above separability criterion as

Theorem 2.5. *A state $|\Psi_{AB}\rangle$ is separable if and only if $\rho_A = \mathrm{Tr}_B[|\Psi_{AB}\rangle\langle\Psi_{AB}|]$ (or, equivalently ρ_B) is a pure state, i.e., $\rho_A^2 = \rho_A$.*

Schmidt number

In the case of bipartite mixed states, the concept of Schmidt rank can be generalised to the so-called Schmidt number.

Definition 2.9. *The bipartite state ρ_{AB} has Schmidt number m if: i) for any decomposition $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ at least one of the vectors $\{|\psi_k\rangle\}$ has at least Schmidt rank m, and ii) there exists a decomposition of ρ with all the vectors $\{|\psi_k\rangle\}$ of Schmidt rank at most m. Equivalently,*

$$m = \inf_{\{p_k, |\psi_k\rangle\}} \max_k \; r(|\psi_k\rangle) \; , \tag{2.77}$$

where $r(|\psi_k\rangle)$ is the Schmidt rank of the pure state $|\psi_k\rangle$.

As for pure states, a bipartite mixed state is separable if and only if it has Schmidt number $m = 1$. Notice that in the case of a pure state, the Schmidt number is equal to its Schmidt rank.

PPT criterion

Before introducing the PPT criterion it is necessary to define the *partial transposition* of a quantum state. This operation possesses the physical interpretation of a partial time reversal [STV98], and can be formally defined as follows:

Definition 2.10. *Let $\rho_{AB} \in \mathcal{B}(\mathcal{H}_{AB})$ be a bipartite state, whose representation, in a chosen product basis, is given by*

$$\rho_{AB} = \sum_{i,j} \sum_{k,l} \rho^{ij}_{kl} |i\rangle\langle j| \otimes |k\rangle\langle l| \; . \tag{2.78}$$

Then, the partial transposition of the state ρ_{AB} with respect to the subsystem B is the operator $\rho_{AB}^{T_B}$, defined as

$$\rho_{AB}^{T_B} = \sum_{i,j} \sum_{k,l} \rho^{ij}_{lk} |i\rangle\langle j| \otimes |k\rangle\langle l| \; . \tag{2.79}$$

Clearly, the partial transposition can also be defined with respect to the subsystem A, i.e., $\rho_{AB}^{T_A}$, and the two operators are related by the simple formula $\rho_{AB}^{T_A} = (\rho_{AB}^{T_B})^T$, where T is the usual transposition of a matrix. Notice that, as in the case of the standard transposition, the expression of the partially transposed matrix depends on the chosen basis, even though its eigenvalues are independent on such a choice.

A bipartite state ρ_{AB} with positive partial transposition, i.e., $\rho_{AB}^{T_A} \succeq 0$, is said a PPT state. On the contrary, states whose partial transposition bears negative eigenvalues are usually referred to as NPT. It is easy to show that PPT states form a convex set, while the same is not true for NPT states. The relation between such sets and the set of separable states is represented schematically in Fig.2.1.

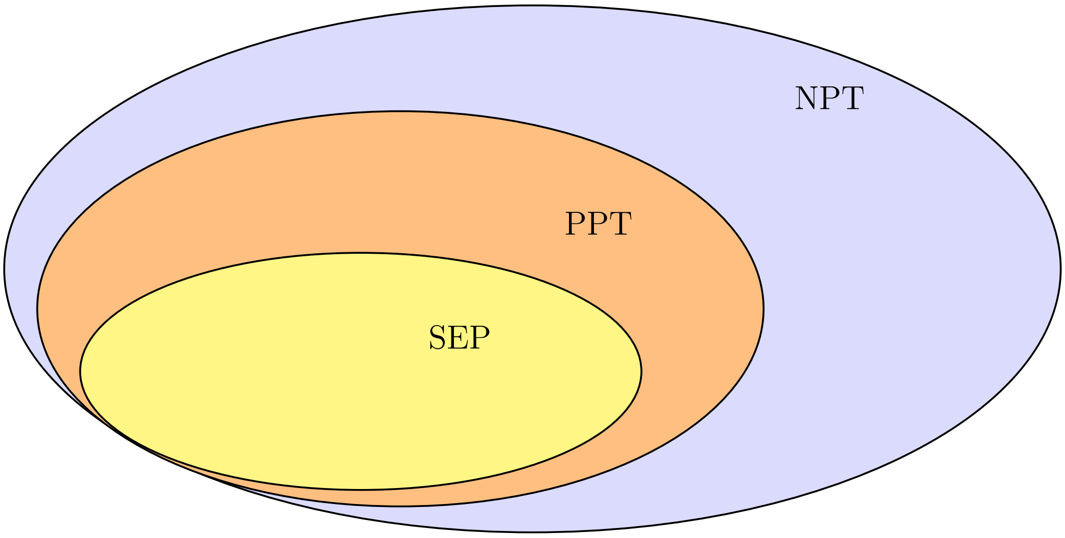

Figure 2.1: Pictorial representation of the convex sets of separable (SEP) and PPT-states (PPT), and the set of NPT states.

With this definitions we are now ready to introduce the PPT-criterion, also called the Peres-Horodecki criterion.

Theorem 2.6 ([Per96; HHH96]). *If $\rho_{AB} \in \mathcal{B}(\mathcal{H}_{AB})$ is a bipartite separable state, then it is PPT.*

Despite its simplicity, the PPT-criterion provides an extremely powerful tool to assess the presence of entanglement in a bipartite state ρ_{AB}. In fact, it is sufficient to compute the spectrum of $\rho_{AB}^{T_A}$ (or, equivalently, of $\rho_{AB}^{T_B}$), and if a negative eigenvalue is found, ρ_{AB} is guaranteed to be entangled. However, when trying to determine if this criterion is also sufficient for separability, some problems arise. In fact, it has been proven [HHH01] that $\rho_{AB}^{T_A}$ does not imply, in general, that the state ρ_{AB} is separable. More formally, we have the following theorem:

Theorem 2.7 ([HHH01]). *Let $\rho_{AB} \in \mathcal{B}(\mathcal{H}_{AB})$ be a bipartite state. If $d = \dim \mathcal{H}_{AB} \leq 6$, ρ_{AB} is separable if and only if $\rho_{AB}^{T_A} \succeq 0$.*

The most remarkable consequence of Th.(2.7) is that there exist some states, dubbed *PPT-entangled*, that display a positive partial transposition but are nevertheless entangled.

PPT-entangled states & bound entanglement

The interest in PPT-entangled states derives from their relation with the so-called *distillation* of entanglement. This problem can be cast as follows: let us suppose we have an arbitrary large (but finite) number of copies of a bipartite entangled state ρ_{AB}, shared between two parties. Is there a way to obtain a singlet using only LOCC? This question is particularly meaningful in the context of quantum communication, where a message, encoded in a register of qubits, is sent to a receiver through a quantum channel. Here, the effective transmission of the message relies crucially on the possibility to dispose of maximally entangled states, i.e., maximally correlated states between the two parties. However, the amount of the entanglement displayed by such states is typically deteriorated when they are sent through the channel, essentially due to the presence of some noise that affects the process. For this reason, techniques to "extract" singlets from an initial large number of entangled states are strongly required to guarantee an effective communication between two distant parties, and indeed there exist protocols of entanglement distillation both for pure and mixed states [BBP+96a; BBP+96b]. Interestingly, not any quantum state can be used for this task: states that allow for entanglement distillation are called distillable, while the others are called undistillable or *bound entangled*, and display the weakest form of entanglement. In [HHH98] it was proved that being PPT is a sufficient condition to be undistillable, and for this reason PPT-entangled states are sometimes referred to as PPT-bound entangled. Examples of PPT-entangled states have been provided using unextendible product basis [BDM+99], and by means of other techniques [BP00; PM07] but their characterisation is, in general, an extremely hard task. Particularly relevant for our analysis are the so-called *edge* states, formally defined as follows:

Definition 2.11. *([LKC+00; LKH+01]) A PPT-entangled state $\delta \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is edge if and only if, for every product vector $|ef\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ and every $\epsilon > 0$, $\delta - \epsilon|ef\rangle\langle ef|$ is not a PPT-entangled state, i.e., it is either $\delta - \epsilon|ef\rangle\langle ef| \ngeq 0$ or $\delta^{T_B} - |ef^*\rangle\langle ef^*| \ngeq 0$, where $*$ denotes the operation of complex conjugation.*

Intuitively, edge states can be found as follows : starting from a PPT-entangled state δ one could subtract projectors $|ef\rangle\langle ef|$ from it until either the resulting state $\delta - |ef\rangle\langle ef|$ or its partial transposition display a negative eigenvalue: in the first case, the state would not be physical, while in the second it would be NPT. Hence, edge states are PPT states that lie on the boundary between the convex sets of PPT and NPT states (see Fig. 2.1). For this reason, they are extreme points in the convex set of PPT states, so that their knowledge is sufficient to construct any other PPT-entangled state. Obviously, being positive under partial transposition, edge states cannot be revealed using the PPT criterion, so that other techniques need to be employed for their detection. Among them, one of the most powerful is known as the range criterion.

Range criterion

When dealing with PPT-entangled states, range criterion [Hor97] is particularly effective in detecting entanglement. Let us first recall the definition of the range of a matrix.

Definition 2.12. *Given a density matrix $\rho \in \mathcal{B}(\mathcal{H})$ we define its range as $\mathcal{R}(\rho) = \{|\psi\rangle \in \mathcal{H} \mid \rho\,|\psi\rangle = |\phi\rangle\,,$ for some $|\phi\rangle \in \mathcal{H}\}$*

Hence, the range criterion can be cast as follows:

Theorem 2.8 ([Hor97])**.** *If a state $\rho_{AB} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is separable, then there exists a set of product vectors $\{|a_i, b_i\rangle\}$ such that $\{|a_i, b_i\rangle\}$ spans $\mathcal{R}(\rho_{AB})$ and $\{|a_i, b_i^*\rangle\}$ spans $\mathcal{R}(\rho_{AB}^{T_B})$.*

As a consequence of Th.2.8, if there exists a vector $|\alpha, \beta\rangle$ such that $|\alpha, \beta\rangle \in \mathcal{R}(\rho_{AB})$ but $|\alpha, \beta^*\rangle \notin \mathcal{R}(\rho_{AB}^{T_B})$, then the state ρ_{AB} is entangled. Recalling Def.2.11, it is easy to see that edge states maximally violate the range criterion. Indeed, we give an alternative definition of an edge state, i.e,

Definition 2.13. *The state $\delta \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is edge if and only if there is no product vector $|ef\rangle \in \mathcal{R}(\delta)$ such that $|ef^*\rangle \in \mathcal{R}(\delta^{T_B})$.*

CCNR criterion

Besides the range criterion, there exists other criteria that are able to detect PPT-entangled states. One of them is the so-called *computable cross norm* or *realignment* (CCNR) criterion [CW03; Rud05]. Before proceeding with its formulation, let us observe that a bipartite state ρ_{AB} can always be decomposed as [Rud05]

$$\rho_{AB} = \sum_k \xi_k F_k^A \otimes F_k^B \,, \tag{2.80}$$

where $\xi_k \geq 0$, and the operators $\{F_k^J\}$ satisfy $\mathrm{Tr}[F_k^J F_{k'}^J] = \delta_{kk'}$ and form an orthonormal basis for the space of the Hermitian operators over $\mathcal{H}_J$, with $J \in \{A, B\}$. Eq.(2.80) represents the analogue of the Schmidt decomposition in the space of Hermitian operators. Hence, the CCNR criterion can be cast as follows:

Theorem 2.9 ([CW03; Rud05]). *If ρ_{AB} is a separable state then*

$$\sum_k \xi_k \leq 1 , \tag{2.81}$$

where ξ_k are the coefficients of the Schmidt decomposition of Eq.(2.80).

Obviously, a violation of condition (2.81) signals the presence of entanglement. The reason for the name of this criterion derives from the fact that it can be recast equivalently in terms of the norm of a matrix $\mathcal{M}(\rho_{AB})$, whose elements are given by

$$\mathcal{M}(\rho_{AB})_{kl}^{ij} \equiv \langle ij|\mathcal{M}(\rho_{AB})|kl\rangle = \langle ik|\rho_{AB}|lj\rangle \equiv (\rho_{AB})_{lj}^{ik} \ . \tag{2.82}$$

Hence, Th.2.9 can be recast equivalently as

Theorem 2.10. *If ρ_{AB} is a separable state then*

$$\|\mathcal{M}(\rho_{AB})\| \leq 1 , \tag{2.83}$$

where $\|\rho\| \equiv \mathrm{Tr}\left[\sqrt{\rho\rho^\dagger}\right]$ is the trace norm of the operator ρ.

Interestingly, in [HHH06] it was shown that the above condition can be generalised to the case of linear *contractions* in the trace norm, i.e., maps $\mathcal{E}$ such that $\|\mathcal{E}(\rho)\| \leq \|\rho\|$. In particular, any linear map that does not increase the trace norm of product states, can be used to deduce a sufficient criterion for separability.

Positive but not completely positive maps

The PPT criterion is a particular case of a separability criterion based on the use of positive but not completely positive maps. Such criterion is based on the observation that for any separable state ρ_{AB} and any positive map $\mathcal{E}$, it must be

$$(\mathbb{1}_A \otimes \mathcal{E})\,[\rho_{AB}] \succeq 0 \ . \tag{2.84}$$

Moreover, it was shown in [HHH96] that the reverse implication must hold for any positive map, i.e.,

Theorem 2.11 ([HHH96]). *A state $\rho_{AB} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is separable if and only if, for every positive map $\mathcal{E} : \mathcal{H}_B \to \mathcal{H}_B$, it holds that $(\mathbb{1}_A \otimes \mathcal{E})\,[\rho_{AB}] \succeq 0$.*

It is clear that the violation of Th.2.11 can be used as a separability criterion. In particular, the characterisation of an entangled state σ can be accomplished by searching for a positive but not completely positive map $\mathcal{E}$ such that $(\mathbb{1}_A \otimes \mathcal{E})\,[\sigma] \not\succeq 0$. An example of such map is the usual transposition $T : \mathcal{B}(\mathcal{H}_B) \to \mathcal{B}(\mathcal{H}_B)$. Indeed, it is easy to check that $T(\rho) = \rho^T \succeq 0$ for all positive operators $\rho \in \mathcal{B}(\mathcal{H}_B)$, although $(\mathbb{1} \otimes T)[\rho_{AB}] \equiv \rho_{AB}^{T_B} \not\succeq 0$, where the last inequality expresses the fact that there exist PPT states that are nevertheless entangled. The use of positive but not completely positive maps as entanglement detectors is a topic that has been widely explored in the literature [Stø63; Wor76; Cho75] and it has been shown that the sufficiency of the PPT criterion relies upon the observation that every positive but not completely positive map in $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C}^2 \otimes \mathbb{C}^3$ is decomposable (see Def.2.5). Another example of a map of this kind is the *reduction map* $\mathcal{E}^R$ [HH99], defined as:

$$\mathcal{E}^R(\rho) = \mathbb{1}\mathrm{Tr}[\rho] - \rho. \tag{2.85}$$

A separable state ρ_{AB} must satisfy condition (2.84) which, in the case of the reduction map, becomes

$$\left(\mathbb{1}_A \otimes \mathcal{E}^R\right)[\rho_{AB}] = \rho_A \otimes \mathbb{1}_B - \rho_{AB} \succeq 0\,, \tag{2.86}$$

a condition known as the *reduction criterion*. Hence, in order to check the separability of a state ρ_{AB}, it is sufficient to compute the spectrum of the reduced density matrix ρ_A (or, equivalently, of ρ_B). As we will see explicitly when dealing with the closely related topic of entanglement witnesses, decomposable maps are not able to detect PPT-entangled states. Nevertheless, starting from the reduction map, one can construct a family of other maps that allow to detect PPT-entangled states in $\mathbb{C}^d \otimes \mathbb{C}^d$, for any even $d \geq 4$. Such maps, dubbed *Breuer-Hall maps* [Bre06; Hal06], are defined as:

$$\mathcal{E}^{BH}(\rho) = \mathbb{1}\mathrm{Tr}[\rho] - U\rho^T U^\dagger\,, \tag{2.87}$$

where U is a unitary operator such that $U^T = -U$. In particular, these maps can certify entanglement in states that the PPT criterion fails to detect.

2.3.4 Entanglement witness

Closely related to positive but not completely positive maps is the concept of entanglement witness (EW).

Definition 2.14. *An Hermitian operator $W \in \mathcal{B}(\mathcal{H}_{AB})$ is said an entanglement witness if:*

- $\mathrm{Tr}[W\rho_{\text{sep}}] \geq 0$, *for every separable state* $\rho_{\text{sep}} \in \mathcal{B}(\mathcal{H}_{AB})$,
- *there exists at least an entangled state* ρ_{ent} *such that* $Tr[W\rho_{\text{ent}}] < 0$.

EWs are endowed with an interesting geometrical interpretation. Let us first introduce the following variant of the celebrated Hahn-Banach theorem [BB11]:

Theorem 2.12. *Let $\mathcal{S}_1, \mathcal{S}_2$ be two disjoint convex closed sets in a Hilbert space, one of them being compact. Then there exists a bounded functional that separates $\mathcal{S}_1$ and $\mathcal{S}_2$.*

Recalling that the set of separable states $\mathcal{S}$ is a closed convex set, the Hahn-Banach theorem states that for every entangled state $\rho_{\text{ent}} \notin \mathcal{S}$ there exists an hyperplane that separates it from $\mathcal{S}$. In particular, choosing W to be the normal vector to the hyperplane, it is possible to quantify the distance of a state ρ from the hyperplane by means of the trace distance, i.e., $\mathrm{Tr}[W\rho]$. Hence, it follows that $\mathrm{Tr}[W\rho_{\text{sep}}] \geq 0$ for all separable states ρ_{sep}, while there exists at least one entangled state ρ_{ent} such that $\mathrm{Tr}[W\rho_{\text{ent}}] < 0$ (see Fig.2.2)

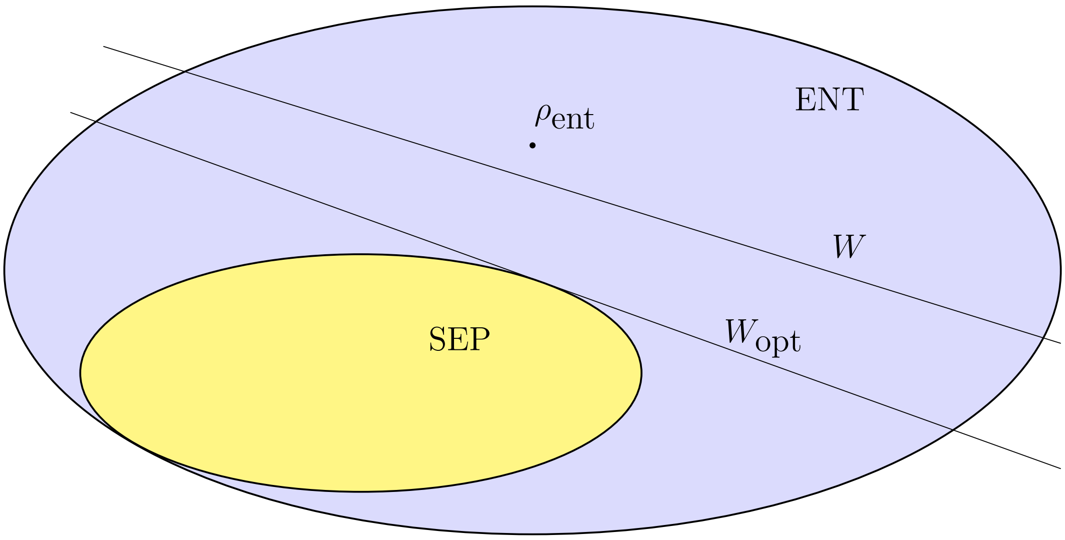

Figure 2.2: Pictorial representation of the convex set of separable states (SEP) and the set of entangled states (ENT). An optimal entanglement witness, W_{opt}, corresponds to a hyperplane which is tangent to the set of separable states.

It is worth to stress that the correspondence between entangled states and EWs is by no means unique and there may exist different witnesses that detect the same state. Moreover, the explicit expression of the witness depends on the entangled state that one wants to detect, a fact that makes the construction of EWs a hard task. Within the set of EWs we distinguish decomposable and non-decomposable.

Definition 2.15. *An EW W is said decomposable if it can be written as $W = P + Q^{T_B}$, with $P, Q \succeq 0$ and where T_B denotes the partial transposition with respect to the subsystem B. Otherwise, W is said non-decomposable.*

Non-decomposable EWs are the only candidates able to detect PPT-entanglement. In fact, given a PPT-entangled state ρ, any decomposable EW fails to detect it since it holds:

$$\mathrm{Tr}[(P + Q^{T_B})\rho] = \mathrm{Tr}[P\rho] + \mathrm{Tr}[Q^{T_B}\rho] = \mathrm{Tr}[P\rho] + \mathrm{Tr}[Q\rho^{T_B}] \geq 0 \,, \tag{2.88}$$

where the last equality follows from the relation $\mathrm{Tr}[XY^{T_B}] = \mathrm{Tr}[X^{T_B}Y]$. For this reason, we can provide an alternative definition of a non-decomposable EW, i.e.,

Definition 2.16. *An EW W is said non-decomposable if and only if it detects at least one PPT-entangled state.*

The definition of decomposability for EWs bears some resemblance with the one that we have introduced in the previous section. Indeed, EWs and positive but not completely positive maps are linked together through the CJS isomorphism, which provide the following relations:

Theorem 2.13 ([SSL+06]). *Given an operator $W \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and its associated map $\mathcal{E}_W : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_A)$ through the CJS isomporphism, the following relations hold:*

- *W is an EW $\iff$ $\mathcal{E}_W$ is positive but not completely positive,*
- *W is a decomposable EW $\iff$ $\mathcal{E}_W$ is a decomposable map*
- *W is a non-decomposable EW $\iff$ $\mathcal{E}_W$ is a positive, non-decomposable map.*

As a consequence, the properties of an EW W can be characterised in terms of those of its related positive but not completely positive map $\mathcal{E}_W$. However, despite their equivalence, it can be shown that they do not detect the same set of entangled states and indeed, a positive but not completely positive map $\mathcal{E}_W$ detects more states than its corresponding EW W [SSL+06].

Another concept of particular interest is that of optimal EW. In order to define this class let us introduce the set Δ_W of the states detected by the EW W, i.e.,

$$\Delta_W = \{\rho \in \mathcal{B}(\mathcal{H}) \mid \mathrm{Tr}[W\rho] < 0\} \; . \tag{2.89}$$

Given two EWs, W_1, W_2, we say that W_1 is finer than W_2 if $\Delta_{W_2} \subset \Delta_{W_1}$, i.e., if W_1 detects more states than W_2. If there exists no other witness finer than W_{opt}, we say that W_{opt} is an optimal EW. More formally, one has the following definition:

Definition 2.17 ([LKC+00]). *An EW W_{opt} is said optimal if and only if for every $\epsilon > 0$ and every $P \succeq 0$, the operator $W' = (1+\epsilon)W_{\mathrm{opt}} - \epsilon P$ is not an EW.*

Interestingly, there exists a sufficient criterion to decide whether an EW is optimal or not.

Theorem 2.14 ([LKC+00]). *Let $W \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ be an EW, and $\{|\alpha_k, \beta_k\rangle\}$ a set of vectors such that*

$$\langle \alpha_k, \beta_k | W | \alpha_k, \beta_k \rangle = 0 \; . \tag{2.90}$$

If $\{|\alpha_k, \beta_k\rangle\}$ spans $\mathcal{H}_A \otimes \mathcal{H}_B$, then W is optimal.

In [LKC+00] a characterisation of optimal witnesses was provided, both for the decomposable and non-decomposable case, along with a method to optimise a generic EW. Notice that, from a geometrical point of view, optimal EWs correspond to the normal vectors to those hyperplanes that are tangent to the convex set of separable states $\mathcal{S}$ (see Fig.2.2).

2.3.5 PPT-symmetric extensions

When one is interested in PPT-entanglement detection, entanglement witnesses are not the only available tool. Another technique, originally propsed in [DPS04] by Spedalieri, Parrilo and Doherty, is based on the construction of *PPT-symmetric extensions* for a given quantum state. Such method is based on the following observation. Let us recall that any separable state $\rho \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ can be decomposed as in Eq.(2.75). If one considers the state $\tilde{\rho} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A)$ given by

$$\tilde{\rho} = \sum_k p_k |\alpha_k\rangle\langle\alpha_k| \otimes |\beta_k\rangle\langle\beta_k| \otimes |\alpha_k\rangle\langle\alpha_k| \; , \tag{2.91}$$

it is easy to see that $\tilde{\rho}$ satisfies three properties:

1. $\mathrm{Tr}_3[\tilde{\rho}] = \rho$, where Tr_3 denotes the trace over the third Hilbert space, which has been chosen equal to $\mathcal{H}_A$.

2. $P_{13}\tilde{\rho}P_{13} = \tilde{\rho}$, where P_{13} is the swap operator exchanging the first with the third party, i.e.,
$$P_{13}\left|i\right\rangle\left|j\right\rangle\left|k\right\rangle = \left|k\right\rangle\left|j\right\rangle\left|i\right\rangle \ . \tag{2.92}$$

3. $(\tilde{\rho})^{T_i} \succeq 0$, where T_i denotes the partial transposition with respect to the i-th party, with $i \in \{1, 2, 3\}$. Notice that, since the first and the third parties coincide, it follows $(\tilde{\rho})^{T_1} = (\tilde{\rho})^{T_3}$.

This procedure can be generalised to the case of any state ρ. In particular, we say that a state $\tilde{\rho}$ that satisfies the three above properties defines a *PPT-symmetric extension* of ρ to two copies of $\mathcal{H}_A$. Obviously, one could consider extensions to more copies of $\mathcal{H}_A$ (or, equivalently, $\mathcal{H}_B$), a procedure that would result in the construction of a hierarchy where each level refers to the number of copies involved in a given extension. Since we have shown that any separable state always admits a PPT-symmetric extension, this observation can be used as a separability criterion, so that any state which does not admit a PPT-symmetric extension at a certain level of the hierarchy must be entangled. Although it is unknown, in general, at which level of the hierarchy an entangled state fails the test, such level is always guaranteed to exist or, stated differently, the hierarchy is complete [DPS02]. More importantly, the structure of these tests can be cast as a semidefinite program (SDP), a class of problems related with the optimization of a convex function. Besides of the possibility to implement them numerically in an effective way, SDP programs possess also an equivalent description in terms of their so-called dual formulation [VB96], a property that allows, given an entangled state, to find the EW that detects it [DPS02].

2.4 Non-locality

The concept of non-locality appeared for the first time in Physics in 1935 when Albert Einstein, Boris Podolsky and Nathan Rosen published a paper that was destined to change forever our understanding of quantum theory [EPR35]. In their seminal work they presented a thought experiment, nowadays referred to as the EPR paradox, where they observed that a measurement on a particle could affect its entangled pair, despite the fact that the two subsystems were spatially separated. This "*spooky action at distance*", as Einstein referred to it, seemed to violate the principles of Relativity, which forbid a superluminal exchange of information between two distant parties. For this reason, the authors concluded that quantum theory must be incomplete, the reason lying in our ignorance of some local properties, dubbed *hidden variables*, whose knowledge would prevent the paradox of an instantaneous communication. Almost thirty years later, in 1964, J.S.Bell showed that the contradiction lied in the requirement that quantum theory had to be compatible with the physical principle of *local realism*, consisting of two assumptions: i) two distant observers cannot exchange information instantaneously (principle of locality), and ii) physical quantities of interest have well defined values before a measurement is performed (realism). Bell's theorem proves that quantum theory is incompatible with local realism, ruling out the existence of a local hidden variable model. As a consequence there are only two possibilities: either one saves realism and admits the presence of non-local correlations between two distant parties, or one retains the principle of locality and thus discards the existence of a hidden variable model. Quoting John S. Bell: "If (a hidden-variable theory) is local it will not agree with quantum mechanics, and if it agrees with quantum mechanics it will not be local" [BA04]. The first experimental proof of Bell's theorem came in 1982 thanks to Alain Aspect [AGR82] and, ever since then, its validity has been confirmed by many other experiments [PBD+00; RKM+01; GMR+13]. Operationally, non-locality is assessed by means of *Bell inequalities*, i.e., mathematical correlations between the measurement outcomes of two or more parties.

2.4.1 The Bell experiment

A multipartite Bell experiment consists of N spatially separated observers, having access to an N-partite shared resource. Each party, labelled by an index $i \in \{1, \ldots, N\}$, performs one out of m possible measurements, i.e., $x_i \in \{1, \ldots, m\}$, yielding one out of Δ possible outcomes, i.e., $a_i \in \{1, \ldots, \Delta\}$. Such a scenario is commonly described by assigning the triplet (N, m, Δ). After repeating this procedure several times, the statistics collected through the experiment can be described in terms of the correlations between the input measurement settings and the obtained outcomes. Labelling $\boldsymbol{x} = (x_1, \ldots, x_N)$ the measurements for the N parties and $\boldsymbol{a} = (a_1, \ldots, a_N)$ the associated outcomes, such correlations can be described in terms of the conditional probability to find the output $\boldsymbol{a}$ given the input setting $\boldsymbol{x}$, i.e.,

$$P(\boldsymbol{a}|\boldsymbol{x}) \equiv P(a_1, \ldots, a_i, \ldots, a_N | x_1, \ldots, x_i, \ldots, x_N) \,. \tag{2.93}$$

Notice that, since $P(\boldsymbol{a}|\boldsymbol{x})$ has to be a valid probabilistic distribution, it must satisfy the positivity constraint $P(\boldsymbol{a}|\boldsymbol{x}) \geq 0$, as well as the normalization condition

$$\sum_{a_1=1}^{\Delta} \cdots \sum_{a_N=1}^{\Delta} P(a_1, \ldots, a_N | x_1, \ldots, x_N) = 1 \ . \tag{2.94}$$

Hence, we can interpret $P(\boldsymbol{a}|\boldsymbol{x})$ as a point in the subspace $\mathcal{P} \subset \mathbb{R}^{(\Delta m)^N}$. It is easy to show that $\mathcal{P}$ is a convex set, that is, for any $P_1, P_2 \in \mathcal{P}$ and any $\lambda \in [0,1]$, we have $\lambda P_1 + (1-\lambda) P_2 \in \mathcal{P}$. Convex sets which are also compact and possess a finite number of extreme points are dubbed (convex) *polytopes*. As a consequence of the Minkowski's theorem [Grü03], polytopes can be either characterised in terms of such extreme points, called *vertices*, or as the intersection of a minimal number of half-spaces, called the *facets* of the polytope, which are strictly related with Bell inequalities. Notice that, so far, the only constraints on $P(\boldsymbol{a}|\boldsymbol{x})$ derive from the mathematical requirement for them to be probabilities. As we will see in the following, the choice of an underlying physical model will result in additional constraints on the set of such correlations.

No-signalling correlations

A first constraint derives from the *no-signalling* principle, which rules out the possibility of an instantaneous communication among the parties. Formally, this requirement translates to the conditions

$$\sum_{a_i=1}^{\Delta} P(\boldsymbol{a}|\boldsymbol{x}) = \sum_{a_i=1}^{\Delta} P(\boldsymbol{a}|\boldsymbol{x}') \quad \forall x_i \neq x'_i \ , \tag{2.95}$$

with $\boldsymbol{x}' = (x_1, \ldots, x'_i, \ldots, x_N)$. Eq.(2.95) has the following physical interpretation: the choice of a measurement setting made by one of the parties cannot influence the outcomes observed by the others. It can be shown that the set of those correlations that satisfy Eq.(2.95) defines the so-called no-signalling polytope, denoted with the symbol $\mathcal{NS}$.

Quantum correlations

Another possible requirement is that the probability distribution $P(\boldsymbol{a}|\boldsymbol{x})$ is obtained from an N-partite quantum state $\rho \in \mathcal{B}(\mathcal{H})$ on which some local measurements

$\{\mathcal{M}^{(i)}_{a_i|x_i}\}$ are performed, i.e.,

$$P(a_1,\ldots,a_i,\ldots,a_N|x_1,\ldots,x_i,\ldots,x_N) = \mathrm{Tr}\left[\bigotimes_{i=1}^{N}\mathcal{M}^{(i)}_{a_i|x_i}\rho\right] . \tag{2.96}$$

Here, $\{\mathcal{M}^{(i)}_{a_i|x_i}\}$ defines a set of positive-operator valued measurements (POVM), satisfying $\mathcal{M}^{(i)}_{a_i|x_i} \succeq 0,\ \sum_{a_i}\mathcal{M}^{(i)}_{a_i|x_i} = \mathbb{1}^{(i)}, \forall i = 1,\ldots,N$. In this case, it is possible to show that the probabilities that satisfy Eq.(2.96) form a convex set, denoted with the symbol $\mathcal{Q}$, which is nothing but the set of quantum states. However, since the boundary of $\mathcal{Q}$ cannot be characterised in terms of a finite number of extreme points, $\mathcal{Q}$ is not a convex polytope.

Local correlations

A further type of correlations derives from the requirement that the parties of the Bell experiment can communicate using only local strategies. Formally, this is equivalent to a scenario where a certain resource λ, commonly referred to as *shared randomness*, is distributed among the parties with a certain probability distribution $p(\lambda)$. Hence, each probability $P(\boldsymbol{a}|\boldsymbol{x})$ which is compatible with this constraint can be cast as

$$P(\boldsymbol{a}|\boldsymbol{x}) = \int_\Lambda d\lambda p(\lambda)\Pi_{i=1}^{N}P(a_i|x_i,\lambda) , \tag{2.97}$$

where $p(\lambda) \geq 0,\ \int_\Lambda d\lambda p(\lambda) = 1$, and Λ is the space associated to the variable λ. The set of probabilities which satisfy Eq.(2.97) defines the so-called local polytope, denoted $\mathcal{L}$.

2.4.2 Bell inequalities

The three sets of correlations introduced so far are not unrelated. In fact, it can be shown (see for example [Pit86]) that any set of local correlations admits a representation of the form of Eq.(2.96), so that $\mathcal{L} \subset \mathcal{Q}$. Moreover, any quantum correlation satisfies the no-signalling constraint, implying that $\mathcal{Q} \subset \mathcal{NS}$. Hence, the following inclusions hold, i.e., $\mathcal{L} \subset \mathcal{Q} \subset \mathcal{NS}$. Since they are all convex sets and, in addition, $\mathcal{L}$ and $\mathcal{NS}$ are also polytopes, we can apply the Hahn-Banach theorem, so that for any probability $\hat{P}(\boldsymbol{a}|\boldsymbol{x}) \notin \mathcal{S} = \{\mathcal{L},\mathcal{Q},\mathcal{NS}\}$ there exists an hyperplane separating $\hat{P}(\boldsymbol{a}|\boldsymbol{x})$ from $\mathcal{S}$. In particular, this separation condition can be expressed in terms of an inequality that is satisfied by every correlation $P(\boldsymbol{a}|\boldsymbol{x}) \in \mathcal{S}$ but is violated by $\hat{P}(\boldsymbol{a}|\boldsymbol{x})$. When $\mathcal{S} = \mathcal{L}$, such inequality is commonly referred to as a

Bell inequality. Sometimes, when $\mathcal{S} = \mathcal{Q}$, the term *quantum Bell inequality* is used. Unless further specified, in this thesis we will deal exclusively with the first type of Bell inequalities.

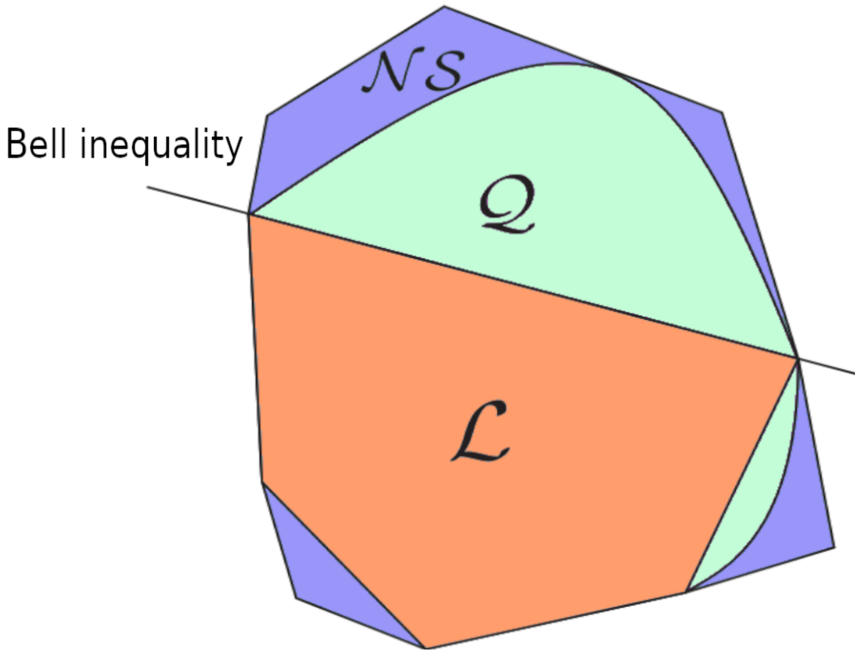

Figure 2.3: Pictorial representation of the convex sets of no-signalling ($\mathcal{NS}$), quantum ($\mathcal{Q}$) and local ($\mathcal{L}$) correlations. (Tight) Bell inequalities correspond to the facets of the local polytope $\mathcal{L}$.

Analogously to the case of EWs, also in this case, due to the Hahn-Banach theorem, we can interpret Bell inequalities as the hyperplanes which are parallel to the facets of the local polytope $\mathcal{L}$ and indeed it can be shown that Bell inequalities are nothing but a particular kind of EWs. Particularly relevant are those Bell inequalities, dubbed *tight*, that are tangent to the facets of $\mathcal{L}$. In fact, exactly as optimal EWs, tight inequalities are those that provide a minimal representation of $\mathcal{L}$, meaning that any other Bell inequality can be written as a convex combination of them (see Fig.2.3). Characterising the facets of the local polytope, and thus the corresponding tight Bell inequalities, is a tremendously hard task whose solution poses a hard challenge even in the case of a small number of parties and measurement settings [Śli03]. In order to get an intuition of this complexity, let us restrict without loss of generality to the case of bipartite outcomes, i.e., $\Delta = 2$. In this case it is possible to recast the original problem in terms of the *correlators* between the parties. If we denote as $\mathcal{M}_{x_i}^{(i)}$ the measurement performed by the i-th party corresponding to the measurement setting x_i, the k-th order correlator is defined as

$$\langle \mathcal{M}_{x_{i_1}}^{(i_1)} \dots \mathcal{M}_{x_{i_l}}^{(i_k)} \rangle = \sum_{a_{i_1}} \cdots \sum_{a_{i_k}} (-1)^{\sum_{j=1}^{k} a_{i_j}} P(a_{i_1} \dots a_{i_k} | x_{i_1} \dots x_{i_k}) \,, \tag{2.98}$$

where $0 \leq i_1 < \dots i_k < N, x_{i_l} \in \{0,1\}, a_{i_l} \in \{-1,1\}, 1 \leq k \leq N$ and $\langle \dots \rangle$ denotes the expectation value of an operator. Hence, in the multipartite scenario, a complete characterisation of a Bell experiment requires the construction of the correlators of any order, a task whose complexity quickly grows with the number of the parties [WW01; ŻB02]. When dealing with experiments, the quantities one has typically access to are correlators of small order. For this reason it becomes natural to ask whether non-locality in many-body systems can be revealed with correlators involving only few parties. As we will discuss thoroughly in section 2.5, we will see that, when dealing with systems of indistinguishable particles, this is indeed the case and the presence of non-local correlations can be assessed by means of only one- and two-body correlators [TAS+14].

2.5 Systems of indistinguishable particles

As we have seen in the previous sections, the characterisation of both entanglement and non-local correlations is, in general, an NP-hard task and usually a solution can be found only in some specific cases. For this reason, it can be argued that dealing with systems endowed with symmetries can reduce the original complexity of both tasks, and indeed, as we shall see in the following chapters, symmetries provide a useful framework where the original problem can be rephrased in an easier way. In this section we discuss the case of systems of indistinguishable particles, along with the mathematical tools that are needed for their description.

2.5.1 Permutationally invariant states

A first natural symmetry one can consider is the permutationally invariance between the parties of a composite system. This symmetry appears in many situations of physical interest, for example when one considers the state of a system of indistinguishable particles (e.g., bosons) which has to remain invariant under the swapping of any pair of subsystems. Formally, this requirement can be expressed by considering the group of permutations N elements, $\mathcal{G}_N$. If $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ is an N-partite Hilbert space, the action of an element $\pi \in \mathcal{G}_N$ on a vector

$|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_N\rangle \in \mathcal{H}$ can be described as

$$P_\pi |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_N\rangle = |\psi_{\pi^{-1}(1)}\rangle \otimes |\psi_{\pi^{-1}(2)}\rangle \otimes \cdots \otimes |\psi_{\pi^{-1}(N)}\rangle \ , \tag{2.99}$$

where P_π is a unitary representation of the permutation π (e.g., a permutation matrix). Hence, we have the following definition:

Definition 2.18. *Let $\rho \in \mathcal{B}(\mathcal{H})$, where $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ is an N-partite Hilbert space. We say that ρ is a permutationally invariant state if, for every $\pi \in \mathcal{G}_N$, the following relation holds, i.e.,*

$$\rho = P_\pi \rho P_\pi^\dagger \, . \tag{2.100}$$

2.5.2 Schur-Weyl duality

In the case of permutationally invariant (PI) states there exists a famous result from representation theory, known as Schur-Weyl duality, which asserts that any N-partite Hilbert space $\mathcal{H} = (\mathbb{C}^d)^N$ admits a decomposition of the form

$$(\mathbb{C}^d)^N \cong \bigoplus_{\lambda \vdash (d,N)} \mathcal{H}_\lambda \otimes \mathcal{K}_\lambda \ , \tag{2.101}$$

where $\mathcal{H}_\lambda$ and $\mathcal{K}_\lambda$ are irreducible representations of the permutation group $\mathcal{G}_N$ and the group $\mathcal{U}_d$ of unitary matrices of order d, respectively. Here the sum runs over the partitions λ of N with at most d elements. As a consequence, a PI state $\rho \in \mathcal{H}$ is block-diagonal in the basis of Eq.(2.101). When dealing with qubits, i.e., $d = 2$, Eq.(2.101) can be written explcitely as

$$(\mathbb{C}^2)^N \cong \bigoplus_{J=J_{min}}^{N/2} \mathcal{H}_J \otimes \mathcal{K}_J \ , \tag{2.102}$$

where the Hilbert spaces $\mathcal{H}_J$ have dimension $\dim \mathcal{H}_J = 2J+1$, and $\mathcal{K}_J$ are called multiplicity spaces, with dimension 1 if $J = N/2$ and

$$\dim \mathcal{K}_J = \binom{N}{N/2 - J} - \binom{N}{N/2 - J - 1} \ , \quad J \neq N/2 \, . \tag{2.103}$$

Notice that Eq.(2.102) corresponds to the decomposition of the Hilbert space of a system of N spin-$\frac{1}{2}$ particles and, for this reason, $\mathcal{H}_J$ are sometimes referred to as spin Hilbert spaces. Hence, a PI state possesses a block-diagonal decomposition in this basis given by

$$\rho = \bigoplus_{J=J_{min}}^{N/2} \frac{p_J}{\dim \mathcal{K}_J} \mathbb{1}_J \otimes \rho_J \ , \tag{2.104}$$

where $\rho_J \in \mathcal{B}(\mathcal{H}_J)$ and p_J defines a probability distribution. Particularly relevant for our analysis is the block of maximum spin, i.e., $J = N/2$, which is spanned by the so-called *Dicke states.*

2.5.3 Dicke states

Dicke states [Dic54] have firstly been introduced in quantum optics to describe the interaction between a single-mode photon and a system of N spin-$\frac{1}{2}$ particles. In this context, denoting $\sigma_\alpha^{(i)}, \alpha \in \{x, y, z\}$ the Pauli matrix σ_α for the i-th subsystem, and $J_\alpha = \frac{1}{2}\sum_{i=1}^N \sigma_\alpha^{(i)}$ the total angular momentum along the direction α, Dicke states are usually defined as the simultaneous eigenstates of the operators J_z and $J^2 = J_x^2 + J_y^2 + J_z^2$. Alternatively, Dicke states correspond to superposition of states with the same number of excitations, according to the following definition:

Definition 2.19. *Let $\mathcal{H} = (\mathbb{C}^d)^{\otimes N}$. The Dicke states correspond to superpositions of k_1 qudits in the state $|0\rangle$, k_1 qudits in the state $|1\rangle$, etc., of the form*

$$|D_{\boldsymbol{k}}\rangle = C(N, \boldsymbol{k})^{-1/2} \sum_{\pi \in \mathcal{G}_N} \pi(|0\rangle^{\otimes k_0} \otimes |1\rangle^{\otimes k_1} \otimes \cdots \otimes |d-1\rangle^{\otimes d-1}) \ , \tag{2.105}$$

where π is a permutation operator, $\boldsymbol{k} = (k_0, \ldots, k_{d-1})$ is a partition of N, i.e., $k_i \geq 0, \sum_{i=0}^{d-1} k_i = N$, and $C(N, \boldsymbol{k})$ is a normalization factor given by

$$C(N, \boldsymbol{k}) = \binom{N}{\boldsymbol{k}} = \frac{N!}{k_0! k_1! \cdots k_{d-1}!} \ . \tag{2.106}$$

The Dicke states, sometimes referred to as *symmetric states*, span the symmetric subspace $\mathcal{S}(\mathcal{H})$, corresponding to the block $\lambda = (N)$ in Eq.(2.101), with dimension $\dim \mathcal{S}(\mathcal{H}) = \binom{N+d-1}{d-1}$.

3

Entanglement in symmetric states

Papà, radice e luce, portami ancora per mano
nell'ottobre dorato del primo giorno di scuola.
Le rondini partivano, strillavano:
fra cinquant'anni ci ricorderai.
Maria Luisa Spaziani

In this chapter we present our results concerning the characterisation of the entanglement for bipartite symmetric states of two qudits for generic dimension d. Remarkably, despite the apparent simplicity of the symmetric subspace due to its reduced dimensionality (namely, $d(d+1)/2$ instead of d^2), the characterisation of entanglement remains, in general, an open problem. In this case, we demonstrate that there exists a set of matrices, known as copositive, that act as entanglement witnesses. Further, we demonstrate that there exists a close relation between copositive matrices and entanglement in symmetric states allowing to construct decomposable, optimal and non decomposable entanglement witnesses from the properties of the copositive cone. In section 3.1 we introduce the basic definitions along with the main results regarding the theory of copositive matrices. In section 3.2.2 we show how to construct an EW for a subclass of symmetric states of two qudits, known as diagonal symmetric states. In section 3.2.3 we discuss the extension of our construction to the the symmetric case, providing some families of PPT-entangled states that are detected by our EWs. Results of section 3.2.2 and section 3.2.3 are based on the work [MAT+21].

3.1 Copositive matrices

Copositive matrices are a set of real matrices that find application in a variety of different fields, ranging from spectral clustering [DHS05] and dynamical systems [MS07; BKS12] to Markovian models of DNA evolution [Kel94], just to name a few. Recently, a renovated interest in copositive matrices has sparked from the possibility to use them as a tool in combinatorial and nonconvex quadratic optimization problems [Bom12; Dür10]. Formally, copositive matrices are defined as follows:

Definition 3.1. *A real symmetric matrix, H, is copositive if and only if $\boldsymbol{x}^T H \boldsymbol{x} \geq 0, \forall \boldsymbol{x} \geq 0$ component-wise.*

Notice that copositive matrices have non-negative diagonal elements. In fact, denoting $\boldsymbol{e}_i = (0, \ldots, 1, \ldots, 0)$ has the basis vector of $\mathbb{R}^+$ with a one in the i-th position, copositivity requires $\boldsymbol{e}_i^T H \boldsymbol{e}_i = H_{ii} \geq 0,\ \forall i = 1, \ldots, d$. It is easy to see that every positive semidefinite matrix is copositive but the converse is not necessarily true. Deciding whether a matrix H is copositive is a difficult task and indeed, it has been proved that checking membership in $\mathcal{COP}_d$ is a co-NP hard problem [MK87]. The connection between the two sets of matrices can be better understood if one introduces the concept of *convex cone*.

Definition 3.2. *A set K in a vector space V is called a convex cone if for every element $\boldsymbol{x}_1, \boldsymbol{x}_2 \in K$ and non-negative scalars α, β, $\alpha \boldsymbol{x}_1 + \beta \boldsymbol{x}_2 \in K$.*

Examples of convex cones are the set of positive semidefinite matrices and the set of non-negative matrices, defined, respectively, as $\mathcal{PSD}_d = \{A \in S_d \mid A \succeq 0\}$, $\mathcal{N}_d = \{A \in S_d \mid A_{ij} \geq 0\ \forall i, j\}$, where S_d denotes the set of symmetric $d \times d$ matrices. Similarly, also the set of copositive matrices forms a convex cone, denoted as $\mathcal{COP}_d$, and the inclusion $\mathcal{PSD}_d + \mathcal{N}_d \subseteq \mathcal{COP}_d$ holds. Surprisingly enough, in his seminal paper of 1962, Diananda proved that the equality holds only for $d < 5$:

Theorem 3.1 ([Dia62])**.** *Let $d < 5$. Then $\mathcal{COP}_d = \mathcal{PSD}_d + \mathcal{N}_d$.*

In $d \leq 4$ there exist sufficient criteria to ensure copositivity.

Theorem 3.2 ([ACE95]). *A symmetric matrix H of order 2 is copositive if and only if*

$$H_{00} \geq 0, \quad H_{11} \geq 0 \tag{3.1}$$

$$H_{01} + \sqrt{H_{00}H_{11}} \geq 0 \tag{3.2}$$

Theorem 3.3 ([CS94]). *A symmetric matrix H of order 3 is copositive if and only if the following inequalities are satisfied*

$$H_{00} \geq 0, \quad H_{11} \geq 0, \quad H_{22} \geq 0\,, \tag{3.3}$$

$$\hat{H}_{01} \equiv H_{01} + \sqrt{H_{00}H_{11}} \geq 0\,, \tag{3.4}$$

$$\hat{H}_{02} \equiv H_{02} + \sqrt{H_{00}H_{22}} \geq 0\,, \tag{3.5}$$

$$\hat{H}_{12} \equiv H_{12} + \sqrt{H_{11}H_{22}} \geq 0\,, \tag{3.6}$$

along with the condition

$$\sqrt{H_{00}H_{11}H_{22}} + H_{12}\sqrt{H_{00}} + H_{02}\sqrt{H_{11}} + H_{01}\sqrt{H_{22}} + \sqrt{2\hat{H}_{01}\hat{H}_{02}\hat{H}_{12}} \geq 0\,. \tag{3.7}$$

A similar result has been proved also for the case $d = 4$ (see [PY93]), but we omit it here for the sake of simplicity. In higher dimension, there exist several other criteria but none of them is sufficient to ensure membership in $\mathcal{COP}_d$ (for a review of some of these criteria see e.g., [HS10; BDS15]).

Exceptional matrices

Theorem 3.1 fails for $d \geq 5$ and a counterexample is given by the so-called Horn matrix [Dia62], i.e.,

$$H_5 = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}. \tag{3.8}$$

Notice that $H_5 \in \mathcal{COP}_d \backslash (\mathcal{PSD}_d + \mathcal{N}_d)$. Matrices of this type are dubbed *exceptional* matrices.

Definition 3.3. *A $d \times d$ copositive matrix H is said to be exceptional if and only if H cannot be decomposed as the sum of a positive semidefinite matrix ($\mathcal{PSD}_d$), and a symmetric entry-wise non-negative matrix ($\mathcal{N}_d$), i.e., $H \in \mathcal{COP}_d \setminus (\mathcal{PSD}_d + \mathcal{N}_d)$.*

As we will see in section 3.2.2, exceptional matrices play a fundamental role in the entanglement detection for bipartite symmetric states and, for this reason, their characterisation is particularly valuable. In [JR08] a method to construct exceptional copositive matrices is proposed but the requirements are quite restrictive and in general there exist only few necessary criteria to check membership in the set of exceptional matrices.

Extreme matrices

Finally, among copositive matrices, we distinguish extreme copositive matrices, that stand out for their impossibility to be decomposed. First, we introduce the definition of an *extreme ray* of a convex cone.

Definition 3.4. *Let K be a convex cone. If $\boldsymbol{x} = \boldsymbol{x}_1 + \boldsymbol{x}_2 \in K$, with $\boldsymbol{x}_1, \boldsymbol{x}_2 \in K$ implies that $\boldsymbol{x}_1 = a\boldsymbol{x}, \boldsymbol{x}_2 = (1-a)\boldsymbol{x}$ for all $a \in [0,1]$, then $\boldsymbol{x}$ is said an extreme vector of K and the cone $\{\boldsymbol{x}\} = \{\alpha\boldsymbol{x}, 0 \leq \alpha \in \mathbb{R}\}$ is called an extreme ray of K.*

Hence, the definition of extreme copositive matrix follows naturally.

Definition 3.5. *A $d \times d$ copositive matrix H is said to be extreme if $H = H_1 + H_2$ with H_1, H_2 copositive, implies $H_1 = aH, H_2 = (1-a)H$ for all $a \in [0,1]$.*

Examples of extreme copositive matrices of order d are:

I. $\boldsymbol{e}_i\boldsymbol{e}_i^T,\ i \in \{1,\dots,d\}$,

II. $\boldsymbol{e}_i\boldsymbol{e}_j^T + \boldsymbol{e}_j\boldsymbol{e}_i^T,\ 1 \leq i < j \leq d$,

III. $\boldsymbol{x}\boldsymbol{x}^T,\ \boldsymbol{x} \in \mathbb{R}^d_+$.

In $d < 5$ the above examples represent the only possible extreme copositive matrices. In fact, recalling that in this case $\mathcal{COP}_d = \mathcal{PSD}_d + \mathcal{N}_d$, it is possible to show that matrices of type I and II are extreme for the cone $\mathcal{N}_d$, while matrices of type III are extreme for $\mathcal{PSD}_d$ [BS03]. However, when $d \geq 5$, other types of extreme matrices are possible, besides the ones considered before. A necessary condition for extremality, which we introduce here for further convenience, is provided by the following theorem:

Theorem 3.4 ([Bau66])**.** *Let $H \in \mathcal{COP}_d$ be an extreme copositive matrix. Then, for every $\varepsilon > 0$ and for every $i \in \{1,\dots,d\}$, it holds*

$$\boldsymbol{x}^T H \boldsymbol{x} - \varepsilon x_i^2 \ngeq 0 , \tag{3.9}$$

for any $\boldsymbol{x} \in \mathbb{R}^d_+$.

Finally, let us conclude this section with an important observation. If we define the boundary of $\mathcal{COP}_d$ as the set

$$\partial\mathcal{COP}_d = \{H \in S_d \mid \boldsymbol{x}^T H \boldsymbol{x} = 0, \forall \boldsymbol{x} \in \mathbb{R}^d_+\}, \tag{3.10}$$

it can be shown that extreme copositive matrices belong to $\partial\mathcal{COP}_d$. However, not every matrix that lies on the boundary of the cone of copositive matrix is necessarily extreme. In Fig.3.1 we illustrate, schematically, the relation between the aforementioned classes of copositive matrices.

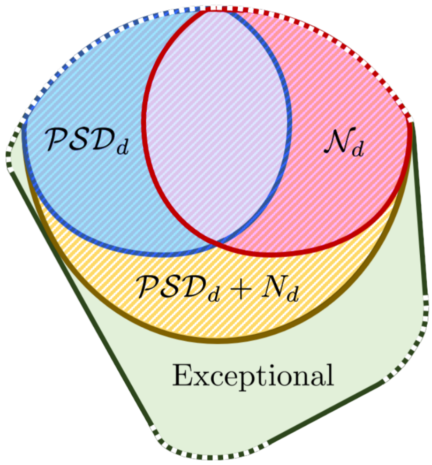

Figure 3.1: Pictorial representation of the cone of copositive matrices, $\mathcal{COP}_d$, and the cones $\mathcal{PSD}_d$ and $\mathcal{N}_d$ of positive semidefinite and non-neegative matrices, respectively. The striped region has been overmagnified for clarity and represents the convex hull of the cones $\mathcal{PSD}_d$ (blue) and $\mathcal{N}_d$ (pink), denoted as $\mathcal{PSD}_d + \mathcal{N}_d$ (yellow). Note that exceptional copositive matrices exist only for $d > 5$ (green). Extremal copositive matrices lie at the border of the cone $\mathcal{COP}_d$ (dashed line).

Completely positive matrices

Completely positive matrices are strictly related to copositive matrices. Formally, one has the following definition.

Definition 3.6. *Let A be a $d \times d$ matrix. A is said completely positive if and only if there exists a non-negative $d \times k$ matrix, C, such that $A = CC^T$, for some $k \geq 1$.*

Notice that the definition of completely positivity for matrices has nothing to do with the same notion for linear maps. Completely positive matrices form a cone, denoted as $\mathcal{CP}_d$, which is the so-called *dual cone* of $\mathcal{COP}_d$.

Definition 3.7. *Let K be a set in a vector space V with inner product $\langle \cdot, \cdot \rangle$. The dual cone of K, denoted as K^*, is the set*

$$K^* = \{\boldsymbol{y} \in V \mid \langle \boldsymbol{x}, \boldsymbol{y} \rangle \geq 0, \forall \boldsymbol{x} \in K\} \,. \tag{3.11}$$

When dealing with cones of matrices it is customary to assume the inner product to be the Hilbert-Schmidt scalar product between two matrices, i.e., $\langle A, B \rangle = \mathrm{Tr}[A^\dagger B]$.

3.2 Entangled states in $\mathbb{C}^d \otimes \mathbb{C}^d$

In what follows we focus on bipartite systems and we denote $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$ the finite dimensional Hilbert space of two qudits. In particular, we are interested in the symmetric subspace $\mathcal{S} \equiv \mathcal{S}(\mathcal{H}) \subset \mathcal{H}$ which, as we have seen in chapter 2, corresponds to the subspace of maximum spin in the Schur-Weyl representation and is spanned by the Dicke states. In the case of two qudits, the Dicke states of Eq.(2.19) take a simpler expression, i.e.,

$$|D_{ii}\rangle \equiv |ii\rangle \;\;, \quad |D_{ij}\rangle \equiv \frac{|ij\rangle + |ji\rangle}{\sqrt{2}} \;\;, \quad i \neq j \;, \tag{3.12}$$

where $\{|i\rangle\}_{i=0}^{d-1}$ is an orthonormal basis of $\mathbb{C}^d$. Notice that the dimension of $\mathcal{S}$ is given by $\dim(\mathcal{S}) = d(d+1)/2$. In an abuse of language, we refer to symmetric quantum states, $\rho_S \in \mathcal{B}(\mathcal{S})$, as the convex hull of projectors onto pure symmetric normalised states, i.e.,

$$\rho_S = \sum_k p_S^{(k)} \, |\Psi_S^{(k)}\rangle \, \langle \Psi_S^{(k)}| \;\;, \tag{3.13}$$

with $p_S^{(k)} \geq 0 \,, \sum_k p_S^{(k)} = 1$ and $|\Psi_S^{(k)}\rangle = \sum_{ij} c_{ij}^{(k)} \, |D_{ij}\rangle$, $c_{ij}^{(k)} \in \mathbb{C}$.
Thus, any $\rho_S \in \mathcal{B}(\mathcal{S})$ is a positive semidefinite operator ($\rho_S \succeq 0$) with unit trace ($\mathrm{Tr}(\rho_S) = 1$), fulfilling the condition

$$\Pi_S \rho_S \Pi_S = \rho_S \;, \tag{3.14}$$

where $\Pi_S = \frac{1}{2}(\mathbb{1} + F)$ is the projector onto the symmetric subspace of two qudits and $F = \sum_{i,j=0}^{d-1} |ij\rangle\langle ji|$ is the so-called flip operator. Notice that, since Π_S is a projector (i.e., $\Pi_S^2 = \Pi_S$), Eq.(3.14) implies that symmetric states satisfy also the following relations

$$\Pi_S \rho_S = \rho_S \Pi_S = \rho_S \tag{3.15}$$

$$F \rho_S = \rho_S F = \rho_S \;. \tag{3.16}$$

Using the Dicke basis, symmetric quantum states can be compactly expressed as follows:

Definition 3.8. *Any bipartite symmetric state, $\rho_S \in \mathcal{B}(\mathcal{S})$, can be written as*

$$\rho_S = \sum_{\substack{0\leq i\leq j<d \\ 0\leq k\leq l<d}} \left(\rho_{ij}^{kl} \left|D_{ij}\right\rangle \left\langle D_{kl}\right| + \text{h.c.}\right) \ , \tag{3.17}$$

with $\rho_{ij}^{kl} \in \mathbb{C}$. Notice that, due to the symmetry of the Dicke states, it holds that $\rho_{ij}^{kl} = \rho_{ji}^{kl} = \rho_{ij}^{lk} = \rho_{ji}^{lk}\ \forall i, j, k, l$.

Convex mixtures of projectors onto Dicke states are denoted as diagonal symmetric (DS) states, since they are diagonal in the Dicke basis. They form a convex subset of $\mathcal{S}$ and are particularly relevant for our analysis.

Definition 3.9. *Any DS state, $\rho_{DS} \in \mathcal{B}(\mathcal{S})$, is of the form*

$$\rho_{DS} = \sum_{0\leq i\leq j<d} p_{ij} \left|D_{ij}\right\rangle \left\langle D_{ij}\right| , \tag{3.18}$$

with $p_{ij} \geq 0,\ \forall\ i, j$ and $\sum_{ij} p_{ij} = 1$.

Due to their explicit structure, symmetric states possess a natural decomposition:

Lemma 3.1. *Every symmetric state, $\rho_S \in \mathcal{B}(\mathcal{S})$, can be written as the sum of a DS state, ρ_{DS}, and a traceless symmetric contribution, σ_{CS}, which contains all coherences between Dicke states, i.e.,*

$$\rho_S = \rho_{DS} + \sigma_{CS} = \sum_{0\leq i\leq j<d} p_{ij} \left|D_{ij}\right\rangle \left\langle D_{ij}\right| + \sum_{\substack{ij \\ (i,j)\neq(k,l)}} \sum_{kl} \left(\alpha_{ij}^{kl} \left|D_{ij}\right\rangle \left\langle D_{kl}\right| + \text{h.c.}\right) , \tag{3.19}$$

with $\alpha_{ij}^{kl} \in \mathbb{C}$ and $\alpha_{ij}^{kl} = (\alpha_{kl}^{ij})^*$.

3.2.1 Separability, EWs & copositive matrices

In this section we rephrase some of the concepts of section 2.3 in the context of bipartite symmetric states on $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$.

Definition 3.10. *A bipartite symmetric state $\rho_S \in \mathcal{B}(\mathcal{S})$ is separable (not entangled) if it can be written as a convex combination of projectors onto pure symmetric product states, i.e.,*

$$\rho_S = \sum_i p_i \left|e_i e_i\right\rangle \left\langle e_i e_i\right| , \tag{3.20}$$

with $p_i \geq 0$, $\sum_i p_i = 1$ and $|e_i\rangle = \sum_i e_i^{(k)} |k\rangle$, where $e_i^{(k)} \in \mathbb{C}$ and $\{|k\rangle\}_{k=0}^{d-1}$ is an orthonormal basis in $\mathbb{C}^d$. If a decomposition of this form does not exist, then ρ_S is entangled.

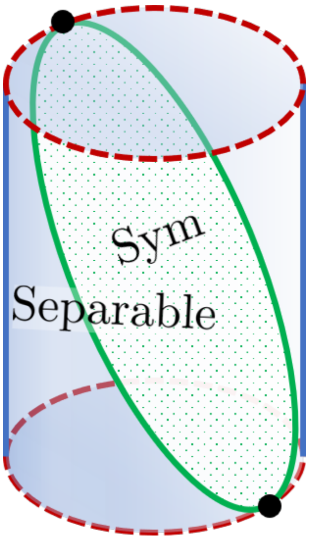

Figure 3.2: Pictorial representation of the set of bipartite symmetric separable states $\mathcal{D}_S$ (Sym) embedded into the set of bipartite separable states. The cylinder represents the separable set $\mathcal{D}$. The discontinuous (red) line corresponds to the extremal points (of the form $|e, f\rangle$) generating the set and the continuous (blue and green) lines corresponds to the respective boundaries (necessarily requiring description as density matrices with rank > 1 but not maximal). Both the separable and the symmetric separable sets share extremal points of the form $|e, e\rangle$, here represented by the black dots.

We denote by $\mathcal{D}$, the compact set of separable quantum states and by $\mathcal{D}_S$, its analogous symmetric counterpart, which is also compact (see Fig.3.2). As a consequence of the Hahn-Banach theorem, the set $\mathcal{D}_S$ admits also a dual description in terms of its dual cone, $\mathcal{P}_S$, defined as the set of the operators W fulfilling

$$\mathcal{P}_S = \{W = W^\dagger \ \text{ s.t } \langle W, \rho\rangle \geq 0 \, , \forall \rho_S \in \mathcal{D}_S\} \, , \tag{3.21}$$

where $\langle W, \rho \rangle \equiv \mathrm{Tr}(W^\dagger \rho)$ is the Hilbert-Schmidt scalar product. Recalling Def.2.14, it is easy to see that $\mathcal{P}_S$ is the set of EWs for symmetric states. Notice that, by definition, the set of separable symmetric states, $\mathcal{D}_S$, satisfies the inclusion $\mathcal{D}_S \subset \mathcal{D}$, but $\mathcal{P} \subset \mathcal{P}_S$, where $\mathcal{P}$ is the dual cone of the convex set $\mathcal{D}$, i.e.,

$$\mathcal{P} = \{W = W^\dagger \;\text{ s.t. } \langle W, \rho \rangle \geq 0 \,, \forall \rho \in \mathcal{D}\} \,. \tag{3.22}$$

In other words, any EW acting on $\mathcal{H}$ that detects an entangled state belongs to $\mathcal{P}_S$, but the converse is not necessarily true (see Fig.3.3).

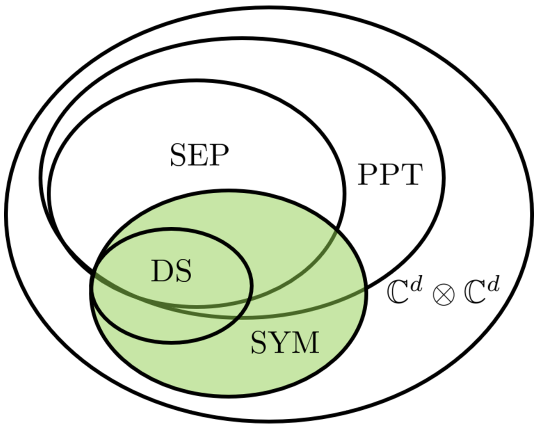

Figure 3.3: Pictorial structure of the quantum states in $\mathbb{C}^d \otimes \mathbb{C}^d$ for $d > 5$. Each set contains the sets displayed inside. The colored region (green) represents the set of symmetric states (SYM). Note that, while for $d > 5$ there exist diagonal symmetric (DS) states that are PPT-entangled, as represented in the figure, for $d < 5$ all PPT-entangled DS state are necessarily separable (SEP) (see the text for details).

For generic symmetric states, sparsity is preserved when the state is expressed in the computational basis but it is lost when the partial transposition is performed. However, for DS states, the corresponding partial transpose remains highly sparse and can be reduced to an associated matrix, $M_d(\rho_{DS})$, of dimension $d \times d$, while generically $\rho_S^{T_B}$ is a matrix of dimension $d^2 \times d^2$.

Definition 3.11. *The partial transpose of every $\rho_{DS} \in \mathcal{B}(\mathcal{S})$ has the form*

$$\rho_{DS}^{T_B} = M_d(\rho_{DS}) \bigoplus_{0 \leq i \neq j < d} \frac{p_{ij}}{2} \,, \tag{3.23}$$

where $M_d(\rho_{DS})$ is a $d \times d$ matrix with non-negative entries defined as

$$M_d(\rho_{DS}) = \begin{pmatrix} p_{00} & p_{01}/2 & \cdots & p_{0,d-1}/2 \\ p_{01}/2 & p_{11} & \cdots & p_{1,d-1}/2 \\ \vdots & \vdots & \ddots & \vdots \\ p_{0,d-1}/2 & p_{1,d-1}/2 & \cdots & p_{d-1,d-1} \end{pmatrix} . \tag{3.24}$$

It has been proven that, in the case of DS states, the properties of the state ρ_{DS} can be rephrased in terms of equivalent properties of the matrix $M_d(\rho_{DS})$ [Yu16; TAQ+18]. In particular, we have the following results:

Theorem 3.5 ([Yu16; TAQ+18])**.** *Let $\rho_{DS} \in \mathcal{B}(\mathcal{S})$ be a DS state. Then,*

$$\rho_{DS} \text{ separable} \iff M_d(\rho_{DS}) \in \mathcal{CP}_d\ . \tag{3.25}$$

Theorem 3.6 ([TAQ+18])**.** *Let $\rho_{DS} \in \mathcal{B}(\mathcal{S})$ be a DS state. Then,*

$$\rho_{DS}^{T_B} \succeq 0 \iff M_d(\rho_{DS}) \in \mathcal{DNN}_d\ , \tag{3.26}$$

where $\mathcal{DNN}_d$ denotes the cone of doubly non-negative *matrices, defined as*

$$\mathcal{DNN}_d = \{A \in S_d \mid A \in \mathcal{PSD}_d, A_{ij} \geq 0\}\ . \tag{3.27}$$

In particular, it can be shown [BDS15] that for $d \leq 4$, the equality $\mathcal{CP}_d = \mathcal{DNN}_d$ holds, so that we have the following result:

Theorem 3.7 ([TAQ+18])**.** *Let $\rho_{DS} \in \mathcal{B}(\mathcal{S})$ be a DS state, with $d \leq 4$. Then,*

$$\rho_{DS} \text{ separable} \iff \rho_{DS} \text{ PPT}\ . \tag{3.28}$$

Th.3.7 states that PPT condition is sufficient to assess separability in the class of two-qudit DS states for $d \leq 4$. However, in higher dimension, there exist examples of diagonal PPT-entangled states which can be detected by means of copositive matrices.

This result stems from the observation that $\mathcal{COP}_d$ is the dual of the cone of $\mathcal{CP}_d$. For this reason, since deciding if a DS state ρ_{DS} is separable is equivalent to check the membership of $M_d(\rho_{DS})$ to the cone of completely positive matrices, this problem can be recast, equivalently, in the dual cone of $\mathcal{CP}_d$, i.e., in the cone $\mathcal{COP}_d$ of copositive matrices. As a consequence, copositive matrices act as EWs for DS states, as we will see in further detail in the following section.

3.2.2 Diagonal symmetric states

Using the definitions of the previous section we now present a method to construct an EW for DS states, starting from a copositive matrix. It turns out that the decomposability of the EWs we propose, depends crucially on the type of copositive matrix we consider. Indeed, we show that decomposable (non-decomposable) EWs correspond to non-exceptional (exceptional) copositive matrices. Our findings are summarised in the following theorems.

Theorem 3.8. *Each copositive matrix $H = \sum_{i,j=0}^{d-1} H_{ij} |i\rangle\langle j|$, with at least one negative entry $H_{mn} = H_{nm} < 0$ ($m \neq n$), leads to an EW on $\mathcal{S}$ of the form $W = (H^{\text{ext}})^{T_B} = \sum_{i,j=0}^{d-1} H_{ij} |ij\rangle\langle ji|$.*

Proof. i) We extend H to the symmetric subspace as $H^{ext} = \sum_{i,j=0}^{d-1} H_{ij} |i\rangle \langle j| \otimes |i\rangle \langle j|$, and denote $W = (H^{ext})^{T_B}$. A direct calculation shows that, for every state $|e\rangle = \sum_{i=0}^{d-1} c_i |i\rangle$, with $c_i \in \mathbb{C}$, it holds $\langle ee|W|ee\rangle = \langle ee^*|H^{ext}|ee^*\rangle = \sum_{ij} |c_i|^2 H_{ij} |c_j|^2 = \boldsymbol{x}^T H \boldsymbol{x} \geq 0$, where $\boldsymbol{x} = (|c_0|^2, |c_1|^2, |c_2|^2)$ and the last inequality follows from the copositivity of H. As a consequence, $\text{Tr}[W\rho_S] \geq 0$ for all $\rho_S \in \mathcal{D}_S$; ii) The diagonalization of W shows that its eigenvectors are given by $\{|ii\rangle, |\psi_{ij}^{\pm}\rangle = (|ij\rangle \pm |ji\rangle)/\sqrt{2}\}$, with corresponding eigenvalues $\{H_{ii}, \pm H_{ij}\}$, i.e.,

$$W = (H^{ext})^{T_B} = \sum_{i=0}^{d-1} H_{ii} |ii\rangle \langle ii| + \sum_{i<j}^{d-1} H_{ij} |\psi_{ij}^{+}\rangle \langle \psi_{ij}^{+}| - \sum_{i<j}^{d-1} H_{ij} |\psi_{ij}^{-}\rangle \langle \psi_{ij}^{-}|, \tag{3.29}$$

where $|\psi_{ij}^{+}\rangle = |D_{ij}\rangle$ and $|ii\rangle = |D_{ii}\rangle$. Notice that the $d(d-1)/2$ eigenvectors corresponding to the projectors $|\psi_{ij}^{-}\rangle \langle \psi_{ij}^{-}|$, are orthogonal to the symmetric subspace and, therefore, can be discarded by projecting on $\mathcal{S}$, i.e.,

$$W_S = \Pi_S W \Pi_S = \sum_{i=0}^{d-1} H_{ii} |D_{ii}\rangle \langle D_{ii}| + \sum_{i<j}^{d-1} H_{ij} |D_{ij}\rangle \langle D_{ij}|. \tag{3.30}$$

Finally, since copositivity requires that $H_{ii} \geq 0 \, \forall i$, W_S is an EW if and only if at least one of the remaining eigenvalues is negative, that is if H has at least one negative element $H_{mn} = H_{nm} < 0$ for some $m \neq n$. It is now trivial to see that W_S indeed detects, at least, the entangled state $|\psi_{mn}^{+}\rangle$ since $\text{Tr}[W_S |\psi_{mn}^{+}\rangle \langle \psi_{mn}^{+}|] = H_{mn} < 0$. To conclude, if W_S is an EW in the symmetric subspace, so it is W given by Eq.(3.29). □

The following theorem establishes a correspondence between decomposable EWs and non-exceptional matrices.

Theorem 3.9. *If $H = H_{\mathcal{N}} + H_{\mathcal{PSD}}$ (i.e., H is non-exceptional) with at least one negative element, then $W = \Pi_S \, (H_{\mathcal{N}}^{\text{ext}})^{T_B} \, \Pi_S + (H_{\mathcal{PSD}}^{\text{ext}})^{T_B}$ is a decomposable EW. The converse is also true, that is, if $W = P + Q^{T_B}$ with $P, Q \succeq 0$, then it is always possible to find a copositive matrix $H = H_{\mathcal{N}} + H_{\mathcal{PSD}}$ with at least one negative element, such that $P = \Pi_S \, (H_{\mathcal{N}}^{\text{ext}})^{T_B} \, \Pi_S$ and $Q = (H_{\mathcal{PSD}}^{\text{ext}})^{T_B}$.*

Proof. ($\Longrightarrow$) Let H be a non-exceptional copositive matrix, i.e., $H = H_{\mathcal{N}} + H_{\mathcal{PSD}}$. Since H has a negative element it must be $(H_{\mathcal{PSD}})_{mn} = (H_{\mathcal{PSD}})_{nm} < 0$. The operator $W = \Pi_S \, (H_{\mathcal{N}}^{ext})^{T_B} \, \Pi_S + (H_{\mathcal{PSD}}^{ext})^{T_B}$ is a decomposable EW on the symmetric subspace:

i) W is positive semidefinite over symmetric separable states. In fact, for any $\rho_{sep} \in \mathcal{S}$ it holds:

$$\begin{aligned} \mathrm{Tr}[W \rho_{sep}] &= \mathrm{Tr}[W \Pi_S \rho \Pi_S] = \mathrm{Tr}[\Pi_S W \Pi_S \rho_{sep}] = \mathrm{Tr}[\Pi_S (H^{ext})^{T_B} \Pi_S \rho_{sep}] = \\ &= \mathrm{Tr}[(H^{ext})^{T_B} \rho_{sep}] = \boldsymbol{x}^T H \boldsymbol{x} \geq 0 \ , \end{aligned}$$

where the result follows from the cyclic property of the trace and the copositivity of H;

ii) W has at least one negative eigenvalue. In fact, it is not hard to see that the spectrum of W is given by $\{(H_{\mathcal{N}})_{ij} + (H_{\mathcal{PSD}})_{ij}, -(H_{\mathcal{PSD}})_{ij}\}$. However, since we are interested exclusively in symmetric states, we can discard the latter eigenvalues, i.e., $\{-(H_{\mathcal{PSD}})_{ij}\}$, since they correspond to anti-symmetric states. As a consequence, since there exists, for hypothesis, at least one negative element $H_{ij} \equiv (H_{\mathcal{N}})_{ij} + (H_{\mathcal{PSD}})_{ij} < 0$, W has at least one negative eigenvalue on $\mathcal{S}$;

iii) W is decomposable. Setting $Q^{T_B} = (H_{\mathcal{PSD}}^{ext})^{T_B}$ it follows $Q = (H_{\mathcal{PSD}}^{ext}) \succeq 0$. Hence, if $P = \Pi_S \, (H_{\mathcal{N}}^{ext})^{T_B} \, \Pi_S \succeq 0$, then W is a decomposable EW. It is easy to see that $\Pi_S \, (H_{\mathcal{N}}^{ext})^{T_B} \, \Pi_S = \sum_{ij} (H_{\mathcal{N}}^{ext})_{ij} |D_{ij}\rangle\langle D_{ij}|$ so that its eigenvalues are given by $\{(H_{\mathcal{N}})_{ij}\}$. Hence, since $H_{\mathcal{N}} \in \mathcal{N}$, $P \succeq 0$.

($\Longleftarrow$) Let $W = \Pi_S \, (H_{\mathcal{N}}^{ext})^{T_B} \, \Pi_S + (H_{\mathcal{PSD}}^{ext})^{T_B}$ be a decomposable EW for symmetric states. Hence, it must have a negative eigenvalue. Recalling the expression of the spectrum of W, this implies that there exists a negative element $H_{ij} \equiv (H_{\mathcal{PSD}})_{ij} + (H_{\mathcal{N}})_{ij} < 0$, so that $(H_{\mathcal{PSD}})_{ij} < 0$. Moreover, positivity over symmetric separable states implies $\mathrm{Tr}[W \rho_{sep}] = \langle ee|W|ee\rangle = \boldsymbol{x}^T H \boldsymbol{x} \geq 0$, a condition that is satisfied if and only if H is a copositive matrix. $\square$

Notice that W from Theorem 3.9 is not a symmetric operator. In fact, due to the latter term in the decomposition, i.e., $(H^{ext}_{\mathcal{PSD}})^{T_B}$, it follows that $\Pi_S W \Pi_S \neq W$, meaning that $W \notin \mathcal{S}$. Despite one might expect that an entangled symmetric state σ can be detected only by a symmetric EW, a non-symmetric EW W can nonetheless be employed as long as its projection W_S onto the symmetric subspace defines a valid witness and is such that $\mathrm{Tr}[W_S\sigma] < 0$. Indeed, it possible to show that the construction of a symmetric EW of the form $W_S = \Pi_S (H^{ext})^{T_B} \Pi_S$ would lead to a non-decomposable EW for any copositive matrix with at least one negative element. In particular, this would imply the possibility to construct a non-decomposable EW for $d < 5$, a result which contrasts with the fact that PPT-entangled DS states (PPTEDS) can only occur for $d \geq 5$. For this reason, if we want to stick to the usual definition of decomposability for EWs, an anti-symmetric contribution must be taken into account. Although one possibility to overcome these contradictions would be to introduce an alternative definition of decomposability (see, e.g., [CJM+22]), in the rest of this thesis we will stick with the original definition given in section 2.3.

Let us illustrate Theorem 3.9 by considering the following copositive matrix in $d = 3$

$$H = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix} . \tag{3.31}$$

A possible decomposition of $H = H_{\mathcal{PSD}} + H_{\mathcal{N}}$, with $H_{\mathcal{PSD}} \in \mathcal{PSD}_3$ and $H_{\mathcal{N}} \in \mathcal{N}_3$, is given by:

$$H_{\mathcal{PSD}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}, \quad H_{\mathcal{N}} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} . \tag{3.32}$$

The associated EW $W = P + Q^{T_B}$, with $P = \Pi_S (H^{ext}_{\mathcal{N}})^{T_B} \Pi_S$, and $Q = H^{ext}_{\mathcal{PSD}}$, reads

$$P = \frac{1}{2}\left(\begin{array}{ccc|ccc|ccc}
2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right), \quad Q = \left(\begin{array}{ccc|ccc|ccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1
\end{array}\right) \tag{3.33}$$

Notice that the decomposition of H might not be unique. For instance, another possible decomposition of H can be

$$H'_{\mathcal{PSD}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}, \quad H'_{\mathcal{N}} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{3.34}$$

but the resulting EW, $W' = P' + Q'^{T_B}$, detects exactly the same states in the symmetric subspace. The link between non-exceptional copositive matrices and decomposable EWs extends also to exceptional copositive matrices and non-decomposable EWs in the symmetric subspace.

Theorem 3.10. *Associated to each exceptional copositive matrix H (i.e., $H \in \mathcal{COP}_d \setminus (\mathcal{PSD}_d + \mathcal{N}_d)$) with at least one negative entry, there is a non-decomposable EW, $W = (H^{\text{ext}})^{T_B}$, able to detect symmetric PPTES.*

Proof. For any $H \in \mathcal{COP}_d \setminus (\mathcal{PSD}_d + \mathcal{N}_d)$, H always admits a decomposition of the form $H = H_{\mathcal{N}} + H_\star$, where $H_{\mathcal{N}}$ is a non-negative symmetric matrix and $H_\star$ has at least one negative eigenvalue but is not positive semidefinite. The associated EW $W = P + Q^{T_B}$ with $P = \Pi_S (H_{\mathcal{N}}^{ext})^{T_B} \Pi_S$ and $Q = H_\star^{ext}$, is a non-decomposable EW since $P \succeq 0$ but $Q \not\succeq 0$. The operator $W = (H^{ext})^{T_B}$ is also a non-decomposable EW. □

Corollary 3.10.1 (From [TAQ+18]). *Since for $d < 5$ every copositive matrix is not exceptional (i.e., $H = H_{\mathcal{PSD}} + H_{\mathcal{N}}$), all EWs of DS states in $d = 3$ and $d = 4$ are decomposable.*

The above corollary rephrases the fact that PPT criterion is necessary and sufficient to assess separability for bipartite DS states $\rho_{DS} \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$ for $d < 5$.

3.2.3 Symmetric states

Let us briefly summarise what we have seen so far. The fact that each DS state, $\rho_{DS} \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$, is associated to a matrix $M_d(\rho_{DS})$ (see Eq.(3.24)), allows to reformulate the problem of entanglement characterisation as the equivalent problem of checking the membership of $M_d(\rho_{DS})$ to the cone of completely positive matrices $\mathcal{CP}_d$. Equivalently, according to the dual formulation, any entangled state ρ_{DS} is detected by an EW W which can be constructed from a copositive matrix H. PPT entangled diagonal symmetric states (PPTEDS) can only be detected by non-decomposable EWs, which correspond to exceptional copositive matrices. Since for $d < 5$, all copositive matrices H are of the form $H = H_{\mathcal{PSD}} + H_{\mathcal{N}}$, all EWs defined as $W = (H^{ext})^{T_B}$ are necessarily of the form $W = P + Q^{T_B}$, with $P, Q \succeq 0$, meaning that for $d < 5$ there are not PPTEDS.

However, for $d > 5$, this is not the case, since there exist exceptional copositive matrices, i.e., $H \notin \mathcal{PSD}_d + \mathcal{N}_d$. Thus, detecting entanglement of ρ_{DS} in $d \geq 5$, is equivalent to checking membership of the corresponding copositive matrix $H \in \mathcal{COP}_d \setminus (\mathcal{PSD}_d + \mathcal{N}_d)$, which is, in general, a co-NP-hard problem [MK87].

What can we say about symmetric PPTES ρ_S that are not DS? In this section, we tackle the problem of entanglement detection for generic states $\rho_S \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$ in arbitrary dimension d. Since decomposable EWs cannot detect bound entanglement, one is tempted to believe that separability in the symmetric subspace is equivalent to the analysis of exceptional copositive matrices only. However, as we shall see in the following, this is not necessarily the case, and non-exceptional copositive matrices also play a relevant role in detecting bound entanglement. Following the argument given above, we split our analysis in two different scenarios, namely when $d \geq 5$ and $d < 5$. Remarkably, even outside of the DS paradigm, we find that copositive matrices lie at the core of non-decomposable EWs for symmetric PPTES in arbitrary dimensions.

Symmetric PPTES in $d \geq 5$

The fact that for $d \geq 5$ there exist exceptional copositive matrices corresponding to non-decomposable EWs in $\mathcal{S}$, implies that: (i) such EWs can detect a PPTEDS, and (ii) the same EWs are able to detect symmetric, but not DS, PPT-entangled states "around" it.

Theorem 3.11. *Let ρ_{DS} be a PPTEDS. Then any symmetric state $\rho_S = \rho_{DS} + \sigma_{CS}$, such that $\rho_S^{T_B} \geq 0$, is PPT entangled.*

Proof. Since ρ_{DS} is a PPTEDS state there exists an exceptional copositive matrix H and an associated non decomposable EW W such that $\mathrm{Tr}[W\rho_{DS}] < 0$. It follows that $\text{Tr}[W\rho_S] = \text{Tr}[W(\rho_{DS} + \sigma_{CS})] = \text{Tr}[W\rho_{DS}] = \text{Tr}[HM_d(\rho_{DS})] < 0$, so that ρ_S is PPT entangled. $\square$

In [JR08] it was proposed a way to construct exceptional copositive matrices for any odd $d \geq 5$. These matrices bear resemblance with the Horn matix of Eq.(3.8) and are of the form

$$H_{\mathcal{H}} = \begin{pmatrix} 1 & -1 & 1 & 1 & \cdots & \cdots & 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & \ddots & & \ddots & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & & & \ddots & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & \ddots & & & \ddots & 1 \\ \vdots & \ddots & 1 & -1 & 1 & \ddots & & & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 1 & \ddots & & & & \ddots & 1 & -1 & 1 & 1 \\ 1 & 1 & \ddots & & & \ddots & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & \ddots & & & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 & \cdots & \cdots & 1 & 1 & -1 & 1 \end{pmatrix} . \tag{3.35}$$

Since the $H_{\mathcal{H}}$ is exceptional and has negative entries, it leads to a non-decomposable EW, $W = (H^{ext})^{T_B}$, that can be used to detect PPTEDS in any odd dimension $d \geq 5$. Moreover, due to Th.(3.11), by adding suitable coherences to such states, the same EW can be used to certify PPT-entanglement also in whole families of symmetric states. Below we provide one of these families.

Corollary 3.11.1. *Given a PPTEDS state, ρ_{DS}, any symmetric state of the form $\rho_S = \rho_{DS} + \sigma_{CS}$, with $\sigma_{CS} = \sum_{i<j}(\alpha_{ij} |D_{ii}\rangle \langle D_{jj}| + \text{h.c.})$ and $|\alpha_{ij}| \leq \frac{p_{ij}}{2}$ is PPT-entangled.*

Proof. The state ρ_S and its partial transpose, $\rho_S^{T_B}$, can be cast as

$$\rho_S = \tilde{M}_d(\rho_S) \bigoplus_{i<j} \frac{p_{ij}}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} , \tag{3.36}$$

$$\rho_S^{T_B} = M_d(\rho_{DS}) \bigoplus_{0 \leq i<j<d} \begin{pmatrix} p_{ij}/2 & \alpha_{ij} \\ \alpha_{ij}^* & p_{ij}/2 \end{pmatrix} , \tag{3.37}$$

with

$$\tilde{M}_d(\rho_S) = \begin{pmatrix} p_{00} & \alpha_{01} & \cdots & \alpha_{0,d-1} \\ \alpha_{01}^* & p_{11} & \cdots & \alpha_{1,d-1} \\ \vdots & \vdots & \vdots & \ddots \\ \alpha_{0,d-1}^* & \alpha_{1,d-1}^* & \cdots & p_{d-1,d-1} \end{pmatrix},$$

$$M_d(\rho_{DS}) = \begin{pmatrix} p_{00} & p_{01}/2 & \cdots & p_{0,d-1}/2 \\ p_{01}/2 & p_{11} & \cdots & p_{1,d-1}/2 \\ \vdots & \vdots & \vdots & \ddots \\ p_{0,d-1}/2 & p_{1,d-1}/2 & \cdots & p_{d-1,d-1} \end{pmatrix}.$$

Positive semidefiniteness of ${\rho_S}^{T_B}$ implies $|\alpha_{ij}| \leq \frac{p_{ij}}{2}$, so that the state ρ_S, generated from a PPTEDS state, remains PPT-entangled – since it is detected by the same non-decomposable EW – as long as the coherences respect the condition $|\alpha_{ij}| \leq \frac{p_{ij}}{2}$. □

A further connection between copositive matrices and EWs appears when considering extreme copositive matrices. For instance, let us consider the generalised Horn matrix $H_{\mathcal{H}}$ of Eq.(3.35), and the so-called Hoffmann-Pereira matrix $H_{\mathcal{HP}}$ [JR08; HP73], which, besides of being exceptional, is also extreme. For $d = 7$, such copositive matrices take the form

$$H_{\mathcal{H}} = \begin{pmatrix} 1 & -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 & -1 & 1 \end{pmatrix}, \tag{3.38}$$

$$H_{\mathcal{HP}} = \begin{pmatrix} 1 & -1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 1 \end{pmatrix}. \tag{3.39}$$

Let us inspect the action of both matrices, $H_{\mathcal{H}}$ and $H_{\mathcal{HP}}$, on a DS state $\rho_{DS} \in$

$\mathcal{B}(\mathbb{C}^7 \otimes \mathbb{C}^7)$, described by its associated $M_7(\rho_{DS})$ (see Eq.(3.24)):

$$M_d(\rho_{DS}) = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 1/8 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 1/8 & 0 & 1/4 & 0 & 0 & 1 & 1 \end{pmatrix} . \tag{3.40}$$

It can be easily checked that $\mathrm{Tr}[H_{\mathcal{HP}} M_7(\rho_{DS})] = \mathrm{Tr}[(H^{ext}_{\mathcal{HP}})^{T_B}\, \rho_{DS}] = -\frac{1}{4}$. Since both $H_{\mathcal{H}}$ and $H_{\mathcal{HP}}$ are exceptional copositive matrices, $W_{\mathcal{HP}} = (H^{ext}_{\mathcal{HP}})^{T_B}$ and $W_{\mathcal{H}} = (H^{ext}_{\mathcal{H}})^{T_B}$ are non-decomposable EWs, so that ρ_{DS} is a PPT-entangled state. Moreover, as stated by Th.(3.11), $W_{\mathcal{HP}} = (H^{ext}_{\mathcal{HP}})^{T_B}$, detects, as well, many other states around the state given by Eq.(3.40). In contrast, $\mathrm{Tr}[H_{\mathcal{H}} M_d(\rho_{DS})] = \mathrm{Tr}[W_{\mathcal{H}} \rho_S] = 0$, indicating that $H_{\mathcal{H}}$ fails to detect this state. This result is by no means a coincidence. In fact, just like exceptional copositive matrices correspond to non-decomposable EWs, it is possible to show that extreme matrices generate optimal EWs. Before proving this result, we introduce the definition of an *irreducible* copositive matrix:

Definition 3.12 ([DDG+13])**.** *Given a matrix $H \in \mathcal{COP}_d$ and a set $\mathcal{M} \subset S_d$ contained in the space of symmetric matrices of order d, we say that H is M-irreducible if there do not exist $\epsilon > 0$ and $M \in \mathcal{M} \setminus 0$ such that $H - \epsilon M \in \mathcal{COP}_d$.*

For extreme copositive matrices the following theorem applies:

Theorem 3.12 ([DDG+13])**.** *Let H be an extreme copositive matrix. Then, it is $\mathcal{N}_d$-irreducible.*

Finally, making use of Th.3.12, we can prove the following theorem:

Theorem 3.13. *Let H be an extreme copositive matrix. Then the operator $W = (H^{\mathrm{ext}})^{T_B}$ is an optimal EW on the symmetric subspace $\mathcal{S}$.*

Proof. Since H is extreme, then it is also $\mathcal{N}_d$-irreducible. This means that for every $\epsilon > 0$ and for every non-negative matrix $N \in \mathcal{N}_d$, the matrix $H' = H - \epsilon N$ is not copositive, i.e., $H' \notin \mathcal{COP}_d$. Let us now construct the operator $W' = [(H')^{ext}]^{T_B} = (H^{ext})^{T_B} - \epsilon (N^{ext})^{T_B}$. Since we are interested in symmetric states, let us consider its projection onto the symmetric subspace, i.e.,

$$W'_S = \Pi_S W' \Pi_S = W_S - \epsilon \Pi_S (N^{ext})^{T_B} \Pi_S \, , \tag{3.41}$$

where we have set $W_S = \Pi_S (H^{ext})^{T_B} \Pi_S$. Notice that $P = \Pi_S (N^{ext})^{T_B} \Pi_S \succeq$ since its eigenvalues are given by $\{N_{ij}\}$, which are non-negative for hypothesis. Moreover, since $H' \notin \mathcal{COP}_d$, the operator W_S' is not positive semidefinite over the separable states in $\mathcal{S}$, i.e., W_S' is not an EW. Hence, W_S is an optimal EW on $\mathcal{S}$. $\square$

Th.(2.14) allows us to prove the above result in an alternative way. First, notice that restricting to the symmetric subspace $\mathcal{S} \subset \mathbb{C}^d \otimes \mathbb{C}^d$ implies that Eq.(2.90) can be cast as

$$\langle a_k, a_k | W | a_k, a_k \rangle = 0 \, . \tag{3.42}$$

Hence, in the case of an EW of the form $W = (H^{ext})^{T_B}$, setting $|a_k\rangle = \sum_i a_k^{(i)} |i\rangle$, with $a_k^{(i)} \in \mathbb{C}$ and $\{|i\rangle\} \in \mathbb{C}^d$ is an orthonormal basis, Eq.(2.90) can be written as

$$\langle a_k, a_k | W | a_k, a_k \rangle = \sum_{ij} H_{ij} |a_k^{(i)}|^2 |a_k^{(j)}|^2 = \boldsymbol{x}_k{}^T H \boldsymbol{x}_k = 0 \, , \tag{3.43}$$

where $\boldsymbol{x_k} = (|a_k^{(1)}|^2, \dots, |a_k^{(d)}|^2)$. It is evident that the above condition is satisfied by any copositive matrix $H \in \partial\mathcal{COP}_d$ so that, in particular, Eq.(3.43) holds for any extreme copositive matrix. Moreover, since any state $|a_k, a_k\rangle$ can be expressed as a linear combination of the Dicke states $|D_{ij}\rangle$, they set $\{|a_k, a_k\rangle\}$ span the symmetric subspace $\mathcal{S}$. Hence, if H is an extreme copositive matrix, $W = (H^{ext})^{T_B}$ is an optimal EW.

Let us conclude this section with a result regarding the relation between exceptional and extreme copositive matrices.

Theorem 3.14. *Let H be an extreme copositive matrix with at least one negative eigenvalue, and at least one negative element $H_{ij} < 0$. Then H must be exceptional.*

Proof. H cannot belong to neither $H_{\mathcal{PSD}}$ nor to $H_{\mathcal{N}}$ and, while it is extremal, it cannot be a combination of their elements as well. $\square$

In other words, copositive matrices that are both extreme and exceptional lead to optimal non-decomposable EWs in the sense of [LKC+00].

Symmetric PPTES in $d < 5$

In this section, we are interested in symmetric PPTES of the form $\rho_S = \rho_{DS} + \sigma_{CS}$ where ρ_{DS} is separable, so that $\mathrm{Tr}(HM_d(\rho_{DS})) \geq 0$ for all copositive matrices H. Moreover, since for $d < 5$, every copositive matrix is non-exceptional, i.e., $H = H_{\mathcal{N}} + H_{\mathcal{PSD}}$, the corresponding witness $W = (H^{ext})^{T_B}$ will always be decomposable. For this reason, coherences are needed to create PPTES in low dimensional systems.

Here we show that such states symmetric PPTES can nevertheless be detected by EWs which are of the form $W_S = W + W_{CS}$, that is by adding to the decomposable EW, W, a convenient off-diagonal, symmetric contribution W_{CS} which reads the coherences of ρ_S.

For the sake of simplicity, we hereby consider symmetric states of the form

$$\rho_S = \rho_{DS} + \sigma_{CS} = \sum_{ij} p_{ij} \left|D_{ij}\right\rangle \left\langle D_{ij}\right| + \sum_{i \neq j \neq k} \left(\alpha_{ijk} \left|D_{ii}\right\rangle \left\langle D_{jk}\right|\right) + \text{h.c.} \,, \tag{3.44}$$

with $p_{ij} \geq 0 \; \forall i,j$, $\sum p_{ij} = 1$ and $\alpha_{ijk} \in \mathbb{C}$.

Indeed, in this case, both ρ_S and $\rho_S^{T_B}$ can be cast as a direct sum of matrices, which highly simplifies our analysis. For instance, for $d = 3$, ρ_S and $\rho_S^{T_B}$ are of the form

$$\rho_S = \frac{1}{2}\begin{pmatrix} p_{02} & \sqrt{2}\alpha & p_{02} \\ \sqrt{2}\alpha^* & 2p_{11} & \sqrt{2}\alpha \\ p_{02} & \sqrt{2}\alpha^* & p_{02} \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} 2p_{00} & \sqrt{2}\beta & \sqrt{2}\beta \\ \sqrt{2}\beta^* & p_{12} & p_{12} \\ \sqrt{2}\beta^* & p_{12} & p_{12} \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} p_{01} & p_{01} & \sqrt{2}\gamma \\ p_{01} & p_{01} & \sqrt{2}\gamma \\ \sqrt{2}\gamma^* & \sqrt{2}\gamma^* & 2p_{22} \end{pmatrix} , \tag{3.45}$$

$$\rho_S^{T_B} = M_d(\rho_{DS}) \oplus \frac{1}{2}\begin{pmatrix} p_{01} & \sqrt{2}\alpha & \sqrt{2}\beta \\ \sqrt{2}\alpha^* & p_{12} & \sqrt{2}\gamma \\ \sqrt{2}\beta^* & \sqrt{2}\gamma^* & p_{02} \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} p_{02} & \sqrt{2}\beta & \sqrt{2}\gamma \\ \sqrt{2}\beta^* & p_{01} & \sqrt{2}\alpha \\ \sqrt{2}\gamma^* & \sqrt{2}\alpha^* & p_{12} \end{pmatrix} , \tag{3.46}$$

where we have defined, for the easiness of reading, $\alpha \equiv \alpha_{120} = \alpha_{102}$, $\beta \equiv \alpha_{012} = \alpha_{021}$ and $\gamma \equiv \alpha_{201} = \alpha_{210}$. Such structure, which corresponds to a particular direct sum decomposition of the total Hilbert space, bears similitude with the so-called circulant states [CK07].

In order to investigate the existence of PPTES we focus on states with low-dimensional ranks, which allow for a simpler analysis. By using a notation common in the literature, we say that a state ρ_S is of type (p,q) if $p = r(\rho_S)$ and $q = r(\rho_S^{T_B})$ are the ranks of ρ_S and $\rho_S^{T_B}$, respectively. While symmetric states in $d = 3$ are, generically, of type $(6,9)$, PPT-entangled edge states must have lower ranks. When dealing with states of the form of Eq.(3.44), we have found numerically that at least two coherences must be considered to observe a PPTES. For instance, we can set $\gamma = 0$ and choose α and β in such a way to lower the value of (p,q). Indeed, a direct inspection of Eqs.(3.45)-(3.46), shows that, by setting $|\alpha|^2 = p_{11}p_{02}/2$ and $|\beta|^2 = p_{02}(p_{01}p_{12} - 2p_{02}p_{11})/4p_{12}$, it is possible to attain a state of type $(5,7)$. Now, starting from a copositve matrix H, we can construct a non-decomposable EW of the form

$$W_S = W_{DS} + \sum_{i \neq j \neq k} W^i_{jk} \left|D_{ii}\right\rangle \left\langle D_{jk}\right| + \text{h.c.} \,, \tag{3.47}$$

where W_{DS} is given by

$$W_{DS} = \Pi_S \, (H_{\mathcal{N}}^{ext})^{T_B} \, \Pi_S + (H_{\mathcal{PSD}}^{ext})^{T_B} \quad , \tag{3.48}$$

and the coefficients W_{jk}^i can be chosen to be real.

Let us illustrate the above results by providing some explicit examples. We first consider the symmetric PPTES provided in [TG10]. Such state is of the form of Eq.(3.44) for $d = 3$ (*i.e.,* of the same form of Eq.(3.45)) and can be obtained from a DS state ρ_{DS} with parameters

$$\begin{aligned} p_{00} &= 0.22, & p_{01} &= 0.176, \\ p_{11} &= 0.234/3, & p_{02} &= 0.167/3, \\ p_{22} &= 0.183, & p_{12} &= 0.254, \end{aligned}$$

and coherences $\alpha = \sqrt{2} \times 0.167/3, \ \beta = -0.059, \ \gamma = 0.$

In [TG10] the authors showed that ρ_S is a PPT-entangled state of two qutrits, providing also a technique to construct $(\frac{N}{2}+1) \times (\frac{N}{2}+1)$ PPT-entangled states starting from symmetric states of N qubits. A non-decomposable EW, W_S, for such state ρ_S can be found with the method of PPT-symmetric extensions proposed in [DPS02]. A direct inspection of its DS part shows that W_{DS} can be constructed from a non-exceptional copositive matrix H of the form

$$H \approx \begin{pmatrix} 0.003 & 10.39 & 100.57 \\ 10.39 & 59.31 & -21.02 \\ 100.57 & -21.02 & 14.22 \end{pmatrix} , \tag{3.49}$$

while the coefficients W_{jk}^i are given by $W_{02}^1 = 23.20$ and $W_{12}^0 = -37.40$. If we restrict to the DS part of the state ρ_S, it is trivial to check that $\mathrm{Tr}[HM_d(\rho_{DS})] \geq 0$. This is by no means a surprise, since for DS states, in $d < 5$, the PPT condition implies separability. For this reason, the coherences provided by the term σ_{CS} are necessary to induce the PPT entanglement. Remarkably, one can vary the value of the coherences α and β to obtain other symmetric PPTES as certified by the EW, i.e., $\mathrm{Tr}[W_S\rho_S] < 0$. In fact, the EW W_S can be used to derive families of PPT entangled states obtained by adding to the state ρ_S any coherent contribution σ_{CS} of the form of Eq.(3.45) that preserves the positivity of both the state and its partial transpose. Indeed, also in the case $\gamma \neq 0$, as long as the conditions $\rho_S \succeq 0$ and $\rho_S^{T_B} \succeq 0$ hold, the same non-decomposable EW W_S, is able to detect, for suitable values of its entries W_{jk}^i, a whole family of PPTES of the form of Eq.(3.45), as depicted in Fig.3.4.

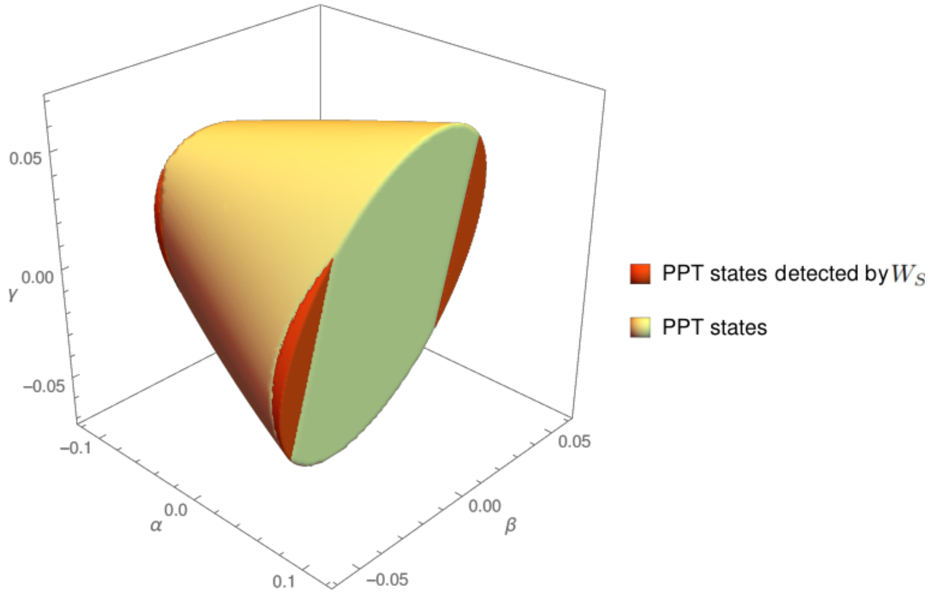

Figure 3.4: The PPT entangled states detected by W_S of Eq.(3.47) with coefficients $|W_{02}^1| = 23.20, |W_{12}^0| = -37.40$ (dark orange) as compared to the whole family of PPT states ρ_S of Eq.(3.45) with $p_{00} = 0.22, p_{11} = 0.234/3, p_{22} = 0.183, p_{01} = 0.176, p_{02} = 0.167/3, p_{12} = 0.254$ (light orange).

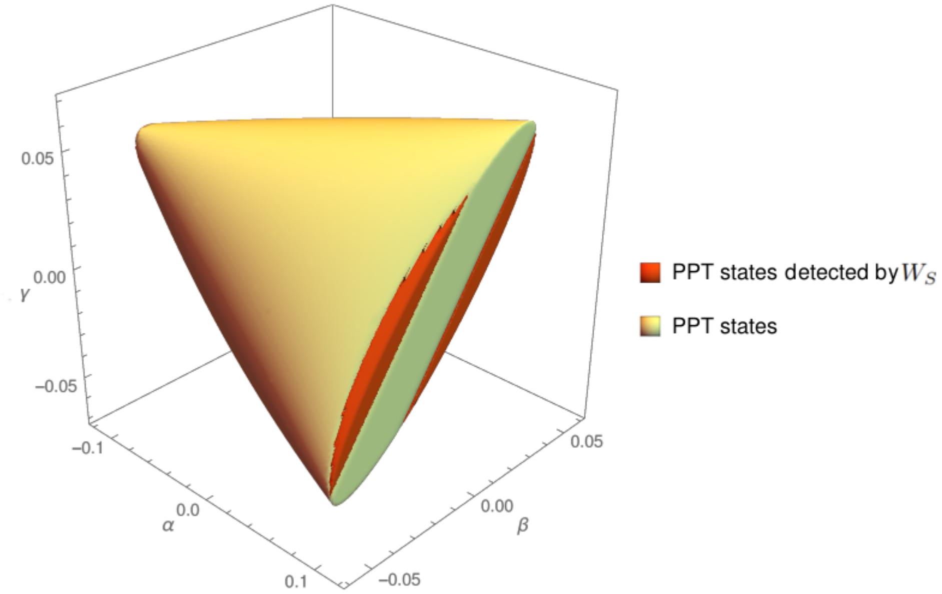

Figure 3.5: The PPT entangled states detected by W_S of Eq.(3.47) with coefficients $|W_{02}^1| = \frac{4595}{191}$, $|W_{12}^0| = \frac{6114}{113}$ (dark orange) as compared to the whole family of PPT states ρ_S of Eq.(3.45) with $p_{00} = p_{11} = p_{12} = \frac{1848}{7625}$, $p_{22} = \frac{464}{7625}$, $p_{01} = \frac{231}{1525}$, $p_{02} = \frac{462}{7625}$ (light orange).

In Fig.3.5, we display a new example of a symmetric PPTES ρ_S of the form of Eq.(3.45), found by semidefinite programming. Also in this case, we have found a non-decomposable EW W_S of the form of Eq.(3.47), with coefficients $W_{02}^1 = \frac{4595}{191}$ and $W_{12}^0 = -\frac{6114}{113}$ and whose associated copositive matrix is given by

$$H = \begin{pmatrix} 1/172 & 1009/151 & 11025/68 \\ 1009/151 & 1803/22 & -5829/65 \\ 11025/68 & -5829/65 & 1224/7 \end{pmatrix} . \tag{3.50}$$

Similarly, we can use the same procedure to derive families of PPT-entangled symmetric states for $d = 4$. In this case, we have found, numerically, that at least three different coherences of the form of Eq.(3.44) are needed in order to get a low-dimensional PPT entangled edge state. To the best of our knowledge, there are no explicit examples of symmetric PPT entangled states in $d = 4$.

The state is given by: i) a DS state ρ_{DS} with $p_{00} = p_{02} = p_{03} = p_{11} = p_{22} = \frac{172+16\sqrt{2}}{1817}$, $p_{01} = p_{13} = \frac{32+172\sqrt{2}}{1817}$, $p_{11} = p_{12} = p_{23} = \frac{86+8\sqrt{2}}{1817}$, $p_{33} = \frac{721-440\sqrt{2}}{1817}$; and ii) a coherence term σ_{CS} with $\alpha = p_{00}$, $\beta = -p_{01}/2$ and $\gamma = p_{01}/4$. Again, to certify its entanglement we have used the PPT-symmetric extension approach [DPS02], which provides a non-decomposable EW, W_S, via semidefinite programming. Such EW is of the form of Eq.(3.47), with coefficients $W^0_{23} = \frac{6526}{321}, W^1_{03} = -\frac{1896}{107}, W^2_{13} = -\frac{549}{1238}$ and has an associated copositive matrix

$$H = \begin{pmatrix} 21/3590 & 9425/1571 & 4853/464 & 1111/28 \\ 9425/1571 & 1293/88 & 2122/145 & 220/323 \\ 4853/464 & 2122/145 & 6/5951 & 1355/3014 \\ 1111/28 & 220/323 & 1355/3014 & 862/7403 \end{pmatrix}. \tag{3.51}$$

Let us observe that, despite the fact that H of Eq.(3.51) does not have any negative matrix element, the corresponding EW has nevertheless a negative eigenvalue. This observation makes clearer, once more, the fact that, in $d < 5$, differently from the case $d \geq 5$, the possibility to detect a PPTES relies exclusively on a convenient choice of the coherences W^i_{jk}.

3.2.4 Symmetric PPTES in $d = 3$: a useful mapping

In this section we provide a complementary approach to tackle the separability problem in the symmetric subspace of two qudits. Making use of a mapping from the symmetric subspace of N qubits, $\mathcal{S}((\mathbb{C}^2)^{\otimes N})$, to the symmetric subspace of a $(N/2+1) \times (N/2+1)$ bipartite system, $\mathcal{S}(\mathbb{C}^{N/2+1} \otimes \mathbb{C}^{N/2+1})$, we provide analytical conditions to decide the separability properties of some families of two-qudit symmetric states. In [TG09] such mapping was used to provide a numerical example of a two-qutrit symmetric bound entangled state. Their technique is based on two steps. First, a symmetric bound entangled state of N qubits is constructed, according to the following lemma:

Lemma 3.2 ([TG09]). *Any symmetric N-qubit state that is PPT with respect to the $\frac{N}{2} : \frac{N}{2}$ partition while NPT with respect to some other partition is bound entangled with respect to the $\frac{N}{2} : \frac{N}{2}$ partition.*

Second, such state is mapped to a symmetric bound entangled state of a $(N/2+1) \times (N/2+1)$ system, where this last step relies on the crucial observation that $\mathcal{S}((\mathbb{C}^2)^{\otimes N}) \subset \mathcal{S}(\mathbb{C}^{N/2+1} \otimes \mathbb{C}^{N/2+1})$ [TG09].
Before moving to our results, let us present a useful theorem regarding the separability of N-qubit symmetric states.

Theorem 3.15 ([Yu16; QRS17]). *Any DS state of N qubits is separable if and only if is PPT w.r.t. partition $\frac{N}{2} : \frac{N}{2}$.*

Notice that Th.3.15 is valid only for DS states of N qubits, i.e., for mixtures of Dicke states that are diagonal in the Dicke basis $\{|D_k^N\rangle\}$. Remarkably, in this case, checking the PPT condition of the largest partition is necessary and sufficient to prove the separability of the state.
Our approach can be summarised as follows. First, we investigate the action of the mapping on a DS state of N qubits, ρ_{DS}^Q. In particular, making use of Th.3.15, we derive necessary and sufficient conditions for the separability of the $(\frac{N}{2}+1)\times(\frac{N}{2}+1)$ symmetric state $\rho_S = \rho_{DS} + \sigma_{CS}$ that results from the mapping. Second, we repeat our analysis considering an initial symmetric state of N qubits, $\rho_S^Q = \rho_{DS}^Q + \sigma_{CS}^Q$. In this case, making use of Lemma 3.2, we provide sufficient conditions to ensure the separability of the mapped symmetric states.
The symmetric subspace of N qubits, $\mathcal{S}((\mathbb{C}^2)^{\otimes N})$, has dimension $N+1$ and a convenient basis is given by the Dicke states $\{|D_k^N\rangle\}_{k=0}^N$, defined as

$$|D_k^N\rangle = \binom{N}{k}^{-1/2} \sum_{\pi\in\mathcal{G}_N} \pi\left(|0\rangle^{\otimes(N-k)}\,|1\rangle^{\otimes k}\right) , \tag{3.52}$$

where $\mathcal{G}_N$ denotes the group of permutations of N elements and π is a permutation operator. Similarly, the symmetric space of two qudits, $\mathcal{S}(\mathbb{C}^d\otimes\mathbb{C}^d)$, has dimension $d(d+1)/2$ and is spanned by the Dicke states $\{|D_{ij}^d\rangle\}$, defined as

$$|D_{ii}^d\rangle = |i\rangle_d\,|i\rangle_d\,, \quad |D_{ij}^d\rangle = \frac{1}{\sqrt{2}}\left(|i\rangle_d\,|j\rangle_d + |j\rangle_d\,|i\rangle_d\right) , \tag{3.53}$$

where the states $\{|i\rangle_d\}\in\mathbb{C}^d$ form an orthonormal basis.
For $d=\frac{N}{2}+1$, the corresponding symmetric space, $\mathcal{S}(\mathbb{C}^{\frac{N}{2}+1}\otimes\mathbb{C}^{\frac{N}{2}+1})$, is spanned by the vectors of Eq.(3.53) with $\{|i\rangle_{N/2+1}\}\in\mathbb{C}^{N/2+1}\cong\mathcal{S}\left((\mathbb{C}^2)^{\otimes N/2}\right)$. Moreover, any Dicke state of N qubits can be expressed as a linear combination of $(\frac{N}{2}+1)\times(\frac{N}{2}+1)$ system. Let us see an explicit example in the case of $N=4$.
The symmetric space of 4 qubits is spanned by the Dicke states $\{|D_k^4\rangle\}_{k=0}^4$ and it holds $\dim(\mathcal{S}((\mathbb{C}^2)^{\otimes 4})=5$. Now consider the bipartite Hilbert space $\mathbb{C}^{N/2+1}\otimes\mathbb{C}^{N/2+1}$ which, for $N=4$, corresponds to the two-qutrit Hilbert space $\mathbb{C}^3\otimes\mathbb{C}^3$. Its symmetric subspace, $\mathcal{S}(\mathbb{C}^3\otimes\mathbb{C}^3)$, has dimension 6 and is spanned by the Dicke states of Eq.(3.53), where $\{|i\rangle_3\}\in\mathbb{C}^3$ is an orthonormal basis. Notice that $\mathbb{C}^3\cong\mathcal{S}(\mathbb{C}^2)^{\otimes 2}$, since it is possible to define

$$|0\rangle_3 = |D_0^2\rangle\ , \quad |1\rangle_3 = |D_1^2\rangle\ , \quad |2\rangle_3 = |D_2^2\rangle\ . \tag{3.54}$$

Now let us consider the 4-qubit Dicke state $|D_1^4\rangle$. Such state can be decomposed as

$$
\begin{aligned}
|D_1^4\rangle &= \frac{1}{2}\left(|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle\right) \\
&= \frac{1}{\sqrt{2}}\left(|D_1^2\rangle\,|D_0^2\rangle + |D_0^2\rangle\,|D_1^2\rangle\right) \equiv |D_{01}\rangle \ .
\end{aligned}
\tag{3.55}
$$

In this way it is possible to map a 4-qubit symmetric state to a two-qutrit symmetric state. Of course, since the dimension of the two spaces are different, this mapping does not correspond, in general, to an isomorphism. Repeating the same steps of Eq.(3.55) for any other states in $\mathcal{S}(\mathbb{C}^2)^{\otimes 4}$ we find the following relations:

$$|D_0^4\rangle = |D_{00}\rangle \ , \tag{3.56}$$

$$|D_1^4\rangle = |D_{01}\rangle \ , \tag{3.57}$$

$$|D_2^4\rangle = \frac{1}{\sqrt{3}}\left(\sqrt{2}\,|D_{11}\rangle + |D_{02}\rangle\right) \ , \tag{3.58}$$

$$|D_3^4\rangle = |D_{12}\rangle \ , \tag{3.59}$$

$$|D_4^4\rangle = |D_{22}\rangle \ . \tag{3.60}$$

Let us begin our analysis by considering a 4-qubit DS state, i.e.,

$$\rho_{DS}^{Q} = \sum_{k=0}^{4} q_k |D_k^4\rangle\langle D_k^4| \ , \tag{3.61}$$

with $q_k \geq 0$ and $\sum_k q_k = 1$. Making use of Eqs.(3.56)-(3.60) we obtain

$$\rho_{DS}^{Q} = \rho_{DS} + \alpha(|D_{11}\rangle\langle D_{02}| + \text{h.c.}) \ , \tag{3.62}$$

where $\alpha = \sqrt{2}q_2/3$ and ρ_{DS} is a two-qutrit DS state, i.e.,

$$\rho_{DS} = \sum_{0\leq i\leq j\leq 2} p_{ij} |D_{ij}\rangle\langle D_{ij}| \ , \tag{3.63}$$

with coefficients

$$p_{00} = q_0 \ , \qquad p_{01} = q_1 \ , \tag{3.64}$$

$$p_{11} = 2p_{02} = 2q_2/3 \ , \qquad p_{22} = q_4 \ . \tag{3.65}$$

Eq.(3.62) shows that a DS state of 4 qubits ρ_{DS}^{Q} is mapped generically to a two-qutrit symmetric state of the form $\rho_S = \rho_{DS} + \alpha(|D_{11}\rangle\langle D_{02}| + \text{h.c.})$. Setting $q_2 = 0$

implies that $p_{11} = p_{02} = \alpha = 0$, and ρ_{DS}^Q is mapped to a DS state of two qutrits ρ_{DS}. Moreover, since in this case ρ_{DS}^Q is not of full rank, by means of Th.1 in [QRS17] we conclude that ρ_{DS}^Q must be either NPT entangled or trivially separable, i.e., a convex combination of the projectors onto the Dicke states $|D_k^4\rangle$ with $k \in \{0,4\}$. The same conclusion is reached when inspecting the matrix $M(\rho_{DS})$ associated to the mapped state ρ_{DS}, which in this case reads

$$M(\rho_{DS}) = \begin{pmatrix} p_{00} & p_{01}/2 & 0 \\ p_{01}/2 & 0 & p_{12}/2 \\ 0 & p_{12}/2 & p_{22} \end{pmatrix} . \tag{3.66}$$

Since a two-qutrit DS state ρ_{DS} is separable if and only if $M(\rho_{DS}) \in \mathcal{DNN}$, it is easy to see that it is either $M(\rho_{DS}) \succeq 0 \iff p_{01} = p_{12} = 0$ and the state is trivially separable, or ρ_{DS} is NPT-entangled.
In the case $q_2 \neq 0$, we can apply Th.3.15 to ρ_{DS}^Q to deduce separability conditions for the two-qutrit state ρ_S that results from the mapping. Let us first inspect the structure of the partial transposition of ρ_{DS}^Q with respect to the partition $2:2$, i.e., $\left(\rho_{DS}^Q\right)^{\Gamma_{2|2}}$. An analytical calculation shows that $\left(\rho_{DS}^Q\right)^{\Gamma_{2|2}}$ can be cast as:

$$\left(\rho_{DS}^Q\right)^{\Gamma_{2|2}} = \frac{1}{12}\begin{pmatrix} 12q_0 & 3q_1 & 2q_2 \\ 3q_1 & 2q_2 & 3q_3 \\ 2q_2 & 3q_3 & 12q_4 \end{pmatrix} \oplus \frac{1}{12}\begin{pmatrix} 3q_1 & 2q_2 \\ 2q_2 & 3q_3 \end{pmatrix} \oplus \frac{q_2}{6} , \tag{3.67}$$

where the last two blocks in the decomposition appear with multiplicity 2. Hence, imposing $\left(\rho_{DS}^Q\right)^{\Gamma_{2|2}} \succeq 0$ implies the positivity of each block in Eq.(3.67). Recalling Eqs.(3.45)-(3.46) and making use of Eq.(3.64), ρ_S and $\rho_S^{T_B}$ can be cast as:

$$\rho_S = \frac{1}{6}\begin{pmatrix} q_2 & 2q_2 & q_2 \\ 2q_2 & 4q_2 & 2q_2 \\ q_2 & 2q_2 & q_2 \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} 2q_0 & 0 & 0 \\ 0 & q_3 & q_3 \\ 0 & q_3 & q_3 \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} q_1 & q_1 & 0 \\ q_1 & q_1 & 0 \\ 0 & 0 & 2q_4 \end{pmatrix} , \tag{3.68}$$

$$\rho_S^{T_B} = \frac{1}{6}\begin{pmatrix} 6q_0 & 3q_1 & q_2 \\ 3q_1 & 4q_2 & 3q_3 \\ q_2 & 3q_3 & 6q_4 \end{pmatrix} \oplus \frac{1}{6}\begin{pmatrix} 3q_1 & 2q_2 & 0 \\ 2q_2 & 3q_3 & 0 \\ 0 & 0 & q_2 \end{pmatrix} \oplus \frac{1}{6}\begin{pmatrix} q_2 & 0 & 0 \\ 0 & 3q_1 & 2q_2 \\ 0 & 2q_2 & 3q_3 \end{pmatrix} . \tag{3.69}$$

Notice that the first 3×3 matrix in Eq.(3.69) is positive semidefinite since it can be expressed as

$$\begin{pmatrix} 6q_0 & 3q_1 & q_2 \\ 3q_1 & 4q_2 & 3q_3 \\ q_2 & 3q_3 & 6q_4 \end{pmatrix} = \begin{pmatrix} 12q_0 & 3q_1 & 2q_2 \\ 3q_1 & 2q_2 & 3q_3 \\ 2q_2 & 3q_3 & 12q_4 \end{pmatrix} \star \begin{pmatrix} 1/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 1/2 \end{pmatrix} , \tag{3.70}$$

where the symbol $\star$ denotes the Hadamard product between two matrices and the result follows due to the condition $\left(\rho_{DS}^{Q}\right)^{\Gamma_{2|2}} \succeq 0$ and the Schur product theorem. Similarly, it is straightforward to check that $\left(\rho_{DS}^{Q}\right)^{\Gamma_{2|2}} \succeq 0$ implies $\rho_S \succeq 0$ as well as the positivity of the remaining blocks in Eq.(3.69). As a consequence, the state ρ_S is PPT and separable. Notice that, in this case, the two-qutrit state ρ_S given by

$$\rho_S = \rho_{DS} + \alpha(|D_{11}\rangle\langle D_{02}| + \text{h.c.}) \ , \tag{3.71}$$

with $p_{11} = 2p_{02} = \sqrt{2}\alpha$ has rank 5, so that it is isomorphic to a DS 4-qubit state ρ_{DS}^{Q}. For this reason, the mapping given by Eqs.(3.56)-(3.60) can be inverted. As a result, we find

$$|D_{00}\rangle = |\bar{0}\rangle \ , \tag{3.72}$$
$$|D_{01}\rangle = |\bar{1}\rangle \ , \tag{3.73}$$
$$|D_{02}\rangle = \sqrt{3}\,|\bar{2}\rangle - \sqrt{2}\,|D_{11}\rangle \ , \tag{3.74}$$
$$|D_{12}\rangle = |\bar{3}\rangle \ , \tag{3.75}$$
$$|D_{22}\rangle = |\bar{4}\rangle \ , \tag{3.76}$$

and the state of Eq.(3.71) can be mapped to a 4-qubit DS state ρ_{DS}^{Q} with coefficients

$$q_0 = p_{00} \ , q_1 = p_{01} \ , \tag{3.77}$$
$$q_2 = 3p_{02} \ , q_3 = p_{12} \ , q_4 = p_{22} \ . \tag{3.78}$$

Repeating a similar analysis of the previous paragraph, we can see that $\rho_S^{T_B} \succeq 0$ implies $\left(\rho_{DS}^{Q}\right)^{\Gamma_{2|2}} \succeq 0$, so that the PPT condition is both necessary and sufficient to ensure the separability of the state ρ_S of Eq.(3.71). This result can be easily generalised to the case of other coherences of the same form by considering an alternative mapping in Eq.(3.54). For instance, defining

$$|0\rangle_3 = |D_2^2\rangle \ , \quad |1\rangle_3 = |D_0^2\rangle \ , \quad |2\rangle_3 = |D_1^2\rangle \ , \tag{3.79}$$

would correspond to a mapped state $\rho_S = \rho_{DS} + \sigma_{CS}$ with $\sigma_{CS} = \gamma(|D_{22}\rangle\langle D_{01}| +$ h.c.). These results can be resumed in the following theorem:

Theorem 3.16. *Let $\rho_S \in \mathcal{B}(\mathcal{S}(\mathbb{C}^3 \otimes \mathbb{C}^3))$ be a symmetric state of the form $\rho_S = \rho_{DS} + \alpha_{jk}^{i}\,(|D_{ii}\rangle\langle D_{jk}| + h.c.)$, with $p_{ii} = 2p_{jk} = \sqrt{2}\alpha_{jk}^{i}$ for $i \neq j \neq k$. The state ρ_S is separable if and only if is PPT.*

Let us now consider the case where the mapping is applied to a symmetric state of 4 qubits. Making use of Lemma 3.2, we can derive sufficient conditions for the separability of the resulting state through the mapping. For instance, consider an initial symmetric state of 4 qubits of the form:

$$\rho_S^Q = \rho_{DS}^Q + \beta(|D_0^4\rangle\langle D_3^4| + \text{h.c.}) \ . \tag{3.80}$$

Making use of Eqs.(3.56)-(3.60) we find

$$\rho_S^Q = \rho_{DS} + \alpha(|D_{11}\rangle\langle D_{02}| + \text{h.c.}) + \beta(|D_{00}\rangle\langle D_{12}| + \text{h.c.}) \ , \tag{3.81}$$

so that applying the mapping we obtain a symmetric state of two qutrits. Now, we require $(\rho_S^Q)^{\Gamma_{2|2}} \succeq 0$ as well as $(\rho_S^Q)^{\Gamma_{1|3}} \not\succeq 0$. An explicit calculation shows that $(\rho_S^Q)^{\Gamma_{2|2}}$ can be written as

$$(\rho_S^Q)^{\Gamma_{2|2}} = \frac{1}{12}\left(M_0^{2|2} \oplus M_1^{2|2} \oplus M_2^{2|2}\right) \ , \tag{3.82}$$

with

$$M_0^{2|2} = \begin{pmatrix} 12q_0 & 3q_1 & 2q_2 \\ 3q_1 & 2q_2 & 3q_3 \\ 2q_2 & 3q_3 & 12q_4 \end{pmatrix} \ , \tag{3.83}$$

$$M_1^{2|2} = \begin{pmatrix} 3q_1 & 2q_2 & 6\beta \\ 2q_2 & 3q_3 & 0 \\ 6\beta & 0 & 2q_2 \end{pmatrix} \ , \tag{3.84}$$

$$M_2^{2|2} = \begin{pmatrix} 2q_2 & 6\beta & 0 \\ 6\beta & 3q_1 & 2q_2 \\ 0 & 2q_2 & 3q_3 \end{pmatrix} \ . \tag{3.85}$$

Similarly, $(\rho_S^Q)^{\Gamma_{1|3}}$ can be cast as

$$(\rho_S^Q)^{\Gamma_{1|3}} = \frac{1}{12}\left(M_0^{1|3} \oplus M_1^{1|3} \oplus M_2^{1|3}\right) \ , \tag{3.86}$$

with

$$M_0^{1|3} = \begin{pmatrix} 3q_1 & 2q_2 \\ 2q_2 & 3q_3 \end{pmatrix} \ , \tag{3.87}$$

$$M_1^{1|3} = \begin{pmatrix} 12q_0 & 6\beta & 3q_1 \\ 6\beta & 3q_3 & 0 \\ 3q_1 & 0 & 2q_2 \end{pmatrix} \ , \tag{3.88}$$

$$M_2^{1|3} = \begin{pmatrix} 2q_2 & 6\beta & 3q_3 \\ 6\beta & 3q_1 & 0 \\ 3q_3 & 0 & 12q_4 \end{pmatrix} \ . \tag{3.89}$$

Finally, the two-qutrit symmetric state ρ_S and its partial transposition $\rho_S^{T_B}$ can be decomposed as: ρ_S and $\rho_S^{T_B}$ can be cast as:

$$\rho_S = \frac{1}{6}\begin{pmatrix} q_2 & 2q_2 & q_2 \\ 2q_2 & 4q_2 & 2q_2 \\ q_2 & 2q_2 & q_2 \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} 2q_0 & \sqrt{2}\beta & \sqrt{2}\beta \\ \sqrt{2}\beta & q_3 & q_3 \\ \sqrt{2}\beta & q_3 & q_3 \end{pmatrix} \oplus \frac{1}{2}\begin{pmatrix} q_1 & q_1 & 0 \\ q_1 & q_1 & 0 \\ 0 & 0 & 2q_4 \end{pmatrix} , \tag{3.90}$$

$$\rho_S^{T_B} = \frac{1}{6}\begin{pmatrix} 6q_0 & 3q_1 & q_2 \\ 3q_1 & 4q_2 & 3q_3 \\ q_2 & 3q_3 & 6q_4 \end{pmatrix} \oplus \frac{1}{6}\begin{pmatrix} 3q_1 & 2q_2 & 3\sqrt{2}\beta \\ 2q_2 & 3q_3 & 0 \\ 3\sqrt{2}\beta & 0 & q_2 \end{pmatrix} \oplus \frac{1}{6}\begin{pmatrix} q_2 & 3\sqrt{2}\beta & 0 \\ 3\sqrt{2}\beta & 3q_1 & 2q_2 \\ 0 & 2q_2 & 3q_3 \end{pmatrix} . \tag{3.91}$$

Analogously to what we have seen in the previous case, it is easy to see that $(\rho_S^Q)^{\Gamma_{2|2}} \succeq 0$ implies $\rho_S, \rho_S^{T_B} \succeq 0$. Moreover, a tedious but straightforward calculation shows that

$$(\rho_S^Q)^{\Gamma_{1|3}} < 0 \iff \det(M_1^{1|3}) < 0 \text{ or } \det(M_2^{1|3}) < 0 . \tag{3.92}$$

These conditions can be reformulated in terms of equivalent bounds on β, i.e.,

$$\det(M_1^{1|3}) < 0 \iff \beta^2 > q_0 q_3 - \frac{3q_1^2 q_3}{8q_2} , \tag{3.93}$$

or

$$\det(M_2^{1|3}) < 0 \iff \beta^2 > \frac{q_1 q_2}{6} - \frac{q_1 q_3^2}{16 q_4} , \tag{3.94}$$

where in both cases the right hand sides are non-negative real quantities. Hence, any β that fulfils either Eq.(3.93) or Eq.(3.94), while preserving the PPT condition $(\rho_S^Q)^{\Gamma_{2|2}} \succeq 0$, leads to a two-qutrit PPT-entangled state. Making use of Eq.(3.64), we can rephrase this result as the following theorem:

Theorem 3.17. *Let $\rho_S \in \mathcal{B}(\mathcal{S}(\mathbb{C}^3 \otimes \mathbb{C}^3))$ be a PPT symmetric state of the form*

$$\rho_S = \rho_{DS} + \alpha_{jk}^i \left(|D_{ii}\rangle\langle D_{jk}| + \text{h.c.} \right) + \alpha_{ik}^j \left(|D_{jj}\rangle\langle D_{ik}| + \text{h.c.} \right) , \tag{3.95}$$

with $p_{ii} = 2p_{jk} = \sqrt{2}\alpha_{jk}^i$ for $i \neq j \neq k$. If α_{ik}^j is such that it is either

$$(\alpha_{ik}^j)^2 > \frac{p_{ik}}{4p_{ii}}(4p_{ii}p_{jj} - p_{ij}^2) , \tag{3.96}$$

or

$$(\alpha_{ik}^j)^2 > \frac{p_{ij}}{16p_{kk}}(4p_{ii}p_{kk} - p_{ik}^2) , \tag{3.97}$$

then ρ_S is PPT-entangled.

Let us conclude this section with a final remark regarding the mapping we have presented. Notice that Lemma 3.2 provides a sufficient but not necessary condition for a symmetric N-qubit state to be bound entangled w.r.t. the $\frac{N}{2}:\frac{N}{2}$ partition, and indeed there exist states of this kind that are PPT w.r.t. all partitions. For instance, in [TAQ+18], it was found a 4-qubit PPTES with all positive partial transpositions. Interestingly, when mapped to a two-qutrit symmetric state, we obtain a $(5,8)$ state of the same form of Eq.(3.45) with coefficients

$$p_{00} = p_{22} = \frac{7}{50}, \qquad p_{11} = \frac{4}{25},$$
$$p_{01} = p_{12} = \frac{6}{25}, \qquad p_{02} = \frac{2}{25},$$

and coherences $\alpha = 2\sqrt{2}/25, \beta = 0,\ \gamma = (-1/25)\sqrt{15/7}$. Using the method of PPT-symmetric extensions we have numerically checked that this state is indeed PPT-entangled, although α and γ violate both of the requirements of Th.3.17.

4

Non-locality in open quantum systems

Dove ti sei perduta
da quale dove non torni,
assediata
bruci senza origine.
Questo fuoco
deve trovare le sue parole
pronunciare condizioni
di smarrimento dire:
"Sei l'unica me che ho
torna a casa".
Chandra Livia Candiani

As we have seen in section 2.4, the characterisation of non-locality in many-body systems requires the construction of N-body correlators, a fact which makes this task NP-hard already for few parties. Surprisingly enough, when dealing with systems of indistinguishable particles, it has been demonstrated [TAS+14] that non-locality in the many-body scenario can be assessed by using only one- and two-body correlators, a result which greatly reduces the complexity of this task. A natural question is whether the same technique can be used to detect non-locality also when the system under exam interacts with an external environment, acting as a source of noise. In this chapter we investigate this scenario, providing several examples of many-body open quantum systems where non-local correlations can be detected also in the presence of noise. In section 4.1 we introduce the family of permutatationally-invariant Bell inequalities, which represent the main tool we will use to detect non-locality. After introducing the physical model for the open quantum system (section 4.2), we analyse both the stationary (section 4.3) and the dynamical regime (section 4.4), as well as the out of equilibrium scenario (section 4.5), showing how, in all cases, non-local correlations can be detected by the aforementioned class of Bell inequalities. Finally, in section 4.6, we inspect the case of a system undergoing repeated measurements and discuss the robustness of non-locality in this scenario.

4.1 Permutationally-invariant Bell inequalities

In what follows, we restrict to the Bell scenario $(N, 2, 2)$, i.e., a multipartite Bell experiment with N parties, each of them able to perform at most two measurements, yielding at most two possible outcomes. As already discussed, even in this case, Bell inequalities for many-body systems are extremely difficult to devise. The reason behind this complexity stems from the fact that tight Bell inequalities correspond to the facets of the local polytope $\mathcal{L}$, an object which is incredibly hard to characterise for increasing values of N. In order to simplify this task, in [TAS+14] the authors considered an approach where $\mathcal{L}$ is projected onto a simpler object by: i) disregarding any correlator of order strictly greater than 2; and ii) requiring the remaining correlators to be invariant under any permutation of the parties. As a consequence, $\mathcal{L}$ is projected onto a simpler object, dubbed the permutationally invariant polytope, whose facets correspond to Bell inequalities of the form [TAS+15]

$$\beta_{cl} + \alpha \mathcal{C}_0 + \beta \mathcal{C}_1 + \frac{\gamma}{2} \mathcal{C}_{00} + \delta \mathcal{C}_{01} + \frac{\epsilon}{2} \mathcal{C}_{11} \geq 0 \,, \tag{4.1}$$

where $\alpha, \beta, \gamma, \delta, \epsilon \in \mathbb{R}$, $\beta_{cl} \in \mathbb{R}$ is the so-called classical bound of the associated Bell inequality and

$$\mathcal{C}_r = \sum_{i=0}^{N-1} \langle \mathcal{M}_r^{(i)} \rangle \,, \quad \mathcal{C}_{rs} = \sum_{i \neq j=0}^{N-1} \langle \mathcal{M}_r^{(i)} \mathcal{M}_s^{(j)} \rangle \,, \tag{4.2}$$

are the one- and two-body permutationally-invariant correlators, respectively, with measurement settings $r, s \in \{0, 1\}$.
Since we are dealing with only two dichotomic measurements for each party, it can be shown [TV06; Mas05] that it is enough to consider traceless real observables, so that we can write

$$\mathcal{M}_0^{(i)} = \cos(\phi_i)\sigma_z^{(i)} + \sin(\phi_i)\sigma_x^{(i)} \ , \tag{4.3}$$

$$\mathcal{M}_1^{(i)} = \cos(\theta_i)\sigma_z^{(i)} + \sin(\theta_i)\sigma_x^{(i)} \ , \tag{4.4}$$

where $\sigma_\mu^{(i)}$ denotes the Pauli matrix at site i along the direction $\mu \in \{x, y, z\}$ and (ϕ_i, θ_i) are the measurement angles of each party. Moreover, it is possible to introduce a Bell operator $\mathcal{B}(\{\phi_i, \theta_i\})$, associated to the family of inequalities (4.1), i.e.,

$$\beta_{cl}\mathbb{1}_{2^N} + \alpha\hat{\mathcal{C}}_0 + \beta\hat{\mathcal{C}}_1 + \frac{\gamma}{2}\hat{\mathcal{C}}_{00} + \delta\hat{\mathcal{C}}_{01} + \frac{\epsilon}{2}\hat{\mathcal{C}}_{11} \ , \tag{4.5}$$

where the correlators are replaced by the operators $\hat{\mathcal{C}}_r$,$\hat{\mathcal{C}}_{rs}$, defined as

$$\hat{\mathcal{C}}_r = \sum_{i=0}^{N-1} \mathcal{M}_r^{(i)} \ , \quad \hat{\mathcal{C}}_{rs} = \sum_{i \neq j=0}^{N-1} \mathcal{M}_r^{(i)}\mathcal{M}_s^{(j)} \ . \tag{4.6}$$

Hence, whenever condition $\mathrm{Tr}[\mathcal{B}(\{\phi_i, \theta_i\})\rho] < 0$ holds, the state ρ is non-local (and thus, entangled).

Notice that, even though the Bell inequalities of Eq.(4.1) are invariant with respect to any permutation of the parties, neither the Bell operator $\mathcal{B}(\{\phi_i, \theta_i\})$ nor the non-local states that it detects, share necessarily the same symmetry. However, it has been argued [TAS+15; ATB+19; PAL+19] that the maximal violation of the Bell inequality of Eq.(4.1) occurs in the case of a permutationally invariant state, when all the parties perform the same measurements, i.e., $\theta_i = \theta_j = \theta$, $\phi_i = \phi_j = \phi$ for all $i \neq j$. Under this assumptions, it is possible to show that $\mathcal{B}(\{\phi_i, \theta_i\})$ now depends only on two angles, i.e., $\mathcal{B}(\phi, \theta)$, and becomes a permutationally invariant operator. Hence, as a consequence of the Schur-Weyl duality, it admits a block-diagonal decomposition, a result which is particularly relevant when dealing with many-body systems, since, in this case, the Bell operator can be stored in a sparse matrix, thus allowing for an effective numerical treatment of the problem.

When one is interested in probing non-locality in symmetric states of N qubits, it turns out that there exists a convenient description in terms of an associated reduced density matrix. First, notice that, given an N-qubit symmetric state, ρ_{SYM}, its two-body reduced density matrix, $\rho_2 = \mathrm{Tr}_{1,\ldots,N-2}(\rho_{SYM})$, is the same regardless of which $N-2$ systems have been traced out. Hence, if ρ_{SYM} is represented in the Dicke bases for N-qubits, then the two-body reduced density matrix reads [TAS+15]

$$(\rho_2)_{\mathbf{i}',\,\mathbf{j}'} = \sum_{k=0}^{N-2} \frac{\binom{N-2}{k}\,(\rho_{SYM})_{k+|\mathbf{i}'|,\,k+|\mathbf{j}'|}}{\sqrt{\binom{N}{k+|\mathbf{i}'|}\binom{N}{k+|\mathbf{j}'|}}}\,, \tag{4.7}$$

where $0 \leq \mathbf{i}',\,\mathbf{j}' < 2^2$, $\mathbf{i}' = i_0 i_1$, $\mathbf{j}' = j_0 j_1$ are the binary representations of the labels associated to the matrix entries and $|\mathbf{i}|'$, $|\mathbf{j}|'$ are their Hamming weights, i.e., the number of ones in this representation.
Analogously, we can associate to $\mathcal{B}(\phi,\theta)$ a two-qubit Bell operator, $\mathcal{B}_2(\phi,\theta)$, whose explicit expression is given by [TAS+15]

$$\begin{aligned}\mathcal{B}_2(\phi,\theta) = {} & \beta_{cl}\,(\mathbb{1}_2\otimes\mathbb{1}_2) + \frac{N}{2}\left[\alpha\,(\mathcal{M}_0\otimes\mathbb{1}_2+\mathbb{1}_2\otimes\mathcal{M}_0)+\beta\,(\mathcal{M}_1\otimes\mathbb{1}_2+\mathbb{1}_2\otimes\mathcal{M}_1)\right] \\ & + \frac{N(N-1)}{2}[\gamma\mathcal{M}_0\otimes\mathcal{M}_0+\delta(\mathcal{M}_0\otimes\mathcal{M}_1+\mathcal{M}_1\otimes\mathcal{M}_0)+\epsilon\mathcal{M}_1\otimes\mathcal{M}_1]\,.\end{aligned} \tag{4.8}$$

Again, if condition $\mathrm{Tr}[\mathcal{B}_2(\phi,\theta)\rho_2] < 0$ holds, then the state ρ_2 is non-local and the same goes true for the full state ρ, an observation which allows to greatly reduce the computational cost required to probe non-locality. Nonetheless, let us remark that in order to perform a fully device-independent Bell experiment, one should still be able address all the parties individually. In [TAS+15] it has been proven that the family of Bell inequalities 4.1 exhibits maximal violation in the block of maximum spin, which corresponds to the symmetric subspace of N qubits spanned by the set of Dicke states $\{|D_k^N\rangle\}$. Since Dicke states appear naturally in physically relevant models, such as the Lipkin-Meshkov-Glick (LMG) Hamiltonian, the relevance of Bell inequalities (4.1) is clear in the context of many-body physics. We now want to take a step further and show that, also in the open scenario, Bell inequalities (4.1) play a crucial role in the detection of non-local correlations. In what follows, we restrict to the Bell inequality that is obtained by setting $\beta_{cl} = 2N, \alpha = -2, \beta = 0, \gamma = 1, \delta = -1, \epsilon = 1$ in Eq.(4.1), i.e.,

$$2N - 2\mathcal{C}_0 + \frac{1}{2}\mathcal{C}_{00} - \mathcal{C}_{01} + \frac{1}{2}\mathcal{C}_{11} \geq 0\,, \tag{4.9}$$

whose associated Bell operator is given by

$$\mathcal{B}(\phi,\theta) = 2N\mathbb{1}_{2^N} - 2\hat{\mathcal{C}}_0 + \frac{1}{2}\hat{\mathcal{C}}_{00} - \hat{\mathcal{C}}_{01} + \frac{1}{2}\hat{\mathcal{C}}_{11}\,. \tag{4.10}$$

Since we are interested in the subspace of symmetric states, where the maximal violation occurs, we can make use of the two-qubit Bell operator, i.e.,

$$\begin{aligned}\mathcal{B}_2(\phi,\theta) &= 2N\left(\mathbb{1}_2\otimes\mathbb{1}_2\right)+\frac{N}{2}\left[-2\left(\mathcal{M}_0\otimes\mathbb{1}_2+\mathbb{1}_2\otimes\mathcal{M}_0\right)\right] \\ &+\frac{N(N-1)}{2}\left[\mathcal{M}_0\otimes\mathcal{M}_0+\mathcal{M}_1\otimes\mathcal{M}_1-\left(\mathcal{M}_0\otimes\mathcal{M}_1+\mathcal{M}_1\otimes\mathcal{M}_0\right)\right].\end{aligned} \tag{4.11}$$

4.2 The main system

As the physical model for the main system S we consider a particular case of the LMG Hamiltonian, i.e.,

$$H_S=\frac{J}{N}S_z^2-hS_x\ , \tag{4.12}$$

where J is the interaction energy scale, h is a magnetic field applied along the x direction and the collective spin operators are $S_\mu=\frac{1}{2}\sum_{i=1}^N\sigma_\mu^{(i)}$, with $\mu\in\{x,y,z\}$. The choice of this specific model are several: first, H_S describes the interaction between N-qubit symmetric states and the ground state of Eq.(4.12) corresponds to a Gaussian superposition of Dicke states, which is known to maximally violate the family of Bell inequalities (4.8) [TAS+14]; furthermore, since H_S depends only on collective spin properties, it admits a block decomposition of the form

$$H_S=\bigoplus_M H_S(M)\ , \tag{4.13}$$

where the sum runs over the total spin number $M=M_{min},\ldots,N/2-1,N/2$, with $M_{min}\in\{0,1/2\}$, depending on whether N is even or odd. This property turns out to be particularly convenient, since, given the symmetrical nature of our Bell inequality, we can restrict our analysis to the block of maximum total spin $M=N/2$, where the global spin operators can be expressed in the Dicke basis.

4.3 The stationary regime

4.3.1 Thermal noise

We start by considering the stationary regime of the LMG model in contact with a bosonic bath at inverse temperature β. Let us denote by $\{b_k\}$ the bosonic operators ($[b_k,b_{k'}^\dagger]=\delta_{k,k'}$) and assume an interaction of the form $V=S_y\otimes(b_k+b_k^\dagger)$. We derive the corresponding QME (see Eq.(2.45)), and find the stationary solutions by

imposing $\mathcal{L}[\rho_S] = 0$.
In the low-temperature limit, we find that the steady states correspond to thermal states given by a Gaussian superposition of Dicke states of the form [TAS+14]

$$\rho_S \approx |\psi_N\rangle\langle\psi_N| \,, \quad |\psi_N\rangle = \sum_{k=0}^{N} \psi_k^N \, |D_k^N\rangle \,, \tag{4.14}$$

with amplitudes $\psi_k^N \approx (1/\sqrt[4]{2\pi\sigma^2})e^{-(k-N/2)^2/4\sigma^2}$, for some variance σ^2.

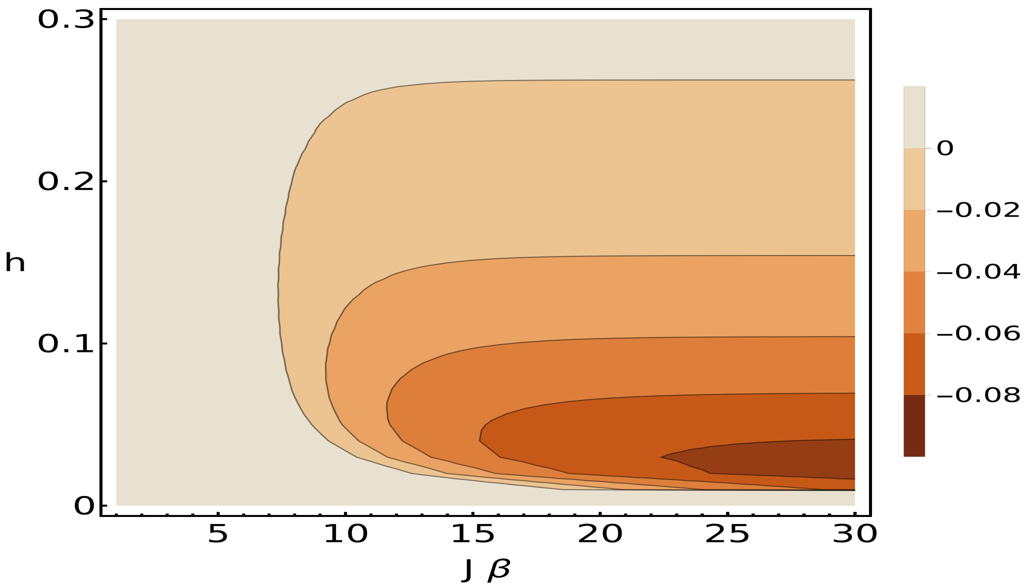

Figure 4.1: Non-local correlations in an OQS described by the Hamiltonian of Eq.(4.12), with $N = 20$, in the case of thermal noise. Negative values indicate the quantum violation (Q_v) of the Bell inequality associated to Eq.(4.8).

In Fig.4.1 we display the detection of non-local correlations as a function of the magnetic field h, the energy coupling J and the inverse temperature β. We observe that there is a significant region of the phase-space for which $\mathrm{Tr}[\mathcal{B}_2(\phi,\theta)\rho_2] < 0$, providing evidence of their robustness against thermal noise. Notice that our results are consistent with the fact that, for $h = 0$, the steady-states of H_S of Eq.(4.12) are clearly separable. Moreover, for high temperatures, i.e., low values of β, thermal fluctuations hinder the possibility to observe non-locality.

4.3.2 Non-thermal noise

Although the coupling with a thermal bath is the most common scenario when dealing with an OQS, we consider the effect of a dissipation that leads to non-thermal steady-states. To this end, referring to Eq.(2.45), we design an *ad hoc* jump operator of the form $\mathcal{J}(\zeta) = \cos(\zeta)\hat{S}_+ + \sin(\zeta)\hat{S}_-$, where $\hat{S}_\pm = U^\dagger S_\pm U$ and U is a unitary transformation from the Dicke basis to the energy basis, i.e., the set of eigenstates of H_S, and $S_\pm = S_x \pm iS_y$. Again, the resulting steady-state solutions are found by imposing $\mathcal{L}[\rho_S] = 0$ for the corresponding GKLS master equation.

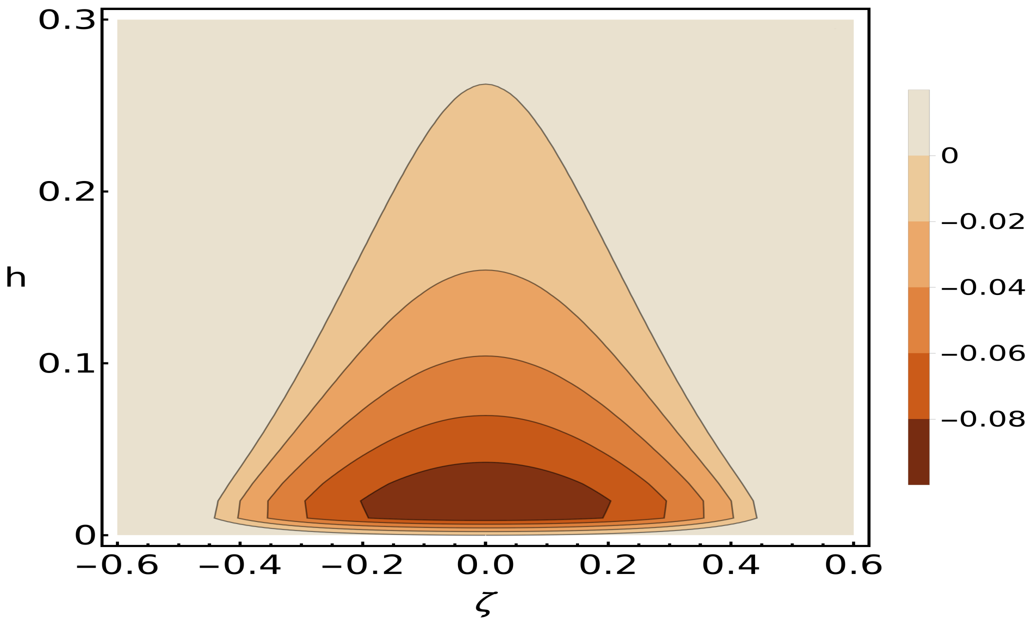

Figure 4.2: Non-local correlations in an OQS described by the Hamiltonian of Eq.(4.12), with $N = 20$, in the case of a non-thermal jump operator $\mathcal{J}(\zeta) = \cos(\zeta)\hat{S}_+ + \sin(\zeta)\hat{S}_-$. Negative values indicate the quantum violation (Q_v) of the Bell inequality associated to Eq.(4.8).

In Fig.4.2 we plot the non-local correlations detected by the Bell operator of Eq.(4.8), and relate them to J, h and the angle ζ. Also in this case, we find that non-locality is present and can be detected for a large range of values of the parameter ζ, showing to be robust against the effect of the magnetic field especially around $\zeta = 0$. Indeed, notice that, for $\zeta = 0$, one gets $\mathcal{J}(0) = \hat{S}_+$, and the effect of the dissipation is to force the evolution towards a thermal steady state given by the same Gaussian superposition of Dicke states of Eq.(4.14). However, for $\zeta \neq 0$, the steady-state solutions are not thermal states, a feature that makes our analysis in this regime particularly valuable.

4.4 The dynamical regime

While in Fig.4.1-4.2 we showed that stationary steady-states exhibit non-local correlations, we are now interested in the somehow opposite regime of the dynamical evolution.

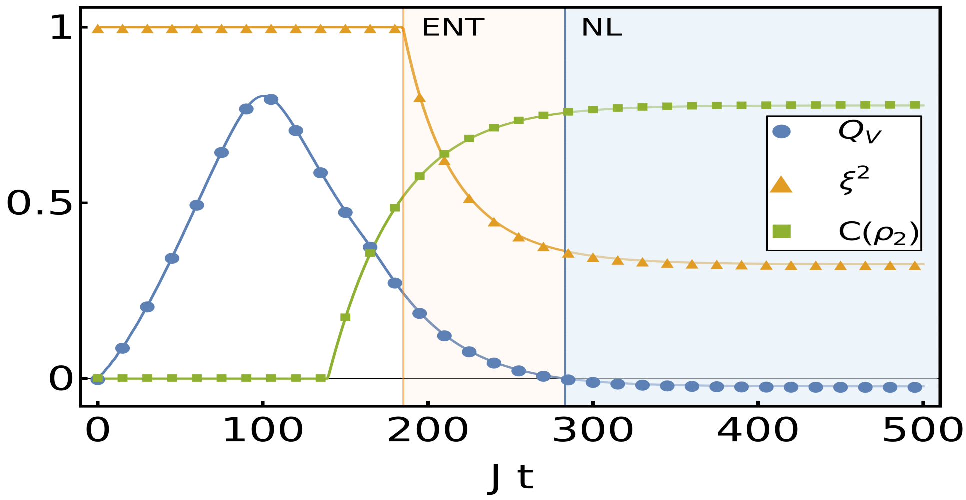

Figure 4.3: Comparison between concurrence (green squares), spin squeezing criterion (orange triangles) and non-local correlations (blue dots) detected by Bell operator (4.8) in the state $\rho_S(t)$ for thermal noise. The value of the violation in the stationary regime corresponds to the steady-state solutions of Fig.4.1 with $N = 20,\ J = 1,\ h = 0.05$ for $\beta = 10$. NL (light blue) and ENT (orange) signal the region of non-locality and entanglement, respectively. Notice that the latter region comprises also the former. For the ease of readability, $C(\rho_2)$ has been multiplied by a factor N and ξ^2 has been chosen equal to 1 for separable states.

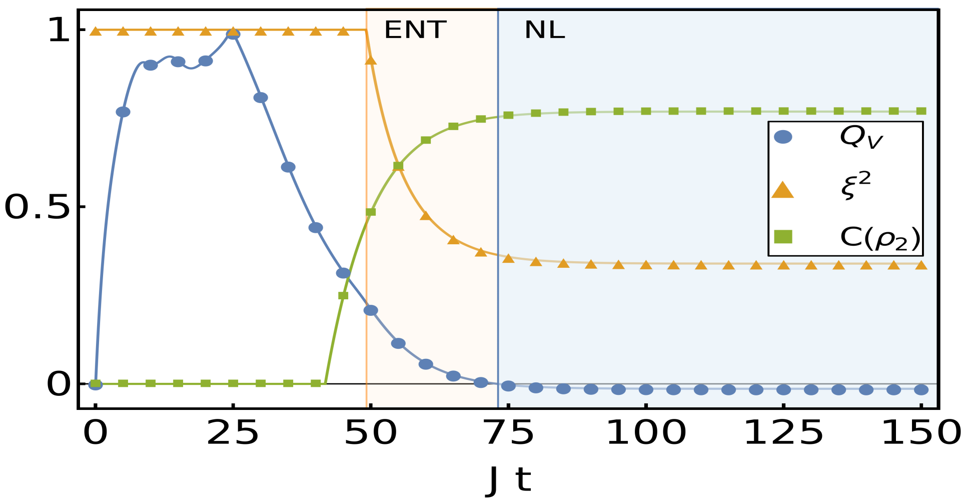

Figure 4.4: Comparison between concurrence (green squares), spin squeezing criterion (orange triangles) and non-local correlations (blue dots) detected by Bell operator (4.8) in the state $\rho_S(t)$ for a non-thermal jump operator $\mathcal{J}(\zeta) = \cos(\zeta)\hat{S}_+ + \sin(\zeta)\hat{S}_-$. The value of the violation in the stationary regime corresponds to the steady-state solutions of Fig.4.2 with $N = 20,\ J = 1,\ h = 0.05$ for $\zeta = 0.35$. NL (light blue) and ENT (orange) signal the region of non-locality and entanglement, respectively. Notice that the latter region comprises also the former. For the ease of readability, $C(\rho_2)$ has been multiplied by a factor N and ξ^2 has been chosen equal to 1 for separable states.

In Fig.4.3-4.4, we show how the stationary steady-state solutions of Fig.4.1-4.2 can be recovered as the result of a dynamical evolution. In particular, starting from a local initial state of the form $\rho_S(0) = |D_N^N\rangle\langle D_N^N|$, we show that non-local correlations can arise in the state $\rho_S(t)$, proving to be robust against the effect of dissipation both in the case of thermal and non-thermal noise. Furthermore, we compare the estimation of the entanglement of $\rho_S(t)$ provided by two distinct criteria. First, with the aid of Eq.(4.7), we derive the two-qubit reduced density matrix ρ_2 and we compute its concurrence, $C(\rho_2)$, defined as

$$C(\rho_2) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)\ , \tag{4.15}$$

where the λ_i's are the eigenvalues of $\rho_2\tilde{\rho}_2$, with $\tilde{\rho}_2 = (\sigma_y \otimes \sigma_y)\, \rho_2^*\, (\sigma_y \otimes \sigma_y)$, ordered in descending order.

Second, we inspect the value of the so-called spin squeezing parameter ξ^2, defined as

$$\xi^2 = N\frac{(\Delta S_z)^2}{\langle S_x\rangle^2 + \langle S_y\rangle^2} \ , \tag{4.16}$$

where $(\Delta S_z)^2 \equiv \langle S_z^2\rangle - \langle S_z\rangle^2$. In this case, if $\xi^2 < 1$, then the state is entangled. Notice that when dealing with symmetric states of N qubits, the spin squeezing criterion is able to detect genuine multipartite entanglement [WS03]. In Fig.4.3-4.4 we display, for both the dissipators previously considered (i.e., thermal and non-thermal), the violation of the Bell inequality (4.8) along with an estimation of the entanglement of $\rho_S(t)$ by means of the concurrence and the spin squeezing criterion. Notice that, in the case of thermal noise (Fig.4.3), non-local correlations manifest at a later time as compared to the case of the non-thermal dissipator (Fig.4.4). Interestingly, we observe a time gap also between the two estimations of the entanglement, a feature which is consistent with the different nature (i.e., two-body versus many-body) of the concurrence and the spin squeezing criterion. In both cases our results provide further evidence that non-locality and entanglement are inequivalent resources, as they clearly manifest at different times scales.

4.5 The out of equilibrium regime

We study the robustness of non-locality in an OQS also in an out of equilibrium scenario, by inspecting the time evolution of the system when dissipation is taken into account. Referring to the Hamiltonian of Eq.(4.12), we consider the simpler case $h = 0$, i.e.,

$$H_S = -\omega S_z^2 + \frac{\omega N}{2}\left(\frac{N}{2}+1\right) \ , \tag{4.17}$$

with $\omega = J/N$.
Starting from a local state of the form $\rho_S(0) = |D^N_{N/2}\rangle\langle D^N_{N/2}| + |D^N_{N/2+1}\rangle\langle D^N_{N/2+1}| + |D^N_{N/2}\rangle\langle D^N_{N/2+1}| + \text{h.c.}$, we consider the evolution of the system in the presence of dissipation.

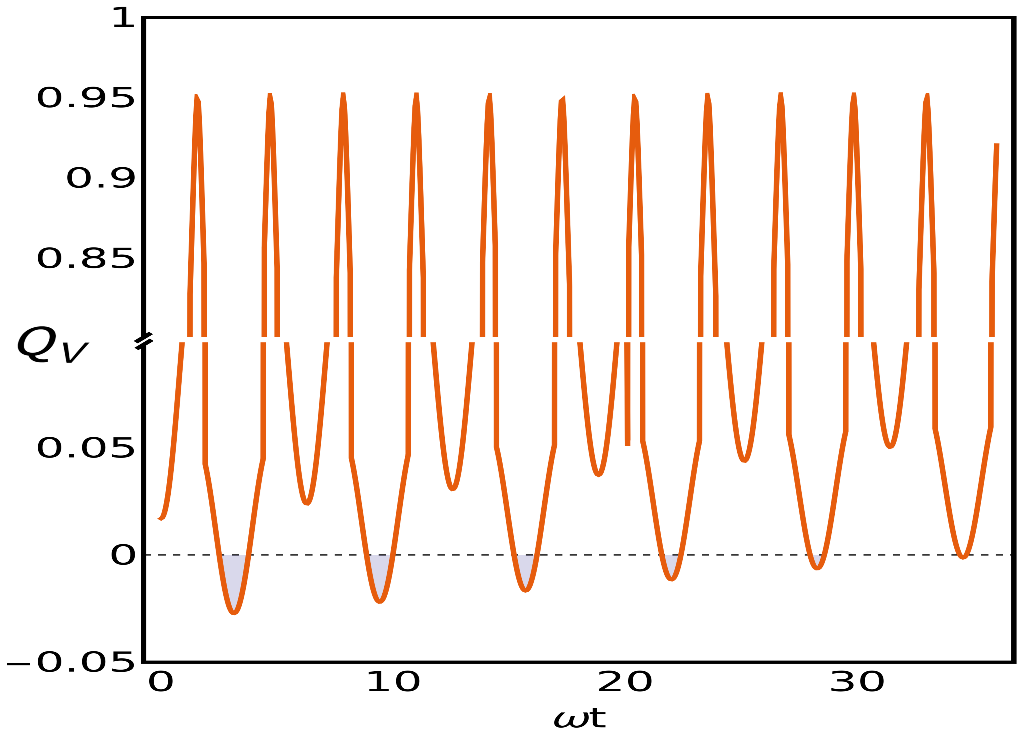

Figure 4.5: Non-local correlations in an OQS described by the Hamiltonian of Eq.(4.17), with $N = 20$ and $\omega = 1$, when a jump operator $\mathcal{J} = S_y/\sqrt{N}$ is considered. Light-blue shaded areas correspond to the negative values of the quantum violation (Q_v) as detected by Bell operator (4.8). The two slanting lines on the y-axis indicate that part of the range has been omitted for the ease of readability.

In Fig.4.5 we plot the quantum violation detected by means of Eq.(4.8) when a jump operator $\mathcal{J} = S_y/\sqrt{N}$ in Eq.(2.45) is considered, with $\gamma = 0.001$. Despite the presence of the dissipation, non-local correlations arise periodically in the system and survive for a certain time. Moreover, the spin squeezing criterion and the analysis of the concurrence attest the presence of entanglement in the dynamical state at all times.

4.6 Repeatedly measured system

Finally, we explore the scenario in which the many-body system S undergoes frequent measurements. From a physical point of view, this setting can be interpreted as the attempt of an eavesdropper to gain information on S while remaining undetected. Interestingly, a system that is weakly and continuously interrogated also obeys an equation of the form (2.45). Namely, given a party Eve that repeatedly performs the measurement $M = \{m_k, \Pi_k\}$ with outcomes m_k and eigenprojectors Π_k, the explicit form of the associated Lindbladian is

$$\partial_t \rho_{\mathrm{S}} = -i[H_{\mathrm{S}}, \rho_{\mathrm{S}}] + \kappa \left(\sum_k \Pi_k \rho_{\mathrm{S}} \Pi_k^\dagger - \rho_{\mathrm{S}} \right) \tag{4.18}$$

where κ is the measurement rate.
This equation was already found in [CBJ+06] but, for completeness, we present an alternative derivation. We denote by δt a very small time step. Then, if the system is not interrogated, the system state evolves according to

$$\rho_{\mathrm{S}}(t+\delta t) = \rho_{\mathrm{S}}(t) - i[H_{\mathrm{S}}, \rho_{\mathrm{S}}(t)]\delta t + \mathcal{O}(\delta t^2) \tag{4.19}$$

Instead, if we perform the measurement $M = \{m_k, \Pi_k\}$ (recall that $\sum_k \Pi_k = \mathbb{1}_{\mathrm{S}}$), the evolved state is given by

$$\rho_{\mathrm{S}}(t+\delta t) = \sum_k \Pi_k \rho_{\mathrm{S}}(t) \Pi_k. \tag{4.20}$$

Now, if the probability of performing a measurement on the interval $[t, t+\delta t]$ is $\kappa\delta t$, we can average the two processes and collect terms to first order in δt to obtain

$$\begin{aligned} \rho_{\mathrm{S}}(t+\delta t) =& (1-\kappa\delta t)\rho_{\mathrm{S}}(t) - i[H_{\mathrm{S}}, \rho_{\mathrm{S}}(t)]\delta t \\ &+ \kappa\delta t \sum_k \Pi_k \rho_{\mathrm{S}}(t) \Pi_k + \mathcal{O}(\delta t^2). \end{aligned} \tag{4.21}$$

Finally, dividing by δt and taking the limit $\delta t \to 0^+$, one recovers Eq.(4.18).

Our analysis is structured as follows: first, we consider an initial state $\rho_{\mathrm{S}}(0)$ derived by numerically solving Eq.(2.45); second, we compute its dynamical evolution under repeated measurements with an operator $\mathcal{M} = S_z$ by means of Eq.(4.18); third, we plot the non-local correlations detected by the Bell operator of Eq.(4.8) for different values of the rate κ as a function of the probability $p = \kappa t$. Our results are shown in Fig.4.6-4.7 where we consider two different initial states: the thermal steady-state for $\beta = 30$ (Fig.4.6); and the non-thermal steady-state for $\zeta = 0.01$ (Fig.4.7).

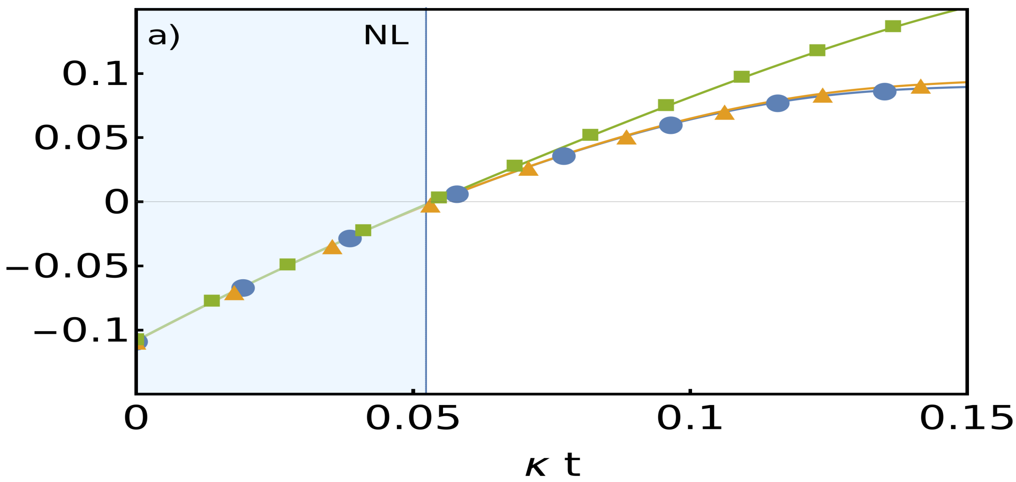

Figure 4.6: Non-local correlations in a many-body system undergoing a repeated measurement $\mathcal{M} = S_z$ at rate k. Blue dots correspond to $\kappa = 1$; orange triangles to $\kappa = 0.1$ and green squares to $\kappa = 0.01$. The initial state has been chosen as the thermal steady-state for $\beta = 30$, $N = 30$, $h = 0.02$ and $J = 1$. NL denotes the non-local region detected by the Bell operator of Eq.(4.8).

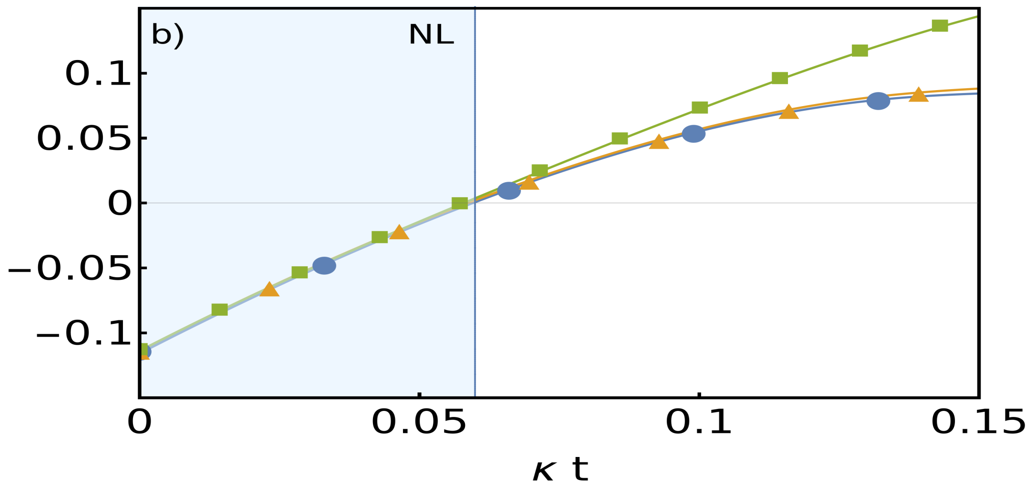

Figure 4.7: Non-local correlations in a many-body system undergoing a repeated measurement $\mathcal{M} = S_z$ at rate k. Blue dots correspond to $\kappa = 1$; orange triangles to $\kappa = 0.1$ and green squares to $\kappa = 0.01$. The initial state has been chosen as the non-thermal steady-state for $\zeta = 0.01$, $N = 30$, $h = 0.02$ and $J = 1$. NL denotes the non-local region detected by the Bell operator of Eq.(4.8).

Our analysis shows that, except for a slight difference in the survival time, the trend is basically the same in the two scenarios. Moreover, we observe that, despite the different values of the measurement rate κ, the slope is identical for all the curves in the non-local region. This can be understood as follows: for sufficiently short times such that $Jt, ht, \kappa t \ll 1$, one can expand the map generated by Eq.(4.18) as

$$\begin{aligned}\partial_t \rho_S(t) &= \rho_S(0) - i[H_S, \rho_S(0)] + \kappa t \left(\sum_k \Pi_k \rho_S(0) \Pi_k^\dagger - \rho_S(0) \right) \\ &= (1 - \kappa t)\rho_S(0) + \kappa t \sum_k \Pi_k \rho_S(0) \Pi_k^\dagger \,, \end{aligned} \tag{4.22}$$

where we have assumed that $[H_S, \rho_S(0)] = 0$.
Hence, with the aid of Eq.(4.22), the state $\rho_S(t)$ can be cast as a convex combination, with probability $p = \kappa t$, of the initial state $\rho_S(0)$ and the dephased state $\bar{\rho}_S(0) = \sum_k \Pi_k \rho_S(0) \Pi_k^\dagger$, i.e., $\rho_S(t) \approx (1-p)\rho_S(0) + p\bar{\rho}_S(0)$. Since we have neglected higher order terms in the exponential map, this result is valid only for $\kappa t \ll 1$, a condition which also guarantees the probability p to be bounded.

5

Quantum maps for neural networks

Ricordami, a settembre – come ricordi l'ultima
stanza della tua casa al mare, in fondo
al corridoio e piccola così
da contenere a malapena un letto.
Sarà il tempo per noi sempre più stretto
rifugio.

Gabriele Galloni

In chapter 2 we have seen how every physical process that describes a change in a quantum state can be represented as the result of the action of a CPTP map on it. As such, quantum channels are ubiquitous and can be used in a variety of different scenarios. Here, we present an application to the case of neural networks, whose evolution, in the case of attractor quantum neural networks (aQNNs) was recently described in terms of quantum channels [LGR+21]. In this way it was demonstrated that aQNNs allow for a storage capacity which scales exponentially with the number of neurons, thus outperforming the one of their classical counterpart [VM98; RBW+18]. In this chapter, using the formalism of quantum channels and their Kraus representation, we show that aQNNs can be analysed using tools from the resource theory of coherence, and discuss their performance both in the error-free and the faulty case, i.e., when some error in the preparation of the network is taken into account. Starting from a brief introduction regarding the major developments in the theory of neural networks (section 5.1), we focus on aQNNs (section 5.2) and establish a link between the associated quantum map and the resource theory of coherence (section 5.3). Within this framework we provide some results regarding the performance of aQNNs both in the error-free (section 5.4) and in the faulty scenario (section 5.5).

5.1 Classical neural networks

Human brain is composed of approximately 10^{11} specialised cells, dubbed neurons, which represent the basic units of the nervous tissue. Each neuron consists of a cell body from which originate some branch-like structures, named dendrites, and a longer termination, called the axon (see Fig.5.1).

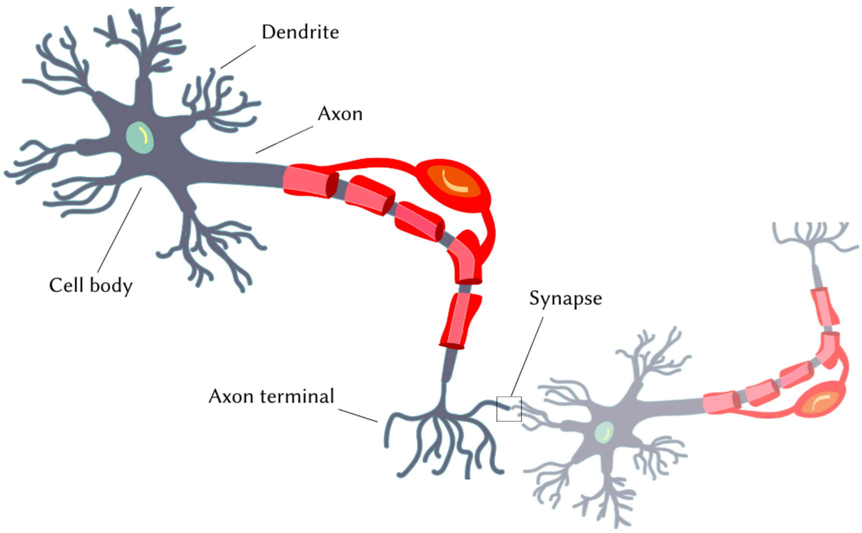

Figure 5.1: The structure of a neuron.

Between the axon terminals of a neuron and the dendrites of another, there exist some structures, called synapses, which allow for the communication of electric signals. In particular, signals can propagate through synapses due to some chemical processes whose effect is to alter the electrical potential in the cell body of the receiving neuron. As a result, if the voltage exceeds a certain threshold, the signal is transmitted and the neuron is said to "fire"; otherwise, the signal is inhibited and the neuron remains in a "rest" state. A collection of interconnected neurons is referred to as a *neural network*. Although this description represents a mere simplification of the functioning of a real neural network, the empirical evidence that a neuron either fires or rests, suggests the possibility to encode its state in a binary variable and, more generally, to describe its behaviour in terms of some mathematical model. Thus, an *artificial* neural network can be conceived as a set of interconnected computational units that mimic the behaviour of real neurons in the nervous system.

5.1.1 The McCulloch-Pitts model

The first attempt to describe mathematically this process is due to McCulloch and Pitts [MP43]. In their model, an artificial neural network consists of a collection of n neurons which can assume binary values $x_i \in \{\pm 1\}$, depending on their status, that is, either active $(x_i = 1)$ or inactive $(x_i = -1)$, respectively. Each neuron collects the incoming inputs, $\{x_1, \ldots, x_n\}$, of the other neurons and emits an output, y_j, depending on the value of the sum $x_1 + \cdots + x_n$: if such value is greater than a certain threshold b_j, then $y_j = 1$, and the neuron fires; otherwise, $y_j = 0$, and the neuron remains inactive (see Fig.5.2). Formally, for the j-th neuron, we have

$$y_j = \begin{cases} 1 & \sum_{i=1}^{n} x_i - b_j \geq 0 \, , \\ 0 & \text{otherwise.} \end{cases} \tag{5.1}$$

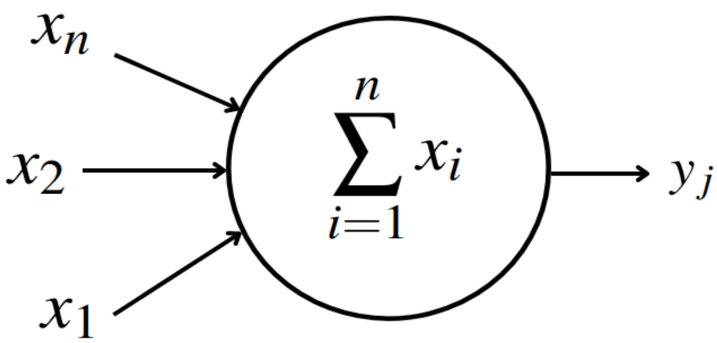

Figure 5.2: Schematic representation of a McCulloch-Pitts neuron. The inputs x_i of each incoming signal are collected by the j-th neuron, whose output y_j depends on the value of the sum $\sum_{i=1}^{n} x_i$.

The comparison between the collected values of the incoming signals and the threshold is typically described in terms of two functions, g and f, that are usually referred to as the *integration* and *activation* functions, respectively: first, g transforms the n-dimensional string $(x_1, \ldots, x_n)$ into a number, and then, the output is obtained by comparing this number with the threshold, i.e., $y_j = f(g(x_1, \ldots, x_n))$. While in general the integration function is taken as the addition between the inputs, i.e., $g(x_1, \cdots, x_n) = x_1 + \ldots x_n$, the activation function can be chosen in several ways. In the McCulloch-Pitts model, f corresponds to the step function $\theta(x)$, defined as

$$\theta(x) = \begin{cases} 1 & x \geq 0 \\ 0 & \text{otherwise} \end{cases} . \tag{5.2}$$

Despite its apparent simplicity, a single McCulloch-Pitts neuron is able to implement basic logical operations such as the AND and OR gates, and it has been demonstrated that any logical function $F : \{0,1\}^n \rightarrow \{0,1\}$ can be computed by a McCulloch-Pitts network of two layers (see e.g., [Roj13]). However, it has been argued that the efficiency of this network depends crucially on the specific task that one wants to solve, and in general it is not possible to intervene dynamically on the network without modifying the neuronal connections or the threshold of each neuron. A natural way to circumvent this drawback is to assign a *weight* w_{ij} between two interacting neurons, that encodes the information regarding the strength of their synaptic connection. Such approach leads to a computational model, known as *perceptron*.

5.1.2 The perceptron

The perceptron is a computational unit introduced for the first time by Rosenblatt in 1958 [Ros58]. From a mathematical point of view, it consists in adding weights to the McCulloch-Pitts model, assigning a factor w_{ij} to each pair of interconnected neurons. Formally, we have

$$y_j = \begin{cases} 1 & \sum_{i=1}^{n} x_i w_{ij} - b_j \geq 0 \, , \\ 0 & \text{otherwise.} \end{cases} \tag{5.3}$$

This process is schematically represented in Fig.5.3, where the basic functioning of a perceptron is depicted.

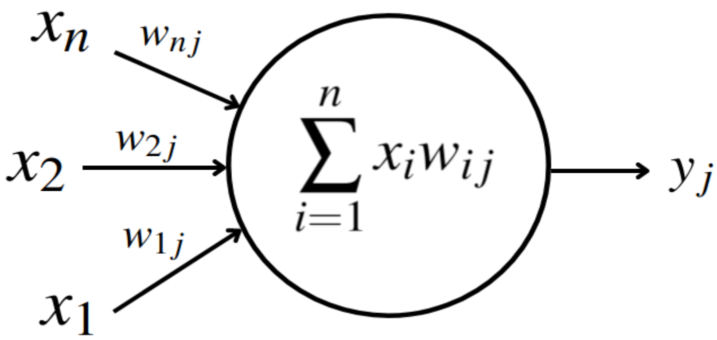

Figure 5.3: Schematic representation of a perceptron. The inputs x_i of each incoming signal are collected by the j-th neuron, whose output y_j depends on the value of the weighted sum $\sum_{i=1}^{n} x_i w_{ij}$.

The conceptual innovation of Rosenblatt's model lies in the possibility to train the network in order to increase its performance when accomplishing a certain task. This feature reflects Hebb's theory to explain synaptic plasticity, that is the capability of human brain to adapt to different situations through experience [Heb05]. According to Hebb, neurons with similar reactions to external stimuli tend to group together, a concept which is sometimes rephrased with the motto "neurons that fire together wire together". Stated differently, if a set of neurons displays a common behaviour, then the connection between them must be stronger than those of a group of unrelated neurons. From a mathematical point of view, this suggests the possibility that the weights w_{ij} in a network can be adjusted according to a *learning algorithm*. As a result of this procedure, some connections will be preferred over others, in such a way that the capability of the network in solving a certain problem can be greatly enhanced. At this point it is evident the advantage offered by the perceptron: while in the McCulloch-Pitts model the only way to train the network is to change its topology, in Rosenblatt's model one can simply update the weights between neurons by assigning a suitable learning rule. The simplest example in this sense is represented by the *Hebbian rule* [Heb05], which consists in updating the weight w_{ij} to a new value w'_{ij}, according to the relation

$$w'_{ij} = w_{ij} + \gamma x_i y_j \ , \tag{5.4}$$

where γ is a parameter dubbed learning constant. As a result, the weight w_{ij} is changed by a factor that correlates the input x_i with the output signal y_j in such a way that the increment is positive for neurons firing or resting at the same time, and negative in the opposite case. The learning process is essential to enhance the performance of a neural network and guarantees a faster convergence of an algorithm towards the desired result. However, even when a suitable learning process is considered, there exist logical operations that a single perceptrons cannot implement. It is the case of the XOR operation between two binary inputs x_1, x_2, defined as $x_1 \oplus x_2$, where the symbol $\oplus$ stands for the addition modulo 2, i.e., $y = x_1 \oplus x_2 \iff y = x_1 + x_2 (\text{mod } 2)$. The possible outcomes of this operation are represented in the following table, i.e.,

x_1	x_2	$y = x_1 \oplus x_2$
0	0	0
0	1	1
1	0	1
1	1	0

.

The reason why a single perceptron fails to implement this operation is strictly related to the way it classifies the input data. In fact, regardless of the specific value of the weighted sum computed by each unit, i.e., $\sum_{ij} x_i w_{ij}$, the output y_j can only assume binary values. From a geometrical point of view, this observation is equivalent to say that the action of the network is to divide the input space in two half subspaces, corresponding to the two possible outputs: if the input data are such that $y_j = 0$ they are assigned to one subspace, otherwise they end up in the complementary subspace.

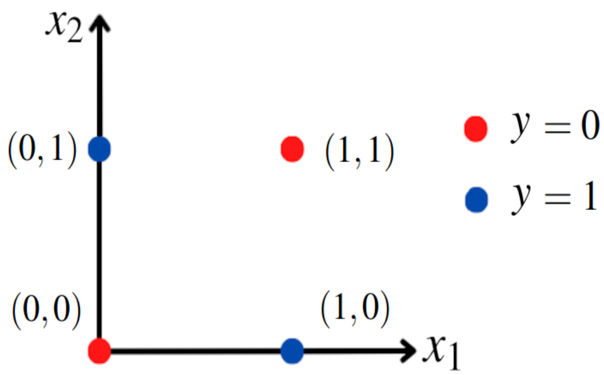

Figure 5.4: The XOR operation $y = x_1 \oplus x_2$ between two binary variables x_1 and x_2 in the input space.

Problems of this kind are known in the literature as *linearly separable*, and represent the class of problems that a single perceptron is able to solve. Hence, it is easy to understand the failure of the perceptron model when implementing the XOR gate. To make this statement clearer, let us represent the XOR operation in the input space (x_1, x_2) (see Fig.5.4). It is evident that it is impossible to separate the input data $(0,1),(1,0)$, corresponding to the output $y = 1$, from the input data $(0,0),(1,1)$, corresponding to the output $y = 0$, with a single line. This simple argument can be made more formal, but is already sufficient to understand why the XOR operation cannot be cast as a linearly separable problem. Clearly, analogously to the case of McCulloch-Pitts neurons, combining together single perceptrons can overcome this problem, an approach that results in the realisation of *multi-layer* neural networks which are able to implement a larger set of Boolean functions as compared to their single-layer counterparts.

5.1.3 The Hopfield model

The simplest example of a multi-layer neural network is dubbed *feed-forward*. As its name suggests, this network consists of different layers where the information can flow only in one direction: once the first layer is initialised in a certain configuration, the output data is fed to the subsequent layer, and this procedure is repeated until a final output is reached. Although they can be effectively used in many practical applications, feed-forward networks display an intrinsic limitation due to the fact that they cannot keep track of the data computed in the previous steps of the algorithm. In other words, they do not allow to store input patterns in order to use them as feedbacks for a learning algorithm. Neural networks of this latter type, where information can propagate backwards along the neurons, are dubbed *recurrent* networks. Of particular interest for our analysis are *attractor* neural networks (aNNs), an example of which is described by the Hopfield model, introduced for the first time in 1980s [Hop82]. In this model, the network consists of a collection of n perceptrons with binary values $x_i \in \{\pm 1\}$, and symmetric weights $w_{ij} = w_{ji}$, for $i \neq j$, and $w_{ii} = 0$. Despite the simplicity of their description, Hopfield neural networks are endowed with a remarkable feature known as *associative memory*, that is the capability to retrieve the pattern $\boldsymbol{x}^p = (x_1^p, \cdots, x_n^p)$ which is the closest to an input state $\boldsymbol{x}^{\text{in}} = (x_1^{\text{in}}, \cdots, x_n^{\text{in}})$, with respect to their Hamming distance, i.e., the numbers of bits one has to flip to turn one string into the other. This property can be better understood by introducing the energy function of the network $E(\boldsymbol{x})$, i.e.,

$$E(\boldsymbol{x}) = -\frac{1}{2}\sum_{i,j=1}^{n} w_{ij} x_i x_j + \sum_{i=1}^{n} b_i x_i \,. \tag{5.5}$$

Eq.(5.5) is nothing but the energy associated to each configuration $\boldsymbol{x} = (x_1, \ldots, x_n)$ of the n computational units that form the network. Notice that Eq.(5.5) is equivalent to the Hamiltonian of an Ising model at zero temperature [Isi25]. Such Hamiltonian describes the behaviour of n spin-$\frac{1}{2}$ particles in a magnetic field h and takes the form

$$H = -\frac{1}{2}\sum_{i,j=1}^{n} J_{ij} s_i s_j - h\sum_{i=1}^{n} s_i \ , \tag{5.6}$$

where the discrete variable $s_i \in \{\pm 1\}$ represents the spin of a particle at the i-th site of a lattice, J_{ij} are the couplings between two interacting particles and h is a magnetic field. Thus, in the same way a magnetic system relaxes to a stable configuration, it can be shown that the same happens in a Hopfield neural network, where an initial input approaches to its attractor. It is important to realise that the weights $\{w_{ij}\}$ or, equivalently, the couplings $\{J_{ij}\}$, are randomly distributed and can have either positive or negative sign. Notice that, in the case of all positive or negative contributions, there would only exist one minimum and the above model would not describe a spin glass. The fact that the couplings can have mixed signs allows to observe several "quasi" minima of energy and, thus, several configurations that can be associated to a a memory. In order to clarify this statement, let us now consider a specific pattern $\boldsymbol{x}^p = (x_1^p, \cdots, x_n^p)$ which we want to store and suppose the weight w_{ij} is updated to a value w'_{ij} according to the Hebbian rule, i.e.,

$$w'_{ij} = w_{ij} + x_i^{(p)} x_j^{(p)} \ . \tag{5.7}$$

If we extend the above equation to multiple patterns we get

$$w'_{ij} = w_{ij} + \frac{1}{P}\sum_{p=1} x_i^{(p)} x_j^{(p)} \ , \tag{5.8}$$

where P denotes the number of patterns that we wish to store. Eq.(5.8) shows that neurons bearing the same state in a large number of patterns will have a weight close to 1. Differently, anticorrelations between them will make their weight to be close to -1. As a consequence, it can be shown that the energy $E(\boldsymbol{x})$ always decreases or stays constant from one computational step to the other, so that an input $\boldsymbol{x}$ will converge to the closest attractor $\boldsymbol{x}^p$, which corresponds to the ground state or to the local quasi-minima of $E(\boldsymbol{x})$.

5.2 Quantum neural networks

Quantum neural networks (QNNs) stem from adding quantum features like correlations, entanglement and superposition to the parallel processing properties of classical neural networks, an approach which is expected to result in an enhancement of their performances [RDR+17; CCC+19; LAT21]. Trying to implement neural computing with quantum computers results, generically, in an incompatibility, since the dynamics of the former is nonlinear and dissipative, while the latter's is linear and unitary, and dissipation can only be introduced by measurements. Nevertheless, a set of desirable properties for QNNs displaying associative memory has been recently proposed [SSP14]: i) QNNs should produce an output state which is the closest to the input state in terms of some distance measure; ii) QNNs should encompass neural computing mechanisms such as training rules or attractor dynamics; and iii) the evolution of QNNs should be based on quantum effects. Remarkably, the quantum analogue of attractor neural networks, which we denote as aQNNs, meet the requirements stated above and represent the main topic of the following sections. In this case, classical bits are replaced by qubits whose evolution is described by the action of a CPTP map. The storage capacity, i.e., the number of attractors of the aQNN, then corresponds to the maximum number of stationary states of such map. The storage capacity of quantum neural networks was analysed for the first time in [LO92]. Recently, the explicit form of the CPTP maps possessing the maximal number of stationary states was derived [LGR+21]. Interestingly, such CPTP maps are described by non-coherence-generating operations, which represent a common tool in the resource theory of coherence and motivates our choice to address aQNNs from a coherence-theoretic approach.

5.2.1 Attractor quantum neural networks

Attractor quantum neural networks (aQNNs) correspond to the quantum version of aNNs where the binary computational units x_i are replaced by qubits. More formally, we define an aQNN of the Hopfield type as a network of n d-dimensional artificial neurons (qudits) which evolve under a quantum channel, i.e., a non-trivial CPTP map $\Lambda : \mathcal{B}(\mathcal{H}_{in}) \to \mathcal{B}(\mathcal{H}_{out})$. The stored memories correspond to the stationary states of the map, that is, the states ρ_S such that $\Lambda(\rho_S) = \rho_S$ [LGR+21]. For an arbitrary input state $\rho \neq \rho_S$, the successive applications of the map will bring the state to one of the stationary states of the map ρ_S. In what follows, we restrict to the case where $\dim(\mathcal{H}_{in}) = \dim(\mathcal{H}_{out}) = N = d^n$. As demonstrated in [LGR+21; LGR+22], a non-trivial CPTP map can have up to N stationary states $\Lambda(|\mu\rangle\langle\mu|) = |\mu\rangle\langle\mu|$, where $\{|\mu\rangle\}_{\mu=0}^{N-1}$ forms an orthonormal basis of $\mathcal{H}_{in}$. Such a map has the form of a generalised decohering map, i.e.,

$$\Lambda(\rho) = \sum_{\mu=0}^{N-1} \rho_{\mu\mu}|\mu\rangle\langle\mu| + \sum_{\substack{\mu,\nu \\ (\mu<\nu)}}^{N-1} \Big[\rho_{\mu\nu}(1+\alpha_{\mu\nu})|\mu\rangle\langle\nu| + \text{h.c.}\Big]\,, \tag{5.9}$$

where $\alpha_{\mu\nu} \in \mathbb{C}$.

To determine the complete-positivity of the map, it is easier to work in terms of its Choi state, $J_\Lambda \in \mathcal{B}(\mathcal{H}_{in} \otimes \mathcal{H}_{out})$, obtained by means of the Choi-Jamiołkowski isomorphism, so that Λ is CPTP iff $J_\Lambda \geq 0$ and $\text{Tr}_{out}(J_\Lambda) = \mathbb{1}_{in}$, where Tr_{out} denotes the partial trace over the subsystem $\mathcal{H}_{out}$. The Choi state of the map of Eq.(5.9) reads

$$J_\Lambda = \sum_{\mu=0}^{N-1} |\mu\mu\rangle\langle\mu\mu| + \sum_{\substack{\mu,\nu \\ (\mu<\nu)}}^{N-1} \Big[(1+\alpha_{\mu\nu})|\mu\mu\rangle\langle\nu\nu| + \text{h.c.}\Big]. \tag{5.10}$$

The positivity requirement, $J_\Lambda \geq 0$, demands that $|1+\alpha_{\mu\nu}|^2 \leq 1\ ,\forall\alpha_{\mu\nu}$ (and $\alpha_{\mu\mu} = 0\ \forall\mu$), as well as the positivity of all minors of $|J_\Lambda|$, which can be checked by, e.g., the Sylvester's condition [LGR+21]. In the most general case checking positivity is evidently hard, but here we simplify our analysis by restricting to the particular cases where $\alpha_{\mu\nu} = \alpha_{\nu\mu} = \alpha \in \mathbb{R}$ for every $\mu \neq \nu$. Upon this requirement, we find that Λ is CPTP whenever $\alpha \in [-N/(N-1), 0]$. We remark that our results are, nevertheless, general and apply also when this restriction is lifted as long as the map Λ is CPTP. Throughout this work, we will only consider aQNNs with maximal storage capacity, that is, those whose evolution is given by Eq.(5.9). With an abuse of language, we will sometimes refer to the map Λ in Eq.(5.9) metonymically as aQNN.

5.3 Resource theory of coherence

In any resource theory, one should firstly introduce the sets of free states and free operations. Given a Hilbert space $\mathcal{H}$ of dimension N, we denote by $\mathcal{B}(\mathcal{H})$ the set of the bounded operators acting on $\mathcal{H}$. The set of free states in the resource theory of coherence, denoted as $\mathbb{I}$, comprises the so-called *incoherent states*, that is, all the states $\delta \in \mathcal{B}(\mathcal{H})$ that are diagonal in a fixed basis $\{|i\rangle\}_{i=0}^{N-1}$ of $\mathcal{H}$, i.e., $\mathbb{I} = \{\delta = \sum_i \delta_i |i\rangle\langle i| \mid \sum_i \delta_i = 1\}$. Free operations are the CPTP maps, $\mathcal{E}$, that leave incoherent states incoherent, i.e., $\mathcal{E}(\mathbb{I}) \subset \mathbb{I}$. Stated differently, $\mathcal{E}$ fulfills $\Delta \circ \mathcal{E} \circ$

$\Delta = \mathcal{E} \circ \Delta$, where $\circ$ denotes the composition between two maps and Δ is the complete-dephasing map in the chosen basis, i.e., $\Delta(\cdot) = \sum_i |i\rangle\langle i| \cdot |i\rangle\langle i|$ [LHL17]. Operations satisfying the above relation are said to be *non-coherence-generating*, since they are unable to create coherence on any incoherent state. In contrast to what happens in the resource theories of asymmetry, athermality or entanglement [CG16], in coherence theory the set of free operations is not unique. This can be grasped by looking at the Kraus structure of the corresponding CPTP maps ($\mathcal{E}(\cdot) = \sum_\alpha K_\alpha \cdot K_\alpha^\dagger$).

The largest class of non-coherence-generating operations are the *maximally incoherent operations* (MIOs), whose Kraus operators, $\{K_\alpha\}$, fulfil $\sum_\alpha K_\alpha \mathbb{I} K_\alpha^\dagger \subset \mathbb{I}$ [Abe06]. A subset of MIOs are the *incoherent operations* (IOs) [BCP14], consisting of all MIOs whose Kraus operators satisfy the relation $K_\alpha \mathbb{I} K_\alpha^\dagger \subset \mathbb{I}$ for all α. Inside the set of IOs we find the *strictly incoherent operations* (SIOs) [WY16], for which the Kraus operators further fulfil that $K_\alpha^\dagger \mathbb{I} K_\alpha \subset \mathbb{I}$ for all α. Finally, *genuinely incoherent operations* (GIOs) [DS16] are SIOs preserving every incoherent state, i.e., $\mathcal{E}_{\text{GIO}}(\delta) = \delta$ for all $\delta \in \mathbb{I}$. As a consequence, GIOs present diagonal Kraus operators.

Besides free states and free operations, one should also introduce a proper measure of the resource considered. To quantify the amount of coherence present in an arbitrary state $\rho \in \mathcal{B}(\mathcal{H})$, a *coherence measure* [BCP14] must be defined as a functional $C : \mathcal{B}(\mathcal{H}) \to \mathbb{R}_{\geq 0}$ satisfying two main conditions: (i) faithfulness, meaning that $C(\delta) = 0$ for all incoherent $\delta \in \mathbb{I}$, and (ii) monotonicity, i.e., $C(\rho) \geq C(\mathcal{E}(\rho))$, for all non-coherence-generating operations $\mathcal{E}$. Among the most typical coherence measures we find the robustness of coherence [NBC+16], the relative entropy of coherence, i.e.,

$$C_{r.e.}(\rho) = S(\Delta(\rho)) - S(\rho), \tag{5.11}$$

where $S(\rho) = -\text{Tr}(\rho \log \rho)$ is the Von Neumann entropy [BCP14], and the l_1-coherence measure,

$$C_{l_1}(\rho) = \sum_{\mu \neq \nu} |\rho_{\mu\nu}|, \tag{5.12}$$

which is a valid measure under IOs, but not MIOs [BX16].

Finally, every coherence measure achieves its maximum value on the set of *maximally coherent states* (S_{MCS}), defined, in dimension N, as $S_{MCS} := \{\frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{i\theta_j} |j\rangle \mid \theta_j \in [0, 2\pi) \; \forall j\}$ [PJF16].

5.4 Error-free aQNNs

A direct inspection of Eq.(5.9) shows that, in the basis $\{|\mu\rangle\}_{\mu=0}^{N-1}$, the condition $\Delta \circ \Lambda \circ \Delta = \Lambda \circ \Delta$ holds, implying that aQNNs are not able to generate coherence on any input state. In particular, since $\Lambda(\delta) = \delta$ for all $\delta \in \mathbb{I}$, it follows that the set of attractors of the aQNN is equivalent to the set of incoherent states $\mathbb{I}$, and that:

Remark 5.1. *aQNNs are described by GIOs.*

As stated in the introduction, this observation justifies addressing aQNNs from a coherence-theoretic perspective. Moreover, analogously to the case of aNNs, aQNNs are *bona fide* models for associative memory. Indeed, in the asymptotic limit, they are able to retrieve the stored attractor which is closest to the input state, in terms of their relative entropy. We show this fact in the following lemma:

Lemma 5.1. *After $r \to \infty$ iterations, an aQNN outputs the stored attractor that minimises the relative entropy with respect to the input state ρ, i.e., $S(\rho|| \lim_{r\to\infty} \Lambda^r(\rho)) = \min_{\delta\in\mathbb{I}} S(\rho||\delta)$, where $S(\rho||\sigma) = \mathrm{Tr}(\rho \log \rho) - \mathrm{Tr}(\rho \log \sigma)$ is the quantum relative entropy of ρ with respect to σ. Equivalently, $C_{r.e.}(\rho)$ quantifies the minimum relative entropy between ρ and the set of the attractors of the aQNN.*

Proof. From Eq.(5.9) one notices that applying Λ a sufficient number of times on an input state ρ results in a complete dephasing of ρ, i.e., $\lim_{r\to\infty} \Lambda^r(\rho) = \Delta(\rho)$. Now, let us write the relative entropy between ρ and an incoherent state δ as $S(\rho||\delta) = S(\Delta(\rho)) - S(\rho) + S(\Delta(\rho)||\delta)$. It is immediate to see that

$$\min_{\delta\in\mathbb{I}} S(\rho||\delta) = S(\Delta(\rho)) - S(\rho) + S(\Delta(\rho)||\Delta(\rho)) = S(\Delta(\rho)) - S(\rho) = C_{r.e.}(\rho) \; , \tag{5.13}$$

that is, the minimum relative entropy between an input state ρ and the set of incoherent states (or attractors) is achieved on $\Delta(\rho)$, i.e., the state retrieved by the aQNN after a sufficient number of applications. As proven above, such minimum distance between the input state and the retrieved attractor is quantified by the relative entropy of coherence of the input. □

5.4.1 Physical realization of aQNNs

Physical operations on a system can always be understood as unitary dynamics and projective measurements on a larger system. Indeed, given a quantum channel

$\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, there always exists an ancillary Hilbert space $\mathcal{A}$ of arbitrary dimension and a unitary operation $U \in \mathcal{B}(\mathcal{H} \otimes \mathcal{A})$ such that

$$\mathcal{E}(\rho) = \mathrm{Tr}_{\mathcal{A}} \left[U(\rho \otimes |a_0\rangle\langle a_0|)U^\dagger \right] \ , \tag{5.14}$$

for any $\rho \in \mathcal{B}(\mathcal{H})$, where $\mathrm{Tr}_{\mathcal{A}}$ denotes the partial trace on the subsystem $\mathcal{A}$ and $|a_0\rangle\langle a_0|$ is the initial state of the ancilla. The corresponding unitary U is known as the Stinespring dilation of the map $\mathcal{E}$ [Pau03]. Thus, aQNNs can be physically realised by appending an ancillary qudit to the network qudits, letting the composite system evolve under the corresponding Stinespring dilation, and finally discarding the ancilla. Knowing that aQNNs are associated to GIOs allows us to derive the Stinespring dilation of the former in a straightforward way:

Proposition 5.2. *The Stinespring dilation of an N-dimensional aQNN is given by*

$$U_{aQNN} = \sum_{\mu=0}^{N-1} |\mu\rangle\langle\mu| \otimes U_\mu, \tag{5.15}$$

where $\{|\mu\rangle\}_{\mu=0}^{N-1}$ is an orthonormal basis and U_μ is a unitary operator such that $U_\mu |a_0\rangle = |c_\mu\rangle$, with $\{|c_\mu\rangle\}_{\mu=0}^{N-1}$ a set of normalised states fulfilling $\langle c_\nu|c_\mu\rangle = 1 + \alpha_{\mu\nu}$, $\forall \mu \neq \nu$.

Proof. Let $\{|\mu\rangle \otimes |a_\mu\rangle\}$ be an orthonormal basis of the composite Hilbert space $\mathcal{H} \otimes \mathcal{A}$. In [YDX+17] it was proven that the action of the Stinespring dilation of a GIO can be expressed as

$$U_{\mathrm{GIO}}(|\mu\rangle \otimes |a_0\rangle) = |\mu\rangle \otimes |c_\mu\rangle \ , \tag{5.16}$$

where $|c_\mu\rangle = \sum_i c_\mu^{(i)} |a_i\rangle$ and $\{|c_\mu\rangle\}$ is a set of normalised but not necessarily orthogonal states. Expressing the state ρ in the basis $\{|\mu\rangle\}_{\mu=0}^{N-1}$, i.e., $\rho = \sum_{\mu\nu} \rho_{\mu\nu} |\mu\rangle\langle\nu|$, and making use of Eq.(5.15), we find that Eq.(5.14) takes the form

$$\mathcal{E}_{\mathrm{GIO}}(\rho) = \sum_{\mu\nu} \left(\sum_k c_\mu^{(k)} \bar{c}_\nu^{(k)} \right) \rho_{\mu\nu} |\mu\rangle \langle\nu| \, . \tag{5.17}$$

Let us observe that, due to the normalization of the states $\{|c_\mu\rangle\}_{\mu=0}^{N-1}$, it holds

$$\sum_k c_\mu^{(k)} \bar{c}_\mu^{(k)} = 1 \ , \quad \sum_k c_\mu^{(k)} \bar{c}_\nu^{(k)} < 1, \ \forall \mu \neq \nu, \tag{5.18}$$

so that $\mathcal{E}_{\mathrm{GIO}}(\rho) = \rho$ for any diagonal state ρ, and the action of $\mathcal{E}_{\mathrm{GIO}}$ does not increase the value of the off-diagonal elements.
A direct comparison between Eq.(5.17) and the map of Eq.(5.9) shows that the two maps are equivalent if

$$1 + \alpha_{\mu\nu} = \sum_k \bar{c}_\nu^{(k)} c_\mu^{(k)} = \langle c_\nu, c_\mu \rangle, \quad \forall \mu \neq \nu, \tag{5.19}$$

which completes the proof. □

5.4.2 Depth of aQNNs and decohering power

Consider the simple case of a maximally coherent qubit $|\Psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ suffering decoherence under the action of an aQNN, i.e., $\Lambda(\Psi_2) = \frac{1}{2}\begin{pmatrix} 1 & 1+\alpha_{01} \\ 1+\bar{\alpha}_{01} & 1 \end{pmatrix}$, where, from now on, we use the notation $\Psi := |\Psi\rangle\langle\Psi|$. From here it is easy to see that an aQNN with a smaller value of $|1+\alpha_{01}|$ needs to be applied less times on a state in order to completely destroy its coherences. To quantify the ability of operations to cause decoherence, the notion of *decohering power* is invoked. The decohering power of a map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, $\dim(\mathcal{H}) = N$, with respect to some coherence measure C was introduced in [MK15]:

$$\begin{aligned} D_C(\mathcal{E}) &= \max_{\Psi_N \in S_{\mathrm{MCS}}} \left(C(\Psi_N) - C(\mathcal{E}(\Psi_N))\right) \\ &= C(\Psi_N) - \min_{\Psi_N \in S_{\mathrm{MCS}}} C(\mathcal{E}(\Psi_N)). \end{aligned} \tag{5.20}$$

When considering the l_1-coherence measure we immediately find:

Proposition 5.3. *The l_1-decohering power of an N-dimensional aQNN described by the CPTP map Λ is given by*

$$D_{C_{l_1}}(\Lambda) = N - 1 - \frac{1}{N}\sum_{\mu\neq\nu} |1+\alpha_{\mu\nu}|, \tag{5.21}$$

fulfilling $0 \leq D_{C_{l_1}}(\Lambda) \leq N-1$.

We define the depth of an aQNN as the minimum number of times, r, that the map Λ has to be applied on a state until it becomes stationary up to some tolerable error η, that is, until the classification process is accomplished with sufficient accuracy (see Fig.5.5a). At that moment, the coherence of the input is small, i.e., $C_{l_1}(\Lambda^r(\rho)) = \eta$, with $0 < \eta \ll 1$.

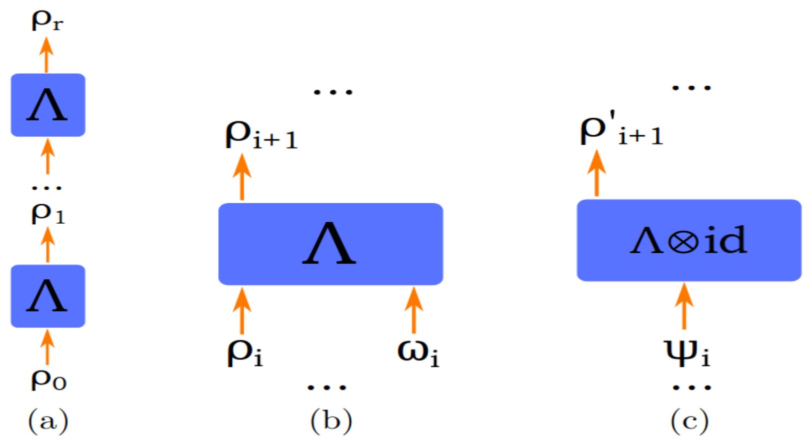

Figure 5.5: (a) Scheme of a typical classification process. The aQNN described by Λ is applied r times until a stationary state ρ_r is reached. (b) Protocol for enhancing the performance of an aQNN associated to Λ at layer i using the coherence present in ω_i: $\rho_{i+1} = \mathcal{N}_i(\rho_i) = \mathrm{Tr}_{\mathcal{A}}(\Lambda(\rho_i \otimes \omega_i))$. (c) Protocol for reducing the depth of an aQNN exploiting the entanglement present in ψ_i s.t. $\rho_i = \mathrm{Tr}_{\mathcal{A}}(\psi_i)$: $\rho'_{i+1} = \mathrm{Tr}_{\mathcal{A}}\{(\Lambda \otimes \mathrm{id})(\psi_i)\}$.

Consider the case where the input state is a maximally coherent state, Ψ_N, which decoheres uniformly under the action of an aQNN, i.e., $\alpha_{\mu\nu} = \alpha_{\nu\mu} \equiv \alpha \, \forall \mu, \nu$. In this case we have $C_{l_1}(\Lambda^r(\Psi_N)) = (N-1)^{1-r}(N-1-D_{C_{l_1}}(\Lambda))^r$. Allowing for stationarity to be reached within a small error η, i.e., $C_{l_1}(\Lambda^r(\Psi_N)) \leq \eta$, immediately yields

Proposition 5.4. *The depth r of an N-dimensional aQNN described by the CPTP map Λ with $\alpha_{\mu\nu} = \alpha_{\nu\mu} \equiv \alpha \, \forall \mu \neq \nu$ acting on a maximally coherent state such that stationarity is reached within η-precision is given by its l_1-decohering power:*

$$r \geq \left\lceil \frac{\log(\eta) - \log(N-1)}{\log(N-1-D_{C_{l_1}}(\Lambda)) - \log(N-1)} \right\rceil . \tag{5.22}$$

Note that the lower bound for r is tight, since in this case $C_{l_1}(\Lambda^r(\Psi_N))$ and $D_{C_{l_1}}(\Lambda)$ are exactly related.

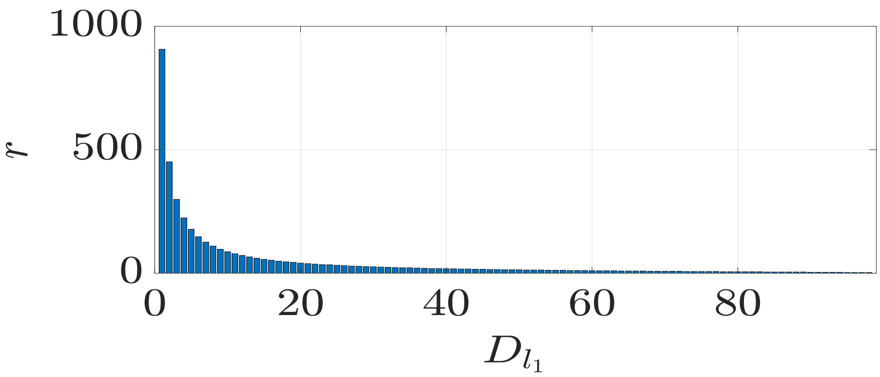

Figure 5.6: Minimum depth of a 100-dimensional aQNN with $\alpha_{\mu\nu} = \alpha_{\nu\mu} \equiv \alpha$ for all $\mu \neq \nu$ acting on a maximally coherent state such that stationarity is reached within error $\eta = 0.01$, as a function of its l_1-decohering power.

Fig.5.6 shows the minimum number of layers that a 100-dimensional aQNN of this kind needs to have in order for stationarity to be achieved within an error $\eta = 0.01$. Moreover, it illustrates how the depth of an aQNN decreases with its decohering power. Turning to generic aQNNs, however, it is not possible to find a tight lower bound for the depth, since under non-uniform decoherence the main quantities $C_{l_1}(\Lambda^r(\Psi_N))$ and $D_{C_{l_1}}(\Lambda)$ are not equivalent.

5.4.3 No-go results for the performance of error-free aQNNs

Throughout this chapter we have assumed already trained aQNNs and we have investigated their properties during the inference phase, i.e., the stage when the output is produced. In this section, we are interested in analysing whether the performance of an aQNN can be improved at the inference stage itself. As it is common in the literature about neural computing, enhancing the performance of a neural network implies: i) increasing its accuracy, and ii) accelerating the inference process, that is, reducing the depth of the network (as we defined it in section 5.4.2). Here we want to investigate whether the performance of an aQNN can be improved by resorting exclusively to quantum resources. To that aim, one can begin by implementing some channel $\mathcal{N}_i$ on a given layer i capable of mitigating some of the errors occurred in previous layers, which results in an increased overall accuracy, and/or reducing the number of layers left until the inference process is accomplished, i.e., decreasing the overall r. We consider a scenario where an aQNN of arbitrary dimension is coupled to an ancillary system $\mathcal{A}$, under the action of a CPTP map $\Lambda : \mathcal{B}(\mathcal{H} \otimes \mathcal{A}) \to \mathcal{B}(\mathcal{H} \otimes \mathcal{A})$, where the ancilla supplies coherent states $\omega_i \in \mathcal{B}(\mathcal{A})$. In this case, one could only exploit the aQNN and the coherent resources in order to realise the target channel $\mathcal{N}_i : \mathcal{B}(\mathcal{H} \otimes \mathcal{A}) \to \mathcal{B}(\mathcal{H})$. The procedure would be as follows: i) append a coherent ancilla $\omega_i \in \mathcal{B}(\mathcal{A})$ to the input state $\rho_i \in \mathcal{B}(\mathcal{H})$, ii) apply Λ on the composite system, and iii) discard the ancillary state (see Fig.5.5b). Formally, we can express this process as

$$\rho_{i+1} = \mathcal{N}_i(\rho_i) = \mathrm{Tr}_{\mathcal{A}}(\Lambda(\rho_i \otimes \omega_i)). \tag{5.23}$$

As discussed in [DDM+17], a non-coherence-generating operation $\mathcal{M}$ is able to realise a coherent channel in this way only if it can activate coherence, i.e., if it fulfills $\Delta \circ \mathcal{M} \circ \Delta \neq \Delta \circ \mathcal{M}$. Noting that GIOs violate this condition [LHL17], the following no-go result holds:

Proposition 5.5. *Coherence cannot be used to enhance the performance of aQNNs.*

Since GIOs are unable to exploit the coherence of ω_i to help implement $\mathcal{N}_i(\rho_i)$ (unlike MIOs [DFW+18] or IOs), aQNNs cannot use coherence to boost their own performance.

Another strategy to reduce the depth of an aQNN by increasing its decohering power relies on the exploitation of initial correlations [TRS22]. Consider an input state $\rho_i \in \mathcal{B}(\mathcal{H})$, purified by the entangled state $\psi_i \in \mathcal{B}(\mathcal{H} \otimes \mathcal{A})$, i.e, $\mathrm{Tr}_{\mathcal{A}}(\psi_i) = \rho_i$. The question is to find whether using such an entangled input state causes a stronger decoherence in the output, thus reducing the number of times that the map $\Lambda : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ has to be applied before the classification task is completed. Stated differently, we want to investigate whether $C(\Lambda(\rho_i))$ is greater than $C(\mathrm{Tr}_{\mathcal{A}}\{(\Lambda \otimes \mathrm{id})(\psi_i)\})$ (see Fig.5.5c). We hereby show this is not possible:

Proposition 5.6. *Initial entanglement cannot be used to reduce the depth of aQNNs.*

Proof. Consider a generally mixed input state $\rho = \sum_k p_k |\phi_k\rangle\langle\phi_k|$, where $p_k \in [0, 1]$ and the states $|\phi_k\rangle$ are not necessarily orthonormal. A purification of ρ is given by $|\psi\rangle = \sum_k \sqrt{p_k}\, |\phi_k\rangle\, |k\rangle$, where $\{|k\rangle\}$ is an orthonormal basis of $\mathcal{A}$. Expressing ρ in this basis, i.e., $\rho = \sum_k p_k \sum_{\mu\nu} c_\mu^{(k)} \bar{c}_\nu^{(k)} |\mu\rangle\langle\nu|$, with $c_\xi^{(k)} = \langle\xi|\phi_k\rangle$, leads to

$$\begin{aligned} \mathrm{Tr}_{\mathcal{A}}[(\Lambda \otimes \mathrm{id})(\psi)] &= \sum_k p_k \left[\sum_\mu |c_\mu^{(k)}|^2 |\mu\rangle\langle\mu| + \sum_{\mu<\nu} \left\{ c_\mu^{(k)} \bar{c}_\nu^{(k)} (1 + \alpha_{\mu\nu}) |\mu\rangle\langle\nu| + \text{h.c.} \right\} \right] \\ &= \Lambda(\rho). \end{aligned} \tag{5.24}$$

Therefore, $C(\Lambda(\rho)) = C(\mathrm{Tr}_{\mathcal{A}}\{(\Lambda \otimes \mathrm{id})(\psi)\}$ and initial correlations cannot produce a faster decoherence in the input state ρ. □

5.5 Faulty aQNNs

We examine now the realistic scenario of non-error-free aQNNs, that is, the case where some error in the implementation of the network is taken into account. In particular, we denote as *faulty* an aQNN such that the associated map, Λ_ϵ, preserves the stationary states up to a certain error $\epsilon \in [0,1]$, i.e.,

$$\Lambda_\epsilon(|\mu\rangle\langle\mu|) = (1-\epsilon)|\mu\rangle\langle\mu| + \frac{\epsilon}{N-1}\sum_{\mu\neq\nu}^{N-1}|\nu\rangle\langle\nu| \,.$$

According to this definition, it is clear that there exist many maps satisfying the above requirement. In what follows we consider one, denoted as $\Lambda_{\epsilon,\gamma}$, whose action over a generic quantum state ρ can be written as

$$\Lambda_{\epsilon,\gamma}(\rho) = \sum_{\mu=0}^{N-1}\rho_{\mu\mu}\Big[(1-\epsilon)|\mu\rangle\langle\mu| + \sum_{\substack{\nu=1\\(\mu\neq\nu)}}^{N-1}\frac{\epsilon}{N-1}|\nu\rangle\langle\nu|\Big] + \sum_{\mu<\nu}^{N-1}\Big\{\rho_{\mu\nu}\Big[(1+\alpha_{\mu\nu})|\mu\rangle\langle\nu| + \gamma|\nu\rangle\langle\mu|\Big] + \text{h.c.}\Big\}\,, \tag{5.25}$$

with $\epsilon \in [0,1]$ and $\gamma \in \mathbb{C}$. Notice that Eq.(5.25) corresponds to a faulty map where ϵ represents the error on achieving the stationary states and γ is a damping factor in the off-diagonal terms. We define a faulty (ϵ,γ)-aQNN as that associated to the map $\Lambda_{\epsilon,\gamma}$ of Eq.(5.25), whose corresponding Choi state is

$$J_{\Lambda_{\epsilon,\gamma}} = \sum_{\mu=0}^{N-1}\Big[(1-\epsilon)|\mu\mu\rangle\langle\mu\mu| + \sum_{\substack{\nu=1\\(\mu\neq\nu)}}^{N-1}\frac{\epsilon}{N-1}|\mu\nu\rangle\langle\mu\nu|\Big] + \sum_{\mu<\nu}^{N-1}\Big[(1+\alpha_{\mu\nu})|\mu\mu\rangle\langle\nu\nu| + \gamma|\mu\nu\rangle\langle\nu\mu| + \text{h.c.}\Big]\,, \tag{5.26}$$

with $|1+\alpha_{\mu\nu}|^2 \leq (1-\epsilon)^2$ for all $\mu \neq \nu$.
Notice that Eq.(5.26) can be cast as a direct sum, i.e., $J_{\Lambda_{\epsilon,\gamma}} = J \bigoplus_{0\leq\mu<\nu\leq N-1} J_{\mu\nu}$, with

$$J = \begin{pmatrix} 1-\epsilon & 1+\alpha_{01} & \cdots & 1+\alpha_{0,N-1} \\ 1+\bar{\alpha}_{01} & 1-\epsilon & \cdots & 1+\alpha_{1,N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1+\bar{\alpha}_{0,N-1} & 1+\bar{\alpha}_{1,N-1} & \cdots & 1-\epsilon \end{pmatrix}, \tag{5.27}$$

$$J_{\mu\nu} = \begin{pmatrix} \epsilon/(N-1) & \gamma \\ \bar{\gamma} & \epsilon/(N-1) \end{pmatrix}, \tag{5.28}$$

where the bar symbol denotes the complex conjugation and each 2×2 matrix $J_{\mu\nu}$ appears with multiplicity $N(N-1)/2$. Following the same arguments of section 5.2, $\Lambda_{\epsilon,\gamma}$ is a CPTP map iff $J_{\Lambda_{\epsilon,\gamma}} \geq 0$. Choosing $|\gamma| \in [0, \epsilon/(N-1)]$ guarantees that $J_{\mu\nu} \geq 0$ for every $\mu \neq \nu$, but finding analytical conditions on the parameters such that $J \geq 0$ is, in general, a cumbersome task. Nevertheless, recalling that $\alpha_{\mu\nu} = \alpha_{\nu\mu} = \alpha \in \mathbb{R}$ for every $\mu \neq \nu$, $\Lambda_{\epsilon,\gamma}$ is a CPTP map whenever $\alpha \in [(\epsilon - N)/(N-1), -\epsilon]$ and $|\gamma| \in [0, \epsilon/(N-1)]$.

Notice that, also in the case of faulty maps $\Lambda_{\epsilon,\gamma}$, the non-coherence-generating condition $\Delta \circ \Lambda_{\epsilon,\gamma} \circ \Delta = \Lambda_{\epsilon,\gamma} \circ \Delta$ holds true. Moreover, it is possible to show that (ϵ,γ)-aQNNs correspond to SIOs:

Lemma 5.2. *(ϵ,γ)-aQNNs are described by SIOs.*

Proof. First, we derive the Kraus operators, defined as $K_i = \sqrt{\lambda^{(i)}}\mathrm{mat}(|\lambda^{(i)}\rangle)$, where $\lambda^{(i)}$ is an eigenvalue of the Choi state and $\mathrm{mat}(|\lambda^{(i)}\rangle)$ the row-by-row matrix representation of the corresponding eigenvector $|\lambda^{(i)}\rangle$. The diagonalization of $J_{\Lambda_{\epsilon,\gamma}}$ can be made simpler thanks to the direct sum decomposition of Eqs.(5.27)-(5.28). Notice that the diagonalization of Eq.(5.27) always yields diagonal Kraus operators. In fact, a generic eigenvector of the $N \times N$ matrix J is of the form

$$|\lambda_J^{(i)}\rangle = \Big((\lambda_J^{(i)})_{00}, (\lambda_J^{(i)})_{11}, \ldots, (\lambda_J^{(i)})_{N-1,N-1}\Big)^T . \tag{5.29}$$

When extending this vector to dimension N^2, we need to add N zeroes between each pair of entries, i.e.,

$$|\lambda_J^{(i)}\rangle_{ext} = ((\lambda_J^{(i)})_{00}, \underbrace{0,\ldots,0}_{N}, (\lambda_J^{(i)})_{11}, \ldots, (\lambda_J^{(i)})_{N-1,N-1})^T . \tag{5.30}$$

Hence, when converting the extended eigenvector into a matrix, it is immediate to find that this operation always yields a diagonal Kraus operator, regardless of the particular eigenvector considered. Let us now inspect the eigenvectors of the operator $J_{\mu\nu}$ of Eq.(5.27). First notice that, for any $0 \leq \mu < \nu \leq N-1$, $J_{\mu\nu}$ can be written in the chosen basis as

$$J_{\mu\nu} = \frac{\epsilon}{N-1}\Big(|\mu\nu\rangle\langle\mu\nu| + |\nu\mu\rangle\langle\nu\mu|\Big) + \gamma|\mu\nu\rangle\langle\nu\mu| + \bar{\gamma}|\nu\mu\rangle\langle\mu\nu| .$$

The diagonalization of $J_{\mu\nu}$ yields a couple of eigenvectors of the form $|\lambda_{J_{\mu\nu}}^{(\pm)}\rangle = (\pm(\lambda_{J_{\mu\nu}})_0, (\lambda_{J_{\mu\nu}})_1)^T$. However, differently from the previous case, when extending these vectors to dimension N^2, we need to add N^2-2 zeroes whose position will vary according to the specific matrix $J_{\mu\nu}$ considered. It is easily found that the zeroes of the extended eigenvector correspond to the elements of the basis of the form $|\mu'\nu'\rangle$ with $\mu', \nu' \neq \mu, \nu$. Thus, the Kraus operators are given by $K_{\mu\nu} = \kappa^{(1)}_{\mu\nu}|\mu\rangle\langle\nu| + \kappa^{(2)}_{\mu\nu}|\nu\rangle\langle\mu|$, for some $\kappa^{(i)}_{\mu\nu} \in \mathbb{C}$. For every incoherent state δ it holds

$$K_{\mu\nu}\delta K^{\dagger}_{\mu\nu} = |\kappa^{(1)}_{\mu\nu}|^2\delta_{\nu\nu}|\mu\rangle\langle\mu| + |\kappa^{(2)}_{\mu\nu}|^2\delta_{\mu\mu}|\nu\rangle\langle\nu| \,, \tag{5.31}$$

and $K^{\dagger}_{\mu\nu}\delta K_{\mu\nu}$ is obtained by relabelling $\mu \to \nu$. Hence, for every $\delta \in \mathbb{I}$, it holds that $K_{\mu\nu}\delta K^{\dagger}_{\mu\nu} \subset \mathbb{I}$, $K^{\dagger}_{\mu\nu}\delta K_{\mu\nu} \subset \mathbb{I}$, with $0 \leq \mu < \nu \leq N-1$. □

Further, we provide the expression of the distance between the two quantum channels Λ and $\Lambda_{\epsilon,\gamma}$. In order to do so, we introduce the *diamond distance*, denoted by $D_{\diamond}$, which is formally defined, for any pair of CPTP maps, as [Wat09; AKN98]

$$D_{\diamond}(\mathcal{E}, \mathcal{F}) = \frac{1}{2}\max_{\rho_{AB}} \|(\mathrm{id}\otimes\mathcal{E})(\rho_{AB}) - (\mathrm{id}\otimes\mathcal{F})(\rho_{AB})\|_1 \ ,$$

where $\rho_{AB} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and $\|X\|_1 = \mathrm{Tr}\sqrt{XX^{\dagger}}$ is the usual trace norm.

Operationally, the diamond distance quantifies how well one can discriminate between two quantum maps. Indeed, it is possible to show that $\mathcal{E}$ and $\mathcal{F}$ become perfectly distinguishable whenever $D_{\diamond}(\mathcal{E}, \mathcal{F}) = 1$ [Wil11]. The computation of the diamond distance between two CPTP maps can be cast as a semidefinite program (SDP) which admits a simple formulation in terms of their Choi states [DFW+18], i.e.,

$$\begin{aligned} \min \quad & \lambda \\ \text{s.t.} \quad & Z \geq J_{\mathcal{E}} - J_{\mathcal{F}} \\ & \lambda \mathbb{1}_A \geq \mathrm{Tr}_B(Z) \\ & Z \geq 0\,. \end{aligned} \tag{5.32}$$

Taking into account Λ and $\Lambda_{\epsilon,\gamma}$, the solution of the above SDP program does not admit, in general, a simple analytical expression. However, upon suitable conditions, we prove the following result:

Proposition 5.7. *Let $\alpha_{\mu\nu} = \alpha_{\nu\mu} \equiv \alpha \in \mathbb{R}$ for all $\mu \neq \nu$ and $\gamma = 0$. Then, the diamond distance between Λ and Λ_{ϵ} is given by $D_{\diamond}(\Lambda, \Lambda_{\epsilon}) = \epsilon$.*

Proof. Notice that, since the difference between the Choi states yields a diagonal matrix, the SDP program (5.32) can be solved by restricting to the diagonal matrices $Z = \mathrm{diag}(z_{00}, \ldots, z_{N-1,N-1})$ satisfying the constraints $Z \geq J_{\Lambda_{\epsilon,\gamma}} - J_{\Lambda}$ and $\lambda\mathbb{1}_A \geq$

$\mathrm{Tr}_B(Z)$. The former condition is easily satisfied by choosing $z_{ii} = \frac{\epsilon}{N-1}$ whenever $\left(J_{\Lambda_{\epsilon,\gamma}} - J_\Lambda\right)_{ii} = \frac{\epsilon}{N-1}$ and $z_{ii} = 0$ elsewhere. With this choice, we find $\mathrm{Tr}_B(Z) = \epsilon\mathbb{1}$, so that the latter condition reduces to $\lambda \geq \epsilon$. Hence, the minimization over λ yields ϵ, which completes the proof. □

Notice that, when restricting to the case of Proposition 5.7, for $\epsilon = 1$ it is possible to fully discriminate between Λ and Λ_ϵ. Moreover, we have numerically found that, also when $\gamma \neq 0$, Proposition 5.7 holds true, thus implying that the diamond distance is independent of the choice of γ.

Regarding the physical realization of (ϵ, γ)-aQNNs, the following result holds:

Proposition 5.8. *The Stinespring dilation of an N-dimensional (ϵ, γ)-aQNN is given by*

$$U_{(\epsilon,\gamma)\text{-}aQNN} = \sum_\mu \sum_k c_\mu^{(k)} |\pi_k(\mu)\rangle\langle\mu| \otimes |a_n\rangle\langle a_0| \,, \tag{5.33}$$

where π_k is a permutation function swapping two states $|\mu\rangle$ and $|\nu\rangle$ $\forall\mu \neq \nu$, i.e., $|\pi_k(\mu)\rangle = |\nu\rangle$, $|\pi_k(\nu)\rangle = |\mu\rangle$, and $\{|c_\mu^{(k)}\rangle\}_{\mu=0}^{N-1}$ is a set of normalised states fulfilling

$$\begin{aligned} &|c_\mu^{(0)}|^2 = 1 - \epsilon \,, \quad c_\mu^{(0)} \bar{c}_\nu^{(0)} = 1 + \alpha_{\mu\nu} \,, \forall \mu \neq \nu \,, \\ &c_\mu^{(k)} \bar{c}_\nu^{(k)} = \gamma, \ \forall k \neq 0 \,. \end{aligned} \tag{5.34}$$

Proof. The Stinespring dilation of a SIO is given by [CG16]

$$U_{\mathrm{SIO}} = \sum_\mu \sum_k c_\mu^{(k)} |\pi_k(\mu)\rangle\langle\mu| \otimes |a_n\rangle\langle a_0| \,, \tag{5.35}$$

where π_k is a permutation function labelled by the index k and the coefficients $\{c_\mu^{(k)}\}$ are such that the vector $|c_\mu\rangle = (c_\mu^{(0)}, \cdots, c_\mu^{(r)})$ is normalised. Inserting Eq.(5.35) in Eq.(5.14) it is easily found that

$$\mathcal{E}(\rho) = \sum_{\mu\nu} \sum_k c_\mu^{(k)} \bar{c}_\nu^{(k)} \rho_{\mu\nu} |\pi_k(\mu)\rangle\langle\pi_k(\nu)| \,. \tag{5.36}$$

In order to relate the above expression with the one of Eq.(5.25), we rewrite it as

$$\mathcal{E}(\rho) = \sum_\mu \sum_k \rho_{\mu\mu} |c_\mu^{(k)}|^2 |\pi_k(\mu)\rangle\langle\pi_k(\mu)| + \sum_{\mu\neq\nu} \sum_k \rho_{\mu\nu} c_\mu^{(k)} \bar{c}_\nu^{(k)} |\pi_k(\mu)\rangle\langle\pi_k(\nu)| \,. \tag{5.37}$$

Let us now denote by $k = 0$ the identical permutation that leaves unchanged the elements of the chosen basis, i.e., $|\pi_0(\mu)\rangle = |\mu\rangle$ for all $\mu = 0, \ldots, N-1$. Hence, the first term of Eq.(5.37) can be cast as

$$\sum_{\mu} \rho_{\mu\mu} |c_{\mu}^{(0)}|^2 |\mu\rangle\langle\mu| + \sum_{\mu} \sum_{k \neq 0} \rho_{\mu\mu} c_{\mu}^{(k)} \bar{c}_{\nu}^{(k)} |\pi_k(\mu)\rangle\langle\pi_k(\nu)| \; . \tag{5.38}$$

Comparing Eq.(5.38) with the diagonal terms in Eq.(5.25), we find

$$|c_{\mu}^{(0)}|^2 = 1 - \epsilon \; , \quad c_{\mu}^{(0)} \bar{c}_{\nu}^{(0)} = 1 + \alpha_{\mu\nu} \; , \; \forall \mu \neq \nu \; .$$

To find the rest of the conditions let us rewrite the second term of Eq.(5.37) as

$$\sum_{\mu \neq \nu} \rho_{\mu\nu} c_{\mu}^{(0)} \bar{c}_{\nu}^{(0)} |\mu\rangle\langle\nu| + \sum_{\mu \neq \nu} \sum_{k \neq 0} \rho_{\mu\nu} c_{\mu}^{(k)} \bar{c}_{\nu}^{(k)} |\pi_k(\mu)\rangle\langle\pi_k(\nu)| \; . \tag{5.39}$$

A direct comparison between Eq.(5.39) and the off-diagonal terms of Eq.(5.25), shows that we need to impose some restrictions on the permutation function. Choosing π_k to be a swap between any two pair of orthogonal states, i.e., $|\pi_k(\mu)\rangle = |\nu\rangle$ and $|\pi_k(\nu)\rangle = |\mu\rangle$ with $\mu \neq \nu$, we find:

$$|c_{\mu}^{(k)}|^2 = \epsilon/(N-1) \; , \quad c_{\mu}^{(k)} \bar{c}_{\nu}^{(k)} = \gamma \; , \; \forall k \neq 0 \; .$$

□

As a consequence of Proposition 5.8, an error-free aQNN may turn faulty if the unitary operator that physically implements it degrades from U_{aQNN} to $U_{(\epsilon,\gamma)\text{-aQNN}}$. We conclude this section by observing that also SIOs are non-coherence-activating operations [LHL17], which results in the following no-go proposition:

Proposition 5.9. *Coherence cannot be used to enhance the performance of* (ϵ, γ)*-aQNNs.*

In addition, entanglement cannot be exploited either to accelerate the inference process in this case:

Proposition 5.10. *Initial entanglement cannot be used to reduce the depth of* (ϵ, γ)*-aQNNs.*

Proof. Consider a generally mixed input state $\rho = \sum_k p_k |\phi_k\rangle\langle\phi_k|$, where $p_k \in [0, 1]$ and the states $|\phi_k\rangle$ are not necessarily orthonormal. A purification of ρ is given by

$|\psi\rangle = \sum_k \sqrt{p_k}\,|\phi_k\rangle\,|k\rangle$, where $\{|k\rangle\}$ is an orthonormal basis of $\mathcal{A}$. Expressing ρ in this basis, i.e., $\rho = \sum_k p_k \sum_{\mu\nu} c_\mu^{(k)} \bar{c}_\nu^{(k)} |\mu\rangle\langle\nu|$, with $c_\xi^{(k)} = \langle\xi|\phi_k\rangle$, leads to

$$\mathrm{Tr}_{\mathcal{A}}[(\Lambda_{\epsilon,\gamma}\otimes \mathrm{id})(\psi)] = \sum_k p_k \Bigg[\sum_\mu |c_\mu^{(k)}|^2[(1-\epsilon)|\mu\rangle\langle\mu| + \sum_{\mu<\nu} \tfrac{\epsilon}{N-1}|\nu\rangle\langle\nu|] \\ + \sum_{\mu<\nu}\Bigg\{ c_\mu^{(k)}\bar{c}_\nu^{(k)}\left[(1+\alpha_{\mu\nu})|\mu\rangle\langle\nu| + \gamma|\nu\rangle\langle\mu|\right] + \mathrm{h.c.}\Bigg\}\Bigg] = \Lambda_{\epsilon,\gamma}(\rho). \quad (5.40)$$

Therefore, $C(\Lambda_{\epsilon,\gamma}(\rho)) = C(\mathrm{Tr}_{\mathcal{A}}\{(\Lambda_{\epsilon,\gamma}\otimes \mathrm{id})(\psi)\}$ and initial correlations cannot produce a faster decoherence in the input state ρ. □

So far, we have considered the case when faulty aQNNs are described by SIOs, showing that neither coherence nor entanglement can be used to enhance the performance of the associated aQNN. Nevertheless, it is possible to show that, when other sources of error are considered, this is not necessarily the case. In particular, we define a map $\Lambda_{\epsilon,\gamma,\lambda}$ defined as:

$$\Lambda_{\epsilon,\gamma,\lambda}(\rho) = \Lambda_{\epsilon,\gamma}(\rho) + \sum_{\mu<\nu}\left[\rho_{\mu\nu}\lambda|\mu+1\rangle\langle\nu+1| + \mathrm{h.c.}\right] \ , \quad (5.41)$$

where $\lambda \in \mathbb{C}$ and $\Lambda_{\epsilon,\gamma}(\rho)$ is the map of Eq.(5.25).
It can be checked numerically that $\Lambda_{\epsilon,\gamma,\lambda}$ corresponds to a MIO, but not IO, thus possibly allowing the use of coherence to enhance the performance of the related aQNN, as proven in [DFW+18].

Conclusion

E me ne devo andare via così?
Non che mi aspetti il disegno compiuto
ciò che si vede alla fine del ricamo
quando si rompe con i denti il filo
dopo averlo su se stesso ricucito
perché non possa più sfilarsi se tirato.
Ma quel che ho visto si è tutto cancellato.
E quasi non avevo cominciato.

Patrizia Cavalli

In this thesis we have analysed different, although related, topics in quantum information theory. In particular, our work has been devoted to three main lines, that is, entanglement characterisation, non-locality detection and quantum neural networks. In all cases, symmetry plays a crucial role in reducing the complexity of the original problems, while providing, as well, an elegant framework for their mathematical description. In the following sections we provide a summary of the main results of this thesis, along with some open questions for each of these topics.

Entanglement in symmetric states: outlook & open questions

In chapter 3 we have tackled the separability problem for symmetric states of two qudits. Motivated by the results of [TAQ+18], where the case of diagonal symmetric states was discussed, we have further explored the connection between this class of states and the cone of copositive matrices. In particular, we have provided the explicit conditions that a copositive matrix has to satisfy to define a valid entanglement witness. Moreover, intrigued by the concept of exceptional copositive matrices, we have shown that they correspond to non-decomposable EWs for diagonal symmetric states, a result which has allowed for the characterisation of new families of PPT-entangled states in arbitrary dimension. We have then turned our analysis to the set of two-qudit symmetric states, focusing on the first non-trivial case, i.e., $d = 3$, where we have been able to provide a new family of two-qutrit PPT-entangled states. Numerical evidence as well as the analytical mapping between two-qutrit and four-qubit symmetric states introduced in chapter 3, strongly suggest that this is the only family of PPT-entangled states in $d = 3$ and indeed, we conjecture that any two-qutrit symmetric PPTES is of the form of Eq.(3.44). Interestingly, also in this case, the diagonal symmetric part of the EW for symmetric states, can be constructed from a copositive matrix, possibly indicating that this class of matrices play a decisive role in the construction of EWs also outside the diagonal symmetric paradigm.

Open questions

A first open question regards the characterisation of PPT-entangled edge states of two symmetric qudits in $d < 5$. In $d = 3$ we conjecture that there exists only one family of such states, a conjecture which is strongly supported by numerical calculations but still requires an analytical proof. In $d = 4$ the numerical examples of PPT-entangled states that we have found are of the same form of their counterpart in $d = 3$, an observation that suggests the possibility to extend the validity of our conjecture also to this latter case. Moreover, it has been recently proven that any two-qutrit PPT-entangled state has Schmidt number 2 [SBL01; YLT16; MMO21]. Hence, it would be interesting to investigate whether a similar result holds also in $d = 4$, that is, if any PPT-entangled state in the symmetric subspace of $\mathbb{C}^4 \otimes \mathbb{C}^4$ has Schmidt number 3. Since in $d = 3$ and $d = 4$ the structure of the copositive cone is the same, we expect that this is the case, but a complete answer to this question certainly requires further investigation. A different, although related topic, refers to the possibility to use bipartite PPT-entangled states in the context of quantum communication. In particular, it has been recently shown [Bra05; SY08] that the combination of two zero-capacity quantum channels can lead to a quantum channel which is useful for communication, a phenomenon known as *superactivation.* Crucially, this effect can be achieved only if one of the two channels is constructed from a bipartite PPT-entangled state. As a consequence, it seems plausible that our characterisation of PPTES can lead to valuable insights into this remarkable phenomenon. Another interesting line of research consists in looking for generalisation of our results to the multipartite scenario of N qudits. While the separability problem for N DS qubits has already been discussed in the literature, this question remains open in the case of N DS qudits. Given the strong symmetry of the problem, we expect that, also in this case, the properties of a multipartite state of N qudits can be rephrased in terms of an associated matrix, and that copositive matrices still act as EWs for PPT-entangled states. Finally, a closely related topic is the prospect to use semidefinite programming not only as a method to tackle the separability problem but also as a tool to characterise exceptional copositive matrices. Indeed, the preliminary results presented in Appendix A suggest that the method of PPT symmetric extension could be particularly useful in this sense, but a more systematic approach to the problem is still needed.

Non-locality in open quantum systems: outlook & open questions

In chapter 4 we have investigated the presence of non-local correlations in open quantum systems. Although one might expect that, given its fragile nature, non-locality is lost when when we consider the interaction with an environment, we prove that this is not necessarily the case and non-local correlations can be detected by means of Bell inequalities involving only one- and two-body correlators. In particular, considering a many-body system described by an LMG Hamiltonian, we have discussed the case where the open quantum system is subjected both to thermal and non-thermal noise. In both case, using quantum master equation methods, we have been able to derive the stationary states of the model and we have shown that they display non-local correlations. Hence, we have compared this result with the dynamics of the entanglement in the evolved state, showing that the violation of a Bell inequality occurs at a later time when compared to the appearance of entanglement in the state of the open system, a behaviour that confirms the inequivalence between entanglement and non-locality. Finally, we have discussed the robustness of non-locality in a scenario where a many-body system undergoes repeated measurements: starting from a state that violates a Bell inequality, non-local correlations survive for a short, though significant, time, to the effect of external noise.

Open questions

When investigating the presence of non-locality in an open quantum system, we have considered both the case of thermal and non-thermal noise. However, the expression for the dissipator in this latter case is the result of an *ad hoc* construction and one might argue that cannot be ascribed to some known physical interaction. For this reason, it would be interesting to consider other examples of environments, outside the paradigm of the thermal bath, that lead to the violation of a Bell inequality in the open system. This might require to change the description of the open system, for instance, considering a different Hamiltonian, and/or a different expression for the dissipator. More importantly, the analysis of alternative sources of non-thermal noise allows to investigate the presence of non-locality in out of equilibrium states. For instance, one could inspect whether our technique can be useful to detect non-local correlations also in open quantum systems whose evolution crosses a phase transition, or in the more complex scenario where a time crystal open quantum system is considered. Another interesting line of research concerns the relation between the scenario where the open quantum system is repeatedly measured and quantum cryptography. In fact, since the disturbance introduced by the measurement bears strong resemblance with the action of an eavesdropper, exploring further the connection between these two settings could lead to new insights into this field and pave the way for innovative avenues of research.

Quantum neural networks & quantum maps: conclusions & outlook questions

The relation between quantum neural networks and the resource theory of coherence is the main topic of chapter 5, where special attention is devoted to the class of attractor quantum neural networks due to the possibility to use their stationary states as associative memories. Motivated by the results in [LGR+21], where the expression of the quantum map with the maximal number of stationary states was derived, we have described such map in the context of the resource theory of coherence. In particular, starting from the error-free case, we have shown that the quantum maps that describe the evolution towards the attractors corresponds to GIOs. Besides, we demonstrate that, for such aQNNs, the equivalent of the Hamming distance is the quantum relative entropy. After deriving their physical implementation, we have defined their depth and established a relation to the concept of decohering power. Further, we show that, in the case of noiseless aQNNs, neither coherence nor entanglement can be exploited as resources to enhance their performance. The same issues were discussed also for the case of faulty aQNNs, where we have shown that the corresponding aQNNs are described either by SIOs or by MIOs, thus opening the possibility, in the latter case, to an enhancement of their performance by using coherence as an external resource.

Open questions

Our analysis of faulty aQNNs shows that the corresponding quantum maps can be described by MIOs, a result which is particularly relevant since it opens the possibility to observe an enhancement of the performance of the network by using coherence as an external resource. For this reason, it would be interesting to provide an explicit example of a quantum neural network where this is indeed the case, deriving the expression of the unitary operators that implement the MIO. A related, although different topic, concerns the training of the network. In particular, since in our approach we deal with trained aQNNs, it would be interesting to discuss how this stage can be taken into account in our description. Another open question regards the characterisation of quantum maps that describe aQNNs with a reduced number of stationary states. This question is particularly relevant for certain tasks, such as image recognition, where restricting the number of stable patterns is a desirable feature to guarantee a higher capability of the network to distinguish between different outcomes. For this reason, it is natural to ask whether the same analysis performed in [LGR+21] can be applied also in this case to deduce the shape of the corresponding maps. Finally, it would be interesting to discuss the generalisation of our results to the case of stationary mixed states. While a partial characterisation of this question was already given in [LGR+21] for the case of error-free aQNNs, a complete answer in the faulty scenario is still missing.

A

Semidefinite programming for the copositive cone

In this Appendix we present a method, based on the construction of PPT-symmetric extensions of [DPS02; DPS04], to generate examples of exceptional copositive matrices in $d \geq 5$. In section A.1 we first recall the formalism used in [DPS02; DPS04]. Then, in section A.2, we focus on the case of two-qudit symmetric states. Finally, in section A.3, we provide a way to construct exceptional copositive matrices using semidefinite programming.

A.1 Semidefinite programming and PPT symmetric extensions

As we have seen in chapter 2, the method of PPT-symmetric extensions allows to cast the separability problem for a quantum state in the form of a hierarchy of SDPs. More specifically, if a quantum state does not admit a PPT-symmetric extension at a certain level of the hierarchy, then it is entangled. A generic semidefinite problem can be cast as

$$\begin{aligned}&\min\, c^T \boldsymbol{x}\\ &\text{s.t. } F(\boldsymbol{x}) \succeq 0\ ,\end{aligned} \tag{A.1}$$

where c is a given vector, $\boldsymbol{x} = (x_1, \dots, x_n)$ is the vector over which the minimization is performed and $F(\boldsymbol{x}) = F_0 + \sum_i x_i F_i \succeq 0$ is a linear constraint over $\boldsymbol{x}$. When $c = 0$, the SDP simply consists in checking whether the linear constraint is satisfied and the SDP is said a *feasibility problem*. The form of the SDP in (A.1) is usually referred to as the primal problem. Each primal problem admits a dual representation of the form

$$\begin{aligned}&\max\nolimits_Z\ \ -\mathrm{Tr}[F_0 Z]\\ &\text{s.t. } Z = Z^\dagger,\ Z \succeq 0\ ,\ \mathrm{Tr}[F_i Z] = c_i\ .\end{aligned} \tag{A.2}$$

The importance of the dual formulation (A.2) lies in the fact that, in the case of a feasibility problem (i.e., $c = 0$), if there exists $Z \succeq 0$ such that $\mathrm{Tr}[F_i Z] = 0$ and $\mathrm{Tr}[F_0 Z] < 0$, then the primal problem must be infeasible. It has been shown [DPS02; DPS04] that such scenario is equivalent to the case where an entangled state violates one of the tests in the hierarchy, thus allowing for the expression of the EW that detects it.

In what follows we will focus on the second test of the hierarchy, that is we look for PPT-symmetric extensions of a state $\rho \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ to two copies of the subsystem A. Introducing two bases for the spaces of Hermitian matrices acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, i.e., $\{\sigma_i^A\}_{i=1}^{d_A^2}$ and $\{\sigma_i^B\}_{i=1}^{d_B^2}$ respectively, we can expand ρ on the basis $\{\sigma_i^A \otimes \sigma_j^B\}$ as $\rho = \sum_{ij} \rho_{ij} \sigma_i^A \otimes \sigma_j^B$. Analogously, we can express $\tilde{\rho} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A)$ as

$$\tilde{\rho} = \sum_{\substack{ijk\\ i<k}} \tilde{\rho}_{ijk} \{\sigma_i^A \otimes \sigma_j^B \otimes \sigma_k^A + \sigma_k^A \otimes \sigma_j^B \otimes \sigma_i^A\} + \sum_{kj} \tilde{\rho}_{kjk} \sigma_k^A \otimes \sigma_j^B \otimes \sigma_k^A\ ,$$

where we have made use of the invariance under the exchange of the first and the third party. Let us now impose that the trace of $\tilde{\rho}$ over the third party yields the initial state, i.e., $\mathrm{Tr}_3[\tilde{\rho}] = \rho$. As a consequence we find

$$\tilde{\rho}_{ij1} = \rho_{ij}\ ,$$

where the result follows from the fact that we have chosen the basis elements in such a way they satisfy the commutation relations of $\mathrm{SU}(n)$, i.e., $\mathrm{Tr}[\sigma_i^X] =$

δ_{i1}, $\mathrm{Tr}[\sigma_i^X \sigma_j^X] = c_X \delta_{ij}$, for some constant c_X, with $X \in \{A, B\}$. Notice that the condition $\mathrm{Tr}_3[\tilde{\rho}] = \rho$ fixes some of the components of $\tilde{\rho}$, the remaining ones being the variables of the SDP over which the minimization is performed.
In order to write the linear constraints of the SDP in the form of (A.1), we define

$$G_0 = \sum_j \rho_{1j} \sigma_1^A \otimes \sigma_j^B \otimes \sigma_1^A + \sum_{i=2,j=1} \rho_{ij} \{\sigma_i^A \otimes \sigma_j^B \otimes \sigma_1^A + \sigma_1^A \otimes \sigma_j^B \otimes \sigma_i^A\} \,, \tag{A.3}$$

$$G_{iji} = \sigma_i^A \otimes \sigma_j^B \otimes \sigma_i^A \,, \quad i \geq 2 \,, \tag{A.4}$$

$$G_{ijk} = (\sigma_i^A \otimes \sigma_j^B \otimes \sigma_k^A + \sigma_k^A \otimes \sigma_j^B \otimes \sigma_i^A) \,, \quad k > i \geq 2 \,, \tag{A.5}$$

so that the condition $\tilde{\rho} \succeq 0$ can be cast as

$$G(\boldsymbol{x}) = G_0 + \sum_J x_J G_J \succeq 0 \,,$$

where J is a multi-index labelling the indices in the above equations.
With the aid of this definitions, the SDP takes the form of the primal problem of Eq.(A.1), where the coefficients $\tilde{\rho}_{ijk} (k \neq 1, k \geq i)$ play the role of the free variables of the SDP. Moreover, if we introduce the matrix $F = \tilde{\rho} \oplus \tilde{\rho}^{T_A} \oplus \tilde{\rho}^{T_B}$, the constraints on the positivity of $\tilde{\rho}$ and its partial transpositions, $\tilde{\rho}^{T_A}$ and $\tilde{\rho}^{T_B}$, can be written in a compact way as $F \succeq 0$, and the primal form for the second test of can be cast as a feasibility problem, i.e.,

$$\begin{aligned} &\min\ 0 \\ &\text{s.t. } F = \tilde{\rho} \oplus \tilde{\rho}^{T_A} \oplus \tilde{\rho}^{T_B} \succeq 0 \,. \end{aligned}$$

Let us now inspect the associated dual form (A.2) with $c = 0$. Given the block structure of F, we can cast

$$F_0 = G_0 \oplus G_0^{T_A} \oplus G_0^{T_B} \,, \tag{A.6}$$

$$F_J = G_J \oplus G_J^{G_A} \oplus G_J^{G_B} \,, \tag{A.7}$$

for every multi-index J. For the same reason, and without loss of generality, the maximization over Z in (A.2) can be restricted to Hermitian matrices of the form

$$Z = Z_0 \oplus Z_1^{T_A} \oplus Z_2^{T_B} \,,$$

and the requirement $Z \succeq 0$ implies $Z_0, Z_1^{T_A}, Z_2^{T_B} \succeq 0$.

An explicit calculation yields

$$\mathrm{Tr}[F_0 Z] = \mathrm{Tr}[G_0(Z_0 + Z_1 + Z_2)] = \mathrm{Tr}[G_0 V] = \mathrm{Tr}[\Lambda(\rho)V] \;,$$

where we have introduced $V = Z_0 + Z_1 + Z_2$ and we have recast G_0 in Eq.(A.3) as $G_0 = \Lambda(\rho)$, that is as the action of a linear map $\Lambda : \mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$ over the state ρ. Denoting by Λ^* the adjoint map of Λ, i.e., the map satisfying $\mathrm{Tr}[\Lambda(X)Y] = \mathrm{Tr}[X\Lambda^*(X)]$, we can write

$$\mathrm{Tr}[F_0 Z] = \mathrm{Tr}[\Lambda(\rho)V] = \mathrm{Tr}[\Lambda^*(V)\rho] = \mathrm{Tr}[W\rho] \;, \tag{A.8}$$

where we have defined $W = \Lambda^*(V)$.
If ρ_{sep} is a separable state, then we know that there exists a PPT symmetric extension or, equivalently, the primal problem (A.1) with $c = 0$ is feasible. As a consequence of Eq.(A.8), for any feasible solution Z it holds that the associated Hermitian operator W satisfies

$$\mathrm{Tr}[W\rho_{sep}] \geq 0 \;. \tag{A.9}$$

On the contrary, whenever the primal problem is infeasible for a given state ρ_{ent}, this implies that such state is entangled. Hence, there exists a feasible solution of the dual problem, i.e. Z, such that $\mathrm{Tr}[F_0 Z] < 0$. This implies that

$$\mathrm{Tr}[W\rho_{sep}] \geq 0 \;, \quad \mathrm{Tr}[W\rho_{ent}] < 0 \;, \tag{A.10}$$

thus defining a valid EW for the state ρ_{ent}.

A.2 PPT symmetric extensions for symmetric states

The separability criterion we have presented so far is based on the construction of PPT symmetric extension for a generic state $\rho \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$. In the following, we focus on the subset of symmetric states of n qudits, i.e, $\rho \in \mathcal{B}(\mathcal{S}(\mathbb{C}^d)^{\otimes n})$. In this case, one should specify how many qudits lie in the state $|0\rangle$, how many in the state $|1\rangle$, etc. For this reason, we introduce an alternative notation where the Dicke states are indexed according to the partitions $\boldsymbol{\lambda}$ of n in d elements, i.e.,

$$|D_{\boldsymbol{\lambda}}\rangle = \sum_{\pi \in \mathcal{G}_n} \binom{n}{\boldsymbol{\lambda}}^{-1/2} \pi\left(|0\rangle^{\lambda_0} \otimes \cdots \otimes |d-1\rangle^{\otimes \lambda_{d-1}}\right) \;,$$

where $\boldsymbol{\lambda} = (\lambda_0, \ldots, \lambda_{d-1}), \sum_i \lambda_i = n, \lambda_i \geq 0$, the sum runs over all possible permutations of n elements, and the multinomial coefficient is given by

$$\binom{n}{\boldsymbol{\lambda}} = \frac{n!}{\lambda_0! \cdots \lambda_{d-1}!} \;.$$

For the ease of notation we will write $|D_{\boldsymbol{\lambda}}\rangle \equiv |\boldsymbol{\lambda}\rangle$, and a generic state $\rho_S \in \mathcal{B}(\mathcal{S}(\mathbb{C}^d)^{\otimes n})$ will be written as

$$\rho = \sum_{\boldsymbol{\lambda},\boldsymbol{\mu} \vdash n} \rho^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} |\boldsymbol{\lambda}\rangle\langle\boldsymbol{\mu}| \ ,$$

where the notation $\boldsymbol{\lambda}, \boldsymbol{\mu} \vdash n$ means that we are considering partitions of n.
Our aim is to solve analytically the SDP associated to the second test of the hierarchy for the class of symmetric states. In order to do so, the first step is to require that a symmetric state of n qudits, $\tilde{\rho}$, is an extension of a symmetric state of m qudits, ρ. In other words, given a state $\tilde{\rho} \in \mathcal{B}(\mathcal{S}(\mathbb{C}^d)^{\otimes n})$ and a state $\rho \in \mathcal{B}(\mathcal{S}(\mathbb{C}^d)^{\otimes m})$, we want to derive under which conditions the equation $\rho = \mathrm{Tr}_{1,\ldots,n-m}[\tilde{\rho}]$ holds true. Such conditions are expressed by the following theorem:

Theorem A.1 ([AFT21]). *Let $\tilde{\rho} = \sum_{\boldsymbol{\lambda},\boldsymbol{\mu} \vdash n} \tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} |\boldsymbol{\lambda}\rangle\langle\boldsymbol{\mu}|$ be a symmetric state of n qudits and let us define $\rho = \mathrm{Tr}_{1,\ldots,n-m}[\tilde{\rho}]$, with $m \leq n$. If*

$$\rho^{\boldsymbol{\alpha}}_{\boldsymbol{\beta}} = \sum_{\boldsymbol{\lambda},\boldsymbol{\mu} \vdash n} \tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} \sum_{\boldsymbol{\kappa} \vdash n-m} \binom{n-m}{\boldsymbol{\kappa}} \sqrt{\frac{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}{\binom{n}{\boldsymbol{\lambda}}\binom{n}{\boldsymbol{\mu}}}} \delta(\boldsymbol{\alpha}+\boldsymbol{\kappa}-\boldsymbol{\lambda})\delta(\boldsymbol{\beta}+\boldsymbol{\kappa}-\boldsymbol{\mu}) \ , \quad \text{(A.11)}$$

then $\rho = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \vdash m} \rho^{\boldsymbol{\alpha}}_{\boldsymbol{\beta}} |\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}|$ is a symmetric state of m qudits.

As a consequence of Th.(A.1), some of the coefficients $\tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}}$ will be referred to as "fixed", since they can be expressed as a function of others, dubbed as "semi-free", and of the $\rho^{\boldsymbol{\alpha}}_{\boldsymbol{\beta}}$. Notice that not every $\tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}}$ will occur in Eq.(A.11), and we will call "free" those coefficients that do not appear in the above equation. Formally, we define:

1. Fixed variables: $\tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} = \tilde{\rho}^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}_{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}$ with $\boldsymbol{\kappa_0}$ arbitrarily chosen,

2. Semi-free variables: $\tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} = \tilde{\rho}^{\boldsymbol{\alpha}+\boldsymbol{\kappa}}_{\boldsymbol{\beta}+\boldsymbol{\kappa}}$ with $\boldsymbol{\kappa} < \boldsymbol{\kappa_0}$ such that $\sum_i \min\{\lambda_i, \mu_i\} \geq n-m$, $\boldsymbol{\lambda}_1 < n-m$ or $\boldsymbol{\mu}_1 < n-m$,

3. Free variables: $\tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}}$ such that $\sum_i \min\{\lambda_i, \mu_i\} < n-m$,

where the notation $\boldsymbol{\kappa} < \boldsymbol{\kappa_0}$ refers to a lexicographic ordering, i.e., $\boldsymbol{\kappa}_i < \boldsymbol{\kappa_0}_i$ for every component of each vector. Notice that the explicit form of the fixed (and, consequently, of the semi-free) variables depends on the choice of the vector $\boldsymbol{\kappa_0}$. Without loss of generality, we choose $\boldsymbol{\kappa_0} = (n-m, 0, \ldots, 0)$, so that it holds $\binom{n-m}{\boldsymbol{\kappa_0}} = 1$.

Expanding the right-hand side of Eq.(A.11) according to the definitions above, we have

$$\rho_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} = \sum_{\boldsymbol{\kappa}<\boldsymbol{\kappa_0}} \binom{n-m}{\boldsymbol{\kappa}} \sqrt{\frac{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa}}}}\tilde{\rho}_{\boldsymbol{\beta}+\boldsymbol{\kappa}}^{\boldsymbol{\alpha}+\boldsymbol{\kappa}} + \sqrt{\frac{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}}\tilde{\rho}_{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}} , \tag{A.12}$$

from which it follows that the fixed variables can be written as a linear combination of the coefficients $\rho_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}}$ and the semi-free variables, i.e.,

$$\tilde{\rho}_{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}} = \sqrt{\frac{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}}\rho_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} - \sqrt{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}} \sum_{\boldsymbol{\kappa}<\boldsymbol{\kappa_0}} \binom{n-m}{\boldsymbol{\kappa}} \frac{\tilde{\rho}_{\boldsymbol{\beta}+\boldsymbol{\kappa}}^{\boldsymbol{\alpha}+\boldsymbol{\kappa}}}{\sqrt{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa}}}} . \tag{A.13}$$

Hence we can write $\tilde{\rho}$ as

$$\begin{aligned}
\tilde{\rho} = &\sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\vdash m} \sqrt{\frac{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}}\rho_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} |\boldsymbol{\alpha}+\boldsymbol{\kappa_0}\rangle\langle\boldsymbol{\beta}+\boldsymbol{\kappa_0}| \qquad \text{(A.14)}\\
&- \sum_{\substack{(\boldsymbol{\alpha},\boldsymbol{\kappa})\in SF\\(\boldsymbol{\beta},\boldsymbol{\kappa})\in SF}} \sqrt{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}\binom{n-m}{\boldsymbol{\kappa}} \frac{\tilde{\rho}_{\boldsymbol{\beta}+\boldsymbol{\kappa}}^{\boldsymbol{\alpha}+\boldsymbol{\kappa}}}{\sqrt{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa}}}} |\boldsymbol{\alpha}+\boldsymbol{\kappa_0}\rangle\langle\boldsymbol{\beta}+\boldsymbol{\kappa_0}|\\
&+ \sum_{\substack{(\boldsymbol{\alpha},\boldsymbol{\kappa})\in SF\\(\boldsymbol{\beta},\boldsymbol{\kappa})\in SF}} \tilde{\rho}_{\boldsymbol{\beta}+\boldsymbol{\kappa}}^{\boldsymbol{\alpha}+\boldsymbol{\kappa}} |\boldsymbol{\alpha}+\boldsymbol{\kappa}\rangle\langle\boldsymbol{\beta}+\boldsymbol{\kappa}| + \sum_{(\boldsymbol{\lambda},\boldsymbol{\mu})\in F} \tilde{\rho}_{\boldsymbol{\mu}}^{\boldsymbol{\lambda}} |\boldsymbol{\lambda}\rangle\langle\boldsymbol{\mu}| ,
\end{aligned}$$

where F and SF refer to the set of free and semi-free variables respectively.
In order to solve the dual formulation of the SDP (A.2) for $c = 0$ we need to derive the expression of the matrices G_0 and G_J. Notice that, differently from the previous case, due to the permutational invariance of the parties, the partial transposition will be the same regardless of the choice of the subsystem. Hence, we can restrict our search over a Hermitian matrix of the form $Z = Z_0 \oplus Z_1^{T_B}$, and the quantities in the previous section will change accordingly, i.e., $F_0 = G_0 \oplus G_0^{T_B}$, $F_J = G_J \oplus G_J^{T_B}$ and $V = Z_0 + Z_1$.
Let us observe that the first element in the right-hand side of Eq.(A.14) is a linear combination of the coefficients $\rho_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}}$. Following the same argument as before, we can write

$$G_0 = \Lambda(\rho) = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\vdash m} \sqrt{\frac{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}}\rho_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} |\boldsymbol{\alpha}+\boldsymbol{\kappa_0}\rangle\langle\boldsymbol{\beta}+\boldsymbol{\kappa_0}| , \tag{A.15}$$

and recalling that $W = \Lambda^*(V)$, we find

$$W = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \vdash m} \sqrt{\frac{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}{\binom{m}{\boldsymbol{\alpha}}\binom{m}{\boldsymbol{\beta}}}} V^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}_{\boldsymbol{\beta}+\boldsymbol{\kappa_0}} |\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}| \,, \tag{A.16}$$

where the last equation follows from the definition of the adjoint map Λ^*, i.e., $\mathrm{Tr}[\Lambda(\rho)V] = \mathrm{Tr}[\Lambda^*(V)\rho]$. A direct inspection of the dual SDP (A.2) with $c = 0$ shows that we still need to impose the constraints $Z \succeq 0$ and $\mathrm{Tr}[F_J Z] = 0$ for every multi-index J labelling the free and semi-free variables of the SDP. Let us observe that, since $F_J = G_J \oplus G_J^{T_B}$, the latter condition can be rewritten as

$$\mathrm{Tr}[F_J Z] = \mathrm{Tr}[G_J(Z_0 + Z_1)] = \mathrm{Tr}[G_J V] = 0 \,. \tag{A.17}$$

The expression of $G_J \equiv G_{\boldsymbol{\lambda},\boldsymbol{\mu}}$ can be found by deriving $\tilde{\rho}$ of Eq.(A.14) with respect to a pair of semi-free variables $\tilde{\rho}^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}}$, i.e.,

$$G_{\boldsymbol{\lambda},\boldsymbol{\mu}} = |\boldsymbol{\lambda}\rangle\langle\boldsymbol{\mu}| \,, \quad \text{if } (\boldsymbol{\lambda},\boldsymbol{\mu}) \in F \,, \tag{A.18}$$

$$G_{\boldsymbol{\lambda},\boldsymbol{\mu}} = |\boldsymbol{\lambda}\rangle\langle\boldsymbol{\mu}| - \sum_{\substack{(\boldsymbol{\alpha},\boldsymbol{\kappa})\in SF \\ (\boldsymbol{\beta},\boldsymbol{\kappa})\in SF}} \delta(\boldsymbol{\alpha}+\boldsymbol{\kappa}-\boldsymbol{\lambda})\delta(\boldsymbol{\beta}+\boldsymbol{\kappa}-\boldsymbol{\mu}) \tag{A.19}$$

$$\sqrt{\frac{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa}}}} \binom{n-m}{\boldsymbol{\kappa}} |\boldsymbol{\alpha}+\boldsymbol{\kappa_0}\rangle\langle\boldsymbol{\beta}+\boldsymbol{\kappa_0}| \,, \quad \text{if } (\boldsymbol{\lambda},\boldsymbol{\mu}) \in SF \,.$$

A straightforward calculation shows that Eq.(A.17) takes the form

$$V^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} = 0 \,, \quad \text{if } (\boldsymbol{\lambda},\boldsymbol{\mu}) \in F \,, \tag{A.20}$$

$$V^{\boldsymbol{\lambda}}_{\boldsymbol{\mu}} = \sum_{\substack{(\boldsymbol{\alpha},\boldsymbol{\kappa})\in SF \\ (\boldsymbol{\beta},\boldsymbol{\kappa})\in SF}} \delta(\boldsymbol{\alpha}+\boldsymbol{\kappa}-\boldsymbol{\lambda})\delta(\boldsymbol{\beta}+\boldsymbol{\kappa}-\boldsymbol{\mu}) \tag{A.21}$$

$$\sqrt{\frac{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa_0}}}{\binom{n}{\boldsymbol{\alpha}+\boldsymbol{\kappa}}\binom{n}{\boldsymbol{\beta}+\boldsymbol{\kappa}}}} \binom{n-m}{\boldsymbol{\kappa}} V^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}_{\boldsymbol{\beta}+\boldsymbol{\kappa_0}} \,, \quad \text{if } (\boldsymbol{\lambda},\boldsymbol{\mu}) \in SF \,.$$

A.3 The diagonal symmetric case

Let us consider the case where ρ is a PPT-entangled diagonal symmetric (PPTEDS) state of m qudits, i.e., $\rho_{DS} = \sum_{\boldsymbol{\alpha}\vdash m} (\rho_{DS})^{\boldsymbol{\alpha}}_{\boldsymbol{\alpha}} |\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}|$, with $\rho_{DS}^{\Gamma} \succeq 0$. In this case

we know that, given a copositive matrix $H = \sum_{ij} H_{ij}|i\rangle\langle j|$, it is always possible to construct an EW, $W_{DS} = \Pi_S(H^{ext})^\Gamma\Pi_S$, where Π_S is the projector onto the symmetric subspace of two qudits, and $H^{ext} = \sum_{ij} H_{ij}|ii\rangle\langle jj|$, is the extension of the copositive matrix to the space $\mathbb{C}^d \otimes \mathbb{C}^d$. In particular, non-decomposable EWs correspond to exceptional copositive matrices, i.e., those matrices that cannot be decomposed as $H = H_{\mathcal{PSD}} + H_{\mathcal{NN}}$, with $H_{\mathcal{PSD}} \in \mathcal{PSD}, H_{\mathcal{NN}} \in \mathcal{NN}$, where $\mathcal{PSD}$, $\mathcal{NN}$ are the cones of positive semidefinite and non-negative matrices, respectively.
In what follows, we restrict to the case $d = 3$ although we stress that, in principle, our approach can be generalized to any other dimension. Since any PPTEDS in $d < 5$ is necessarily separable, we want to prove that the operator $W_{DS} = \Lambda^*(V)$ is a decomposable EW or, equivalently, that its associated copositive matrix is non-exceptional. Let us start by proving that W_{DS} is a decomposable EW.
Since Λ^* is a linear map, we can split its action on $V = Z_0 + Z_1$ in two terms, i.e., $W_{DS} = \Lambda^*(Z_0) + \Lambda^*(Z_1)$. Hence, proving the EW to be decomposable consists in showing that it can be written as $W_{DS} = P + Q^\Gamma$, with $P, Q \succeq 0$. In what follows, we typically construct decompositions where $P = \Lambda^*(Z_0)$ and $Q = \Lambda^*(Z_1)^\Gamma$, although, due to the fact that Z_0 and Z_1 have the same structure, an equivalent result would hold true under the swap $Z_0 \leftrightarrow Z_1$.

Notice that the PPT symmetric extension of n qudits of a DS state must be a DS state, i.e., $\tilde{\rho}_{DS} = \sum_{\boldsymbol{\lambda}\vdash n}(\tilde{\rho}_{DS})^{\boldsymbol{\lambda}}_{\boldsymbol{\lambda}}|\boldsymbol{\lambda}\rangle\langle\boldsymbol{\lambda}|$. Due to the symmetry of the problem, we can now solve the dual formulation of the SDP by restricting our search to Hermitian matrices of the form $Z_{DS} = Z_0 \oplus Z_1^\Gamma$, where each Z_i is a DS state of n qudits, with $Z_0, Z_1^\Gamma \succeq 0$. Moreover, recalling the definitions of fixed and semi-free variables, any Z_i can be cast as

$$Z_i = \sum_{\boldsymbol{\alpha}\vdash m}(Z_i)^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}_{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}|\boldsymbol{\alpha}+\boldsymbol{\kappa_0}\rangle\langle\boldsymbol{\alpha}+\boldsymbol{\kappa_0}| + \sum_{(\boldsymbol{\alpha},\boldsymbol{\kappa})\in SF}(Z_i)^{\boldsymbol{\alpha}+\boldsymbol{\kappa}}_{\boldsymbol{\alpha}+\boldsymbol{\kappa}}|\boldsymbol{\alpha}+\boldsymbol{\kappa}\rangle\langle\boldsymbol{\alpha}+\boldsymbol{\kappa}| \; . \quad \text{(A.22)}$$

The constraint $Z_0 \succeq 0$ implies $(Z_0)^{\boldsymbol{\lambda}}_{\boldsymbol{\lambda}} \geq 0 \; \forall \boldsymbol{\lambda} \vdash 3$, and we can set

$$P \equiv \Lambda^*(Z_0) = \sum_{\boldsymbol{\alpha}\vdash 2}\frac{\binom{3}{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}}{\binom{2}{\boldsymbol{\alpha}}}(Z_0)^{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}_{\boldsymbol{\alpha}+\boldsymbol{\kappa_0}}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}| \succeq 0 \; . \quad \text{(A.23)}$$

The structure of Z_1^Γ can be represented more easily in the Dicke basis of three qutrits, where a generic operator $Z \in \mathcal{S}((\mathbb{C}^3)^{\otimes 3})$ takes the form

$$Z = \sum_{0\leq i\leq j\leq k\leq 2} Z_{ijk}|D_{ijk}\rangle\langle D_{ijk}| \; . \quad \text{(A.24)}$$

Using the same notation, Z_1^Γ can be cast as

$$Z_1^\Gamma = A \oplus B \oplus C \bigoplus_{i<j} \frac{(Z_1)_{iij}}{3} \bigoplus_{i<j<k} \frac{(Z_1)_{ijk}}{3}\,, \tag{A.25}$$

where we have set

$$A = \frac{1}{3}\begin{pmatrix} 3(Z_1)_{000} & \sqrt{2}(Z_1)_{001} & \sqrt{2}(Z_1)_{002} \\ \sqrt{2}(Z_1)_{001} & 2(Z_1)_{011} & (Z_1)_{012} \\ \sqrt{2}(Z_1)_{002} & (Z_1)_{012} & 2(Z_1)_{022} \end{pmatrix},$$
$$B = \frac{1}{3}\begin{pmatrix} 2(Z_1)_{001} & \sqrt{2}(Z_1)_{011} & (Z_1)_{012} \\ \sqrt{2}(Z_1)_{011} & 3(Z_1)_{111} & \sqrt{2}(Z_1)_{112} \\ (Z_1)_{012} & \sqrt{2}(Z_1)_{112} & 2(Z_1)_{122} \end{pmatrix},$$
$$C = \frac{1}{3}\begin{pmatrix} 2(Z_1)_{002} & (Z_1)_{012} & \sqrt{2}(Z_1)_{022} \\ (Z_1)_{012} & 2(Z_1)_{112} & \sqrt{2}(Z_1)_{122} \\ \sqrt{2}(Z_1)_{022} & \sqrt{2}(Z_1)_{122} & 3(Z_1)_{222} \end{pmatrix}.$$

Hence, $Z_1^\Gamma \succeq 0$ implies $A, B, C \succeq 0$, as well as the positivity of the coefficients in Eq.(A.25). We want to show that $Q^\Gamma = \Lambda^*(Z_1)$ with $Q \succeq 0$. The partial transposition of $\Lambda^*(Z_1)$ yields

$$\Lambda^*(Z_1)^\Gamma = H_{Z_1} \oplus \frac{3}{4}(Z_1)_{001} \oplus \frac{3}{4}(Z_1)_{002} \oplus \frac{3}{2}(Z_1)_{012}\,, \tag{A.26}$$

where the matrix H_{Z_1} is given by

$$H_{Z_1} = \frac{3}{4}\begin{pmatrix} 4(Z_1)_{000}/3 & (Z_1)_{001} & (Z_1)_{002} \\ (Z_1)_{001} & 4(Z_1)_{011} & 2(Z_1)_{012} \\ (Z_1)_{002} & 2(Z_1)_{012} & 4(Z_1)_{022} \end{pmatrix}. \tag{A.27}$$

Introducing the matrix G, given by

$$G = \frac{3}{4}\begin{pmatrix} 4/3 & 3/\sqrt{2} & 3/\sqrt{2} \\ 3/\sqrt{2} & 6 & 6 \\ 3/\sqrt{2} & 6 & 6 \end{pmatrix}, \tag{A.28}$$

it is straightforward to see that $H_{Z_1} = G \star A$, where $\star$ denotes the Hadamard product between two matrices. Since $G, A \succeq 0$, by the Schur product theorem it follows that $H_{Z_1} \succeq 0$, thus proving that $W_{DS} = \Lambda^*(Z_0) + \Lambda^*(Z_1)$ is a decomposable EW.

Analogously, we want show that W_{DS} can be constructed from a non-exceptional copositive matrix H. Similarly to the previous case, we expect that the two terms of the decomposition, i.e., $H_{\mathcal{NN}}$ and $H_{\mathcal{PSD}}$, will stem from the operators $\Lambda^*(Z_0), \Lambda^*(Z_1)$. Let us first consider the term $\Lambda^*(Z_0)$, whose expression in the Dicke basis is given by

$$\Lambda^*(Z_0) = \text{diag}\left((Z_0)_{000}, \frac{3}{2}(Z_0)_{001}, \frac{3}{2}(Z_0)_{002}, 3(Z_0)_{011}, 3(Z_0)_{012}, 3(Z_0)_{022} \right) . \tag{A.29}$$

The expression of its associated matrix, H_{Z_0}, in the computational basis can be obtained by stacking the elements of $\Lambda^*(Z_0)$ row by row in a 3×3 matrix an multiplying the off-diagonal elements by a factor $1/2$, i.e.,

$$H_{Z_0} = \frac{3}{4} \begin{pmatrix} 4(Z_0)_{000}/3 & (Z_0)_{001} & (Z_0)_{002} \\ (Z_0)_{001} & 4(Z_0)_{011} & 2(Z_0)_{012} \\ (Z_0)_{002} & 2(Z_0)_{012} & 4(Z_0)_{022} \end{pmatrix} . \tag{A.30}$$

Notice that, as a consequence of the constraint $Z_0 \succeq 0$, it follows that $H_{Z_0} \in \mathcal{NN}$. By the same argument, we can construct the matrix H_{Z_1}, whose expression can be obtained by Eq.(A.30) by relabeling $Z_0 \to Z_1$, thus yielding the same matrix of Eq.(A.27). As before, due to the condition $(Z_1)^\Gamma \succeq 0$, it follows that $H_{Z_1} \in \mathcal{PSD}$, thus concluding the proof.

This result suggests that the separability criterion based on the construction of PPT-symmetric extension can be applied also to the cone of copositive matrices. In fact, if a DS state does not admit a PPT extension at some level of the hierarchy, then it is entangled and can be detected by a witness constructed from an exceptional copositive matrix. Since the characterisation of this class of matrices is, in general, NP-hard, this method can provide a computational method to generate new examples of exceptional copositive matrices in arbitrary dimension $d \geq 5$.

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