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Aabhas GULATI

École doctorale
EDMITT - Ecole Doctorale Mathématiques, Informatique et Télécommunications de Toulouse

Spécialité
Mathématiques et Applications

Unité de recherche
IMT : Institut de Mathématiques de Toulouse

Thèse dirigée par
Clément PELLEGRINI et Ion NECHITA

Composition du jury
Mme Monique LAURENT, Rapporteure, Tilburg Universiteit
Mme Anna SANPERA, Rapporteure, Universitat Autònoma de Barcelona
M. Omar FAWZI, Rapporteur, ENS Lyon
M. Victor MAGRON, Examinateur, CNRS Occitanie Ouest
M. Clément PELLEGRINI, Directeur de thèse, Université de Toulouse
M. Ion NECHITA, Co-directeur de thèse, CNRS Occitanie Ouest

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INTRODUCTION

MOTIVATION AND CONTEXT

This thesis deals primarily with the geometric structure of entanglement and entanglement witnesses in bipartite and multipartite quantum systems. Quantum entanglement is the fundamental phenomenon in quantum theory that exhibits a form of non-classical correlations. Although it was seen as a paradoxical phenomenon in quantum theory for much of the previous century, it now has the status of a *resource* that powers quantum protocols in quantum communication [SN96, BBC$^+$93], cryptography [Eke91], and error correction [BDSW96]. Despite considerable progress in understanding entanglement, various problems in the theory of entanglement remain unsolved [HHHH09], especially when the quantum systems have mixed states due to the presence of noise.

Separable states, or unentangled states, are convex mixtures of pure product states and can be prepared by local operations and classical communication. This simple definition masks significant complexity, as the membership problem for separable states is NP-hard [Gur03, Gha10], thus implying limits on algorithmic solvability. This also implies the impossibility of exact efficiently computable necessary and sufficient conditions for deciding whether a state is entangled or separable (if P $\neq$ NP). Moreover, it was recently established that the geometry of separable states of a system of dimensions $d \times d'$ where $dd' > 6$ cannot be described by a linear matrix inequality or its projections, and hence it is not semidefinite representable [Faw21].

Every convex set (or convex cone) has an associated dual, i.e., the set of hyperplanes that separate the convex set from other points. In the case of separable states, these hyperplanes are called entanglement *witnesses*, and correspond to linear functionals positive on separable states. For bipartite states, these also have a well-known correspondence with positive maps between matrix algebras [HHH01], a well-studied object in operator theory and functional analysis. In general, multipartite witnesses can also be described as homogeneous *complex* positive polynomials.

In general, since the complexity of the separability problem forbids an exact solution, the role of entanglement criteria is central to the theory. These are necessary criteria for separability, and any violation of such a criterion detects entanglement. Many such entanglement criteria have been designed, for example the Peres-Horodecki criterion [Per96, HHH96], which checks if a matrix has a positive partial transpose (PPT); the CCNR (Computable cross norm and realignment) criterion, which checks whether a certain norm is less than 1 [Rud00, CW03]; and other criteria based on covariance matrices [TG09]. Moreover, every entanglement witness forms an entanglement criterion, which can also be directly implemented in the lab.

In this thesis, we will focus on the Peres-Horodecki (PPT) criterion. Although separable states satisfy this in all dimensions, it is also sufficient only if the product of dimensions $dd' \leq 6$ [HHH96]. The convex set of PPT states, i.e., the states that have a positive partial transposition, is a relaxation of the set of separable states, whose membership only involves checking eigenvalues of the partial transpose, and hence is efficiently decided. Although the set of PPT states was only designed to be a mathematical approximation, they were later discovered to have physically interesting properties, and PPT entangled states are at the heart of some open problems in quantum information.

The dual of the bipartite PPT states has a correspondence with the well-known decomposable maps, which can be written as the sum of completely positive and completely co-positive maps. This is analogous to the correspondence between entanglement witnesses and positive maps. Any positive non-decomposable map acts as a witness for PPT entangled states. Moreover, such a map was constructed by Choi in his seminal paper [Cho80a], which also predates the beginning of quantum information theory. In general, it is considered a non-trivial problem to construct examples of non-decomposable maps, and similarly, of PPT entangled states.

Symmetries have played an important role in the entanglement problem, reducing its complexity and enabling exact analytical solutions of the entanglement geometry. For example, bipartite quantum states with unitary symmetries can be described by two parameters in total [Wer89], and the exact parameters for separability of such a state can be computed [VW01]. Moreover, such symmetries can also be exploited to construct entanglement witnesses. The main results in this thesis broadly concern two different types of symmetries: a local diagonal unitary symmetry and/or a global permutation symmetry. In all these cases, we show that the *symmetry* can be used to connect quantum entanglement to various interesting problems in matrix/tensor analysis, positivity of polynomials, and graph theory, leading to novel insights into the complex structure of entanglement.

SUMMARY OF CONTRIBUTIONS

Entanglement in cyclic sign invariant quantum states – Aabhas Gulati, Ion Nechita and Satvik Singh

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We introduce and study bipartite quantum states that are invariant under the local action of the cyclic sign group. Due to symmetry, these states are sparse and can be parameterized

by a triple of *vectors*. Hence, these states have a *linear* number of free parameters, and their important semi-definite properties, such as positivity and positivity under partial transpose (PPT), can be simply characterized in terms of the parametrizing vectors and their discrete Fourier transforms. Moreover, a characterization of separability can be obtained by these vectors satisfying some convolution relations.

We study the bosonic states in this class, the states invariant under permutations of the systems. For these states, separability is equivalent to the *circulant* version of the complete positivity problem, which is equivalent to deciding whether a vector is a sum of cyclic *autocorrelations* of positive vectors. In local dimension $d \leq 5$, we completely characterize the geometry of these sets and construct bosonic entanglement witnesses. We also obtain some partial results about the geometry of these sets for $d = 6, 7$.

The bosonic PPT cone corresponds to the *semi-positive cone* for the Fourier matrix, for which we give a characterization of extremal points.

$$\{a \in \mathbb{R}_d^+ \mid \mathcal{F}a \in \mathbb{R}_d^+\}$$

Our results show that these states have a rich entanglement structure in the bosonic subspace, and provide some new insights into the geometric structures of completely positive and doubly non-negative matrices. Finally, we construct a new family of symmetric entangled states for which the properties of PPT and separability can be characterized for all dimensions. This generalizes some results from [SBSGS22] while also simplifying the proof.

Rank-based entanglement detection for bound entangled states – Aabhas Gulati

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Although PPT entangled states are known to exist for all bipartite systems with dimensions $d \cdot d' \geq 6$, the construction of such entangled states is generally non-trivial. In general, a variety of methods have been used to construct new families of PPT entangled states [Hor97, Bre06, SP18, CK06, HK05, Sin21]. In our article, we show a method for entanglement detection that is useful to detect new families of entangled states, and is based on detection of rank-1 generated property of some matrix convex cones.

The positive-semidefinite matrices form a convex cone that has extremal elements of rank 1. However, convex conic subsets resulting from the presence of linear constraints allow extremal elements of rank greater than or equal to 2. The problem of deciding when a matrix is rank-1 generated, i.e., a sum of rank-1 positive-semidefinite matrices, has been studied extensively in optimization theory for a variety of convex cones.

We show that some faces of PPT density matrices map to convex cones that are not rank-1 generated under a *rank*-preserving map. The main idea we exploit is that such a map sends separable states to rank-1 generated states, while the same is not true for the corresponding mapping of PPT entangled states. We consider mappings of different faces of PPT states to sparse PSD matrices, correlation matrices, and doubly non-negative matrices. These cones are well-known convex cones consisting of elements that are not rank 1 generated. Moreover, if a PPT density matrix is mapped to an extremal point of such a cone that is rank ≥ 2, it is guaranteed to be a PPT edge-state.

These ideas are used to construct new examples of PPT entangled states and PPT edge states in the class of local orthogonal invariant states.

Positive maps and extendibility hierarchies from copositive matrices – Aabhas Gulati, Ion Nechita and Sang-Jun Park

Preprint
https://arxiv.org/abs/2509.15201

In this work, we introduce and systematically study a new convex cone of pairwise copositive (PCOP) matrices. We establish that this cone is dual to the cone of PCP (pairwise completely positive) and, critically, provides a complete characterization for the positivity of the broad class of covariant maps. We provide a way to lift matrices from the cone of COP to PCOP, thereby creating a powerful bridge between the theory of copositive forms and the positive maps, which correspond to *bi*-quadratic positive forms. We develop an analogous framework for decomposable maps, introducing the cone of pairwise decomposable matrices (PDEC).

As a primary application of this framework, we define a novel family of linear maps $\Phi_{G,t}$ parameterized by a graph G and a real parameter t. We derive exact thresholds on t that determine when these maps are positive or decomposable, linking these properties to fundamental graph-theoretic parameters. This construction yields vast new families of positive indecomposable maps, for which we provide explicit examples derived from infinite classes of graphs, notably rank 3 strongly regular graphs such as Paley graphs. We also show that for triangle-free graphs, the thresholds for positivity and decomposability of $\Phi_{G,t}$ differ iff it is not bipartite.

The second main contribution of this work is to understand the properties of extendibility witnesses. We prove that the SOS hierarchies used in polynomial optimization to approximate the cone of copositive matrices correspond precisely to witnesses for different levels of the *bosonic* extendibility hierarchy. In the setting of the Doherty Parillo Spedalieri (DPS) hierarchy for separability, we construct a large family of optimal entanglement

witnesses that are not certifiable at any level, which answers an open question about this hierarchy.

Entanglement in the Dicke subspace – Aabhas Gulati, Ion Nechita and Clément Pellegrini

Preprint

https://arxiv.org/abs/2602.15800

We provide a complete mathematical theory for the entanglement of mixtures of Dicke states. These quantum states form an important subclass of bosonic states arising in the study of indistinguishable particles.

Firstly, we introduced a tensor-based parametrization where the diagonal entries of these states are encoded as a symmetric tensor, to enable a translation between entanglement properties and some well-studied convex cones of tensors. This dictionary maps separability to completely positive tensors, the PPT property to moment tensors, entanglement witnesses to copositive tensors, and decomposable witnesses to sum of squares tensors. This allows us to construct new non-decomposable maps through positive polynomials that are not sum of squares, e.g., the Motzkin polynomial.

In mixtures of Dicke states, we establish that PPT entanglement exists for all multipartite systems with three qutrits or more, disproving a recent conjecture in [RPAR+25]. Due to the bosonic symmetry of the states, these states are also de-facto *genuinely* multipartite entangled.

We also show that, for mixtures of Dicke states, the PPT condition with respect to the most balanced bipartition implies PPT with respect to any other bipartition, which also resolves a conjecture in [RPAR+25] and extends the results obtained in [Yu16] about qubits to general states.

We further connect bosonic extendibility of mixtures of Dicke states to the duals of known hierarchies for non-negative polynomials, such as the ones by Reznick and Polya. We thus provide polynomial-sized semidefinite programming relaxations for separability and entanglement testing in the Dicke subspace.

STRUCTURE OF THESIS

This thesis is organised into Part i : Background and Part ii : Presentation of Articles.

Background

- Chapter 2 discusses some algebraic results in polynomial positivity and sum of squares.
- Chapter 3 consists of some results in matrix analysis and optimization theory concerning complete positivity and copositivity, and some other matrix cones.
- Chapter 4 provides a brief background of quantum information theory, with the main focus on quantum entanglement, PPT and extendibility.
- Chapter 5 discusses some results about entanglement in symmetric states, with a focus on diagonal unitary and orthogonal symmetries, and Bosonic symmetric states.

Presentation of articles

The Chapter 6, Chapter 7, Chapter 8, and Chapter 9 present the articles discussed previously.

Conclusion

The final chapter Chapter 10 provides some future directions and improvements, and lists some open problems.

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Part I

BACKGROUND

1

Notation and Basic Definitions

Basic Notation	
$\mathbb{R},\ \mathbb{C}$	Field of real and complex numbers
$\mathbb{N}$	Natural numbers $\{0, 1, 2, \ldots\}$
$\mathbb{Z}$	Ring of integers $\{\ldots, -2, -1, 0, 1, 2, \ldots\}$
$\mathbb{T}$	$\{z \in \mathbb{C}, \lvert z\rvert = 1\}$
X^d	$X \times X \ldots \times X$ (d times)
$\mathbb{R}_+$	Non-negative real numbers
$[n]$	The set $\{1, 2, \ldots, n\}$ for $n \in \mathbb{N}$
$\mathbb{N}_d^{(k)}$	$\{x \in \mathbb{N}^d \mid \sum_i x_i = k\}$
$\lvert v\rangle$	Vector in $\mathbb{R}^d$ or $\mathbb{C}^d$
$\lvert v\rangle \otimes \lvert w\rangle$	Tensor product; $(\lvert v\rangle \otimes \lvert w\rangle)_{ij} := v_i w_j$
$\langle v \mid w\rangle$	Inner product; $\sum_i \overline{v_i}\, w_i$
$\mathrm{span}_{\mathbb{C}}(A)$	Complex linear span of the set A
$\mathrm{span}_{\mathbb{R}}(A)$	Real linear span of the set A
$\lvert v\rangle\langle w\rvert$	Rank-1 matrix (outer product) with entries $v_i w_j$
$\mathcal{M}_{d,d'}$	Set of $d \times d'$ complex matrices
$\mathcal{M}_d$	Square $d \times d$ complex matrices
$\mathrm{Herm}[\mathcal{M}_d]$	Hermitian $d \times d$ matrices
$\mathrm{Sym}[\mathcal{M}_d(\mathbb{R})]$	Real symmetric $d \times d$ matrices
XY	Matrix product of X and Y

continued on next page

$\ker(M),\ \mathrm{ran}(M)$	Kernel and range of a matrix M
$X \succeq 0$	X has non-negative eigenvalues
$\odot$	Schur (entry-wise) product: $(X \odot Y)_{ij} := X_{ij}Y_{ij}$
T	Transposition map: $X^T_{ij} := X_{ji}$
$\mathbb{I}_d, \mathbb{J}_d$	Identity matrix, all ones matrix (resp.) of size $d \times d$
$\mathrm{Tr}(X),\ \mathrm{rk}(M)$	Trace and rank of a matrix
$\mathrm{supp}(X)$	Support of X: the orthogonal complement of its kernel
$V^{\otimes n}$	n-fold tensor product $V \otimes \cdots \otimes V$
$V + W$	Sum of vector spaces V, W: $\{\|v\rangle + \|w\rangle \mid \|v\rangle \in V,\ \|w\rangle \in W\}$
$\|v\|_p$	p-norm of $\|v\rangle \in \mathbb{C}^d$: $\left(\sum_{i\in[d]} \|v_i\|^p\right)^{1/p}$
$\sigma(M)$	Singular values of a matrix M
$\|M\|_p$	Schatten p-norm of a matrix: $\left(\mathrm{Tr}(\|M\|^p)\right)^{1/p}$
$\mathrm{int}(A)$	Interior of a set A
$\mathrm{cl}(A)$	Closure of a set A
δA	Boundary of a set A

1.1 CONVEX GEOMETRY

Notation	
$\mathrm{cone}(A)$	Conic hull of set A
$\mathrm{conv}(A)$	Convex hull of set A
$\mathrm{ext}(\mathcal{C})$	Set of extreme rays of a convex cone $\mathcal{C}$
$\mathcal{C}^\circ$	Polar dual of $\mathcal{C}$

Let V be a real vector space. A set $\mathcal{S} \subseteq V$ is *convex* if for any two points $|v\rangle, |w\rangle \in \mathcal{S}$, the line segment connecting them also lies in $\mathcal{S}$, i.e., $\lambda|v\rangle + (1-\lambda)|w\rangle \in \mathcal{S}$ for all $\lambda \in [0,1]$. The *convex hull* $\mathrm{conv}(A)$ is the smallest convex set containing A. A subset $\mathcal{C} \subseteq V$ is a *convex cone* if it is closed under non-negative combinations, i.e., for $|v\rangle, |w\rangle \in \mathcal{C}$ and $\alpha, \beta \geq 0$, we have $\alpha|v\rangle + \beta|w\rangle \in \mathcal{C}$. The *conic hull* $\mathrm{cone}(A)$ is the set of all non-

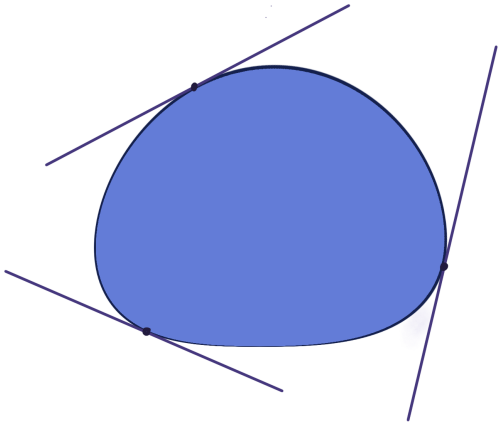


Figure 1: A convex set with some of its supporting hyperplanes

negative linear combinations of elements of A, or equivalently, the smallest convex cone containing A. Sometimes we require the closure of the convex hull, which will be denoted by $\mathrm{cl}(\mathrm{conv}(A))$.

A vector $|v\rangle \in \mathcal{C}$ generates an *extreme ray* of a cone $\mathcal{C}$ if it cannot be decomposed as the sum of two linearly independent vectors in $\mathcal{C}$; that is,

$$|v\rangle = |w\rangle + |z\rangle \text{ with } |w\rangle, |z\rangle \in \mathcal{C} \implies |w\rangle, |z\rangle \propto |v\rangle .$$

The *polar dual* $\mathcal{C}^\circ$ of a cone $\mathcal{C}$ is the set of hyperplanes positive on elements of $\mathcal{C}$:

$$\mathcal{C}^\circ = \{|y\rangle \in V^* \mid \langle y|x\rangle \geq 0 \; \forall \, |x\rangle \in \mathcal{C}\}.$$

A supporting hyperplane is an element $|y\rangle \in \mathcal{C}^\circ$ such that there exists a $|x\rangle \in \mathcal{C}$ that vanishes on $|x\rangle$, i.e, $\langle y|x\rangle = 0$. Then, the supporting hyperplane theorem states that there exists a supporting hyperplane for any point in the boundary $\delta\mathcal{C}$ of the convex cone, as in *Fig.* 1 (see [BV04]).

It follows from the definition of the polar dual that if $K_1 \subseteq K_2$, then $K_2^\circ \subseteq K_1^\circ$. Finally, we recall some important results about convex sets (and cones) that will be useful in this thesis. These facts can be found in popular textbooks on convex geometry/optimization, see [BV04].

Theorem 1.1 (Dual of the dual)**.** Let $\mathcal{C}$ be a convex cone. Then

$$(\mathcal{C}^\circ)^\circ = \mathrm{cl}(\mathcal{C}).$$

A set $A \subseteq \mathcal{S}$ is said to *generate* the convex set $\mathcal{S}$ if $\operatorname{conv}(A) = \mathcal{S}$, and similarly for convex cones.

Theorem 1.2 (Krein–Milman)**.** A compact convex subset of a finite-dimensional[a] vector space is equal to the convex hull of its extreme points:

$$\operatorname{conv}(\operatorname{ext} \mathcal{C}) = \mathcal{C}.$$

a This theorem can be stated for more general vector spaces. Since we consider only finite-dimensional vector spaces in this thesis, we don't include the general result here.

Theorem 1.3 (Duality of intersection and sum)**.** Let $\mathcal{C}_1$ and $\mathcal{C}_2$ be two convex cones. Then

$$(\mathcal{C}_1 \cap \mathcal{C}_2)^\circ = \operatorname{cl}(\mathcal{C}_1^\circ + \mathcal{C}_2^\circ).$$

Note that the closure in the previous result is necessary, even when the cones themselves are closed and finite-dimensional.

1.2 GRAPH THEORY

Notation	
$G = (V, E)$	Graph with vertex set V and edge set E
$\bar{G}$	Complement graph of G
A_G	Adjacency matrix of graph G
$\alpha(G)$, $\omega(G)$	Independence number and clique number of a graph G

In this thesis we restrict our focus to finite, undirected, simple graphs. A graph $G = (V, E)$ consists of a set of vertices V and a set of edges $E \subseteq \{\{i, j\} \mid i \neq j \in V\}$. A graph is *empty* if the edge set is empty, and *complete* if $|E| = \binom{|V|}{2}$, i.e., every pair of vertices is connected. The *complement graph* $\bar{G}$ shares the same vertex set V but contains exactly the edges not present in G. The structure of G is encoded in its *adjacency matrix* $A_G \in \mathcal{M}_{|V|}$, defined by $(A_G)_{ij} = 1$ if $\{i, j\} \in E$ and 0 otherwise.

For a graph $G = (V, E)$, the *induced subgraph* on a vertex set $\tilde{V} \subseteq V$ has edge set $\tilde{E} := \{\{i, j\} \in E \mid i, j \in \tilde{V}\}$. An *independent set* is a subset of vertices, no two of which are adjacent; the maximum size of such a set is the *independence number* $\alpha(G)$. Conversely,

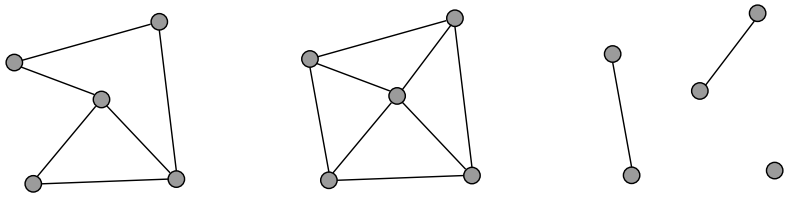


Figure 2: A graph G, its complement graph $\bar{G}$, complete graph K_d

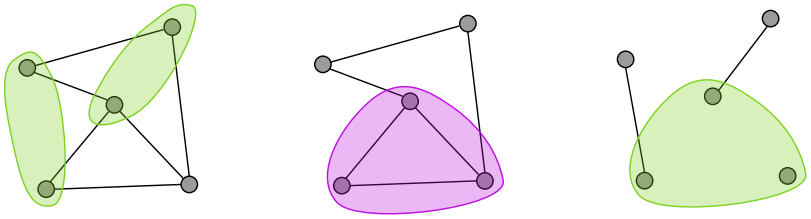


Figure 3: The largest independent set, the largest clique of the graph G, the largest clique is the largest independent set of the complementary graph.

a *clique* is a subset in which every pair of distinct vertices is adjacent, or equivalently, an induced subgraph that is complete. The maximum size of a clique is the *clique number* $\omega(G)$. It holds that $\omega(G) = \alpha(\bar{G})$. For general graphs $\alpha(G)$ is NP-hard to compute, and also NP-hard to approximate.

For $k \geq 3$, a *k-cycle* in a graph is a sequence of vertices $v_0, v_1, \ldots, v_{k-1}, v_k$ with $v_k = v_0$, the vertices $v_0, v_1, \ldots, v_{k-1}$ pairwise distinct, and $\{v_i, v_{i+1}\} \in E$ for every $0 \leq i < k$. A 3-cycle is called a *triangle*, and a graph containing no triangles is called *triangle-free*. A graph is *cyclic* if it contains a cycle and *acyclic* otherwise. A graph is *chordal* if every cycle of length at least 4 has a *chord*, that is, an edge connecting two non-consecutive vertices of the cycle. A graph containing no odd cycles is called *bipartite*; equivalently, its vertex set admits a bipartition such that every edge has one endpoint in each part.

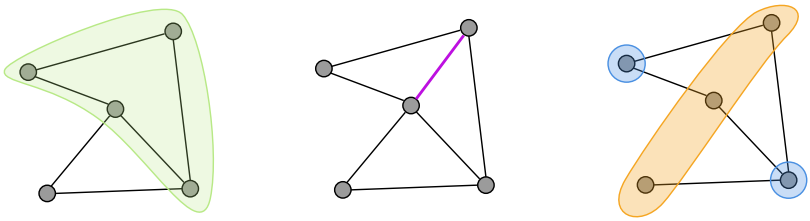


Figure 4: A cycle of a graph G, a chordal graph, and a bipartite graph.

It is a truth universally acknowledged, that a mathematical object whose orderings are non-negative must be in want of a representation as a sum of squares.

Bruce Reznick, inspired by Jane Austen

2

Positivity of Polynomials

The first chapter of the thesis deals with some well-known ideas in polynomial optimization and real algebraic geometry, focusing on positivity of polynomials and their representations as sum-of-squares.

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Notation	
$\mathbb{R}[x]$	Ring of real polynomials in variables $x_1 \dots x_d$
$\mathbb{C}[z, \overline{z}]$	Ring of complex polynomials in variables $z_1, \dots z_d$
$\mathbb{R}[x]_{n,d}$	Space of polynomials in variables $x_1 \dots x_d$ of degree n
$\mathbb{H}[x]_{n,d}$	Space of homogeneous polynomials in variables $x_1 \dots x_d$ of degree n
$\mathbb{C}[z, \overline{z}]_{n,m,d}$	Space of complex polynomials in variables $z_1 \dots z_d$ of degree n, m
$\mathbb{H}[z, \overline{z}]_{n,d}$	Space of bi-homogeneous polynomials in variables $z_1 \dots z_d$ of degree n
$\mathrm{Herm}[z, \overline{z}]_{n,d}$	Real linear space of Hermitian polynomials in variables $z_1 \dots z_d$ of degree n
$\deg(p)$	Degree of a polynomial p
$x^\alpha,\ \overline{z}^\alpha$	Monomial and conjugate monomial for $\alpha \in \mathbb{N}^d$

continued on next page

$P_{d,2n}$	Positive homogeneous polynomials in d variables, degree $2n$
$\Sigma_{d,2n}$	Sum of squares (SOS) polynomials in d variables, degree $2n$
$p^{\mathrm{Re}},\ p^{\mathrm{Im}}$	Real and imaginary parts of a complex polynomial p
c-SOS	Complex sum of squares: $p = \sum_k \lvert f_k\rvert^2$ for $f_k \in \mathbb{C}[z, \overline{z}]$
r-SOS	Sum of squares of Hermitian polynomials

2.1 POSITIVE POLYNOMIALS AND SUM OF SQUARES

In the first section, we focus on the link between positive polynomials and sum of squares; a classic problem that goes back to the work of Hilbert in the nineteenth century, in which he characterized the exact cases when a positive polynomial is a sum of squares [Hil88]. We also discuss the extensions of these notions to complex *Hermitian* polynomials.

Real Polynomials and Sum of Squares. A polynomial $p \in \mathbb{R}[x_1, \ldots, x_d]$ is said to be positive if it is non-negative for all $x \in \mathbb{R}^d$. Of course, a polynomial is positive if it is a sum of squares of other polynomials, that is, it has a decomposition of the following form.

$$p = \sum_{k=1}^{K} f_k^2$$

where $\forall k \in [K],\ f_k \in \mathbb{R}[x]$. Moreover, for any such decomposition, it holds that $\forall k \in [K]$, the degree of polynomials satisfies

$$\frac{\deg(f_k)}{2} \leq \deg(p).$$

Consider the linear space of all real homogeneous polynomials of degree n with d variables, sometimes called the d-ary n-artics, which we denote as $\mathbb{H}[x]_d^n$. We have the convex cone of positive homogenous polynomials,

$$P_{d,2n} := \{p \in \mathbb{H}[x]_d^{2n} \mid \forall x \in \mathbb{R}^d,\ p(x) \geq 0\}$$

and all homogenous polynomials that can be written as a sum of squares,

$$\Sigma_{d,2n} := \{p \in \mathbb{H}[x]_d^{2n} \mid \exists \{f_k\}_{k=1}^K \in \mathbb{H}[x]_d^n,\ p = \sum_{k=1}^{K} f_k^2\}.$$

Then, clearly, we have the inclusion between the convex cones.

$$\Sigma_{d,2n} \subseteq P_{d,2n}. \tag{1}$$

By a celebrated result of Hilbert [Hil88], the equality in Eq. (1) holds if and only if either $d = 2$, or $n = 1$, or $d = 3, n = 2$ [1]

	$2n = 2$	$2n = 4$	$2n \geq 6$
$d = 2$	Yes	Yes	Yes
$d = 3$	Yes	Yes	No
$d \geq 4$	Yes	No	No

Table 5: Can any homogeneous polynomial of degree $2n$ in d variables be represented as a sum of squares?

On the complexity side, it is known that the computational complexity of deciding whether a polynomial is globally non-negative is NP-hard, even in the case when $n = 4$. This follows from the NP-hard complexity of deciding copositivity [MK87], which we discuss in detail later in Section 3.2. In contrast, the sum of squares property can be recast as a semidefinite program, by utilizing the *Gram-Matrix* reformulation [PW98]; see also the notes by Laurent [Lau08, Section 3.3].

Theorem 2.1. A homogeneous polynomial $p \in \mathbb{H}[x]_d^{2n}$ of degree $2n$ is a sum of squares (SOS) if and only if there exists a PSD matrix, $P \in \mathrm{Sym}[\mathcal{M}_d(\mathbb{R})^{\otimes n}]$ such that

$$p(x) = \langle x^{\otimes n} | P | x^{\otimes n} \rangle .$$

Motzkin's Polynomial. Hilbert's approach to show existence of non-negative polynomials that are not sum of squares was non-constructive and did not yield explicit examples. The first explicit example of a positive polynomial that cannot be represented as a sum-of-squares occurred in the literature much later after Hilbert's results [Mot67]; the polynomial was constructed by Theodore Motzkin:

$$p_{\mathrm{mot}}(x, y) = x^2y^4 + x^4y^2 + 1 - 3x^2y^2.$$

This can be homogenized to the following form in 3 variables.

$$p_{\mathrm{mot}}(x, y, z) = x^2y^4 + x^4y^2 + z^6 - 3x^2y^2z^2.$$

1 Any non-homogenous polynomial $p \in \mathbb{R}[x]$ of degree n can be homogenized to $\tilde{p} \in \mathbb{H}[x, z]_{d+1,n}$ by adding an extra variable z, by the map $\tilde{p}(x, z) = z^{\deg(p)} p(\frac{x}{z})$. Moreover, this preserves the positivity and sum of squares property of the polynomial p. Therefore, by homogenization, Hilbert's result can be extended to non-homogenous polynomials as well.

The positivity of this polynomial is easy to check; it follows from the AM-GM [2] inequality applied to the first three terms.

$$\frac{x^2y^4 + x^4y^2 + z^6}{3} \geq (x^6y^6z^6)^{\frac{1}{3}} = x^2y^2z^2.$$

But this polynomial is not a sum of squares. For a simple proof, see [Lau08, Example 3.7]. There are a variety of examples of globally non-negative and non-SOS polynomials available in the literature [Rob73, Cho75b, CLR87, Har99, Bos07], but in general it is considered non-trivial to construct them. For a historical account of such constructions, see the review [Rez00, Section 4].

Hermitian Polynomials. Let $\mathbb{C}[z, \bar{z}]$ denote the ring of complex polynomials in variables z and the conjugate variables $\bar{z}$. We denote the *bi*-degree n *bi*-homogenous polynomials as the polynomials for which each monomial term has a degree n in z and a degree n in $\overline{z}$,

$$p(z) = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} c_{\alpha,\beta} z^\alpha \bar{z}^\beta$$

where $c_{\alpha,\beta} \in \mathbb{C}$. This is also equivalent to the following condition on the polynomial,

$$\forall z \in \mathbb{C}^d, \quad p(\lambda z) = |\lambda|^{2n} p(z).$$

Such a polynomial is called Hermitian when, $p = \bar{p}$; a Hermitian polynomial only outputs real values. A polynomial is Hermitian if and only if the coefficients satisfy the following conditions,

$$\forall \alpha, \beta \in \mathbb{N}_d^{(n)}, \quad c_{\alpha,\beta} = \overline{c_{\beta,\alpha}}.$$

A Hermitian polynomial is called *positive* if it is non-negative over the full complex plane. We define the following polynomials in $\mathbb{R}[x, y]_{2d,2n}$

$$p^{\text{Re}}(x, y) = \text{Re}(p(x + iy))$$

$$p^{\text{Im}}(x, y) = \text{Im}(p(x + iy))$$

Therefore any polynomial in $\mathbb{C}[z, \overline{z}]$ can be decomposed as

$$p = p^{\text{Re}}(x, y) + ip^{\text{Im}}(x, y).$$

For any Hermitian polynomial $p^{\text{Im}}(x, y) = 0$ and for any positive polynomial $p^{\text{Re}}(x, y)$ is positive.

2 In fact, the example was discovered by Motzkin when he inquired if the AM-GM inequality could be written as a sum of squares, which is true for the case of two variables, $a^2 + b^2 - 2ab = (a - b)^2 \geq 0$.

Complex SOS. The complex SOS (or c-SOS for short) polynomials are those Hermitian polynomials that can be expressed as a sum of absolute squares of complex polynomials (which may not be Hermitian).

$$p = \sum_{k=1}^{K} |f_k|^2$$

Real SOS. A Hermitian polynomial is called real-SOS (or r-SOS for short) if it is a sum of squares of other Hermitian polynomials, i.e.,

$$p = \sum_{k=1}^{K} f_k^2$$

where $\forall k \in [K]$, f_k is a Hermitian polynomial. Clearly, a polynomial being r-SOS implies that it is c-SOS, but the reverse implication is false.

Example 2.2. A bi-degree 1 homogenous polynomial is of the form

$$p(z) = \sum_{i,j} c_{ij} \bar{z}_i z_j = \langle z|C|z\rangle \geq 0 \iff C \succeq 0.$$

By the spectral theorem $p(z)$ is c-SOS; we can expand $C = \sum_{k=1}^{K} |\psi_k\rangle\langle\psi_k|$ and we obtain

$$\langle z| \sum_{k=1}^{K} |\psi_k\rangle\langle\psi_k| \, |z\rangle = \sum_{k=1}^{K} |\langle\psi_k|z\rangle|^2.$$

But also note that each square can be written as squares of Hermitian polynomials.

$$|\langle\psi|z\rangle|^2 = \frac{1}{4}(\langle\psi|z\rangle + \langle z|\psi\rangle)^2 + \left(\frac{\langle\psi|z\rangle - \langle z|\psi\rangle}{2i}\right)^2.$$

This implies that it is also r-SOS.

Moreover, the real SOS condition exactly corresponds to the real polynomial p^{Re} being sum of squares.

Theorem 2.3. p is an r-SOS polynomial if and only if p^{Re} is SOS.

Proof. Let p be an r-SOS polynomial, hence it has a decomposition $p = \sum_k f_k^2$ where f_k are Hermitian. Moreover, this implies that $f_k^2(x + iy) = (f_k^{\mathrm{Re}}(x, y))^2$ that shows that

$p^{\mathrm{Re}} = \sum_k (f_k^{\mathrm{Re}})^2$. For the reverse direction, assume that $p^{\mathrm{Re}}(x,y) = \sum_k f_k^2(x,y)$. Consider the following Hermitian polynomials, $\forall k, z \in \mathbb{C}^d$, $p_k(z) = f_k(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2i})$. This shows that $p(z) = p^{\mathrm{Re}}(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2i}) = \sum_k f_k^2(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2i})$ is r-SOS. ■

The real sum of squares property is also intimately connected to the decomposability of positive linear maps, which we discuss next. Let us finish section with the following question.

> **Question 2.4.** What is the analog of Hilbert's theorem for Hermitian polynomials?

Positive and Decomposable Maps. Consider a Hermitian linear map between the matrix algebras, $\Phi : \mathcal{M}_d \to \mathcal{M}_{d'}$. Such a map is called positive if it maps PSD matrices to PSD matrices. We can define the k-ampliation of the map Φ as $\Phi \otimes I_k : \mathcal{M}_d \otimes \mathcal{M}_k \to \mathcal{M}_{d'} \otimes \mathcal{M}_k$. If all the ampliations of a positive map are positive, it is called completely positive. The transposition map $T : \mathcal{M}_d \to \mathcal{M}_d$ defined as

$$(\rho^T)_{ij} := \rho_{ji}$$

is the celebrated example of the map that is positive but *not* completely positive [HHH96, Per96]. The positivity of this map can be inferred from the fact that it preserves the spectrum, while for any non-product vector $|\varphi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$,

$$(T \otimes I_2)(|\varphi\rangle\langle\varphi|) \ngeq 0$$

shows that it is not completely positive. A linear map Φ is called *decomposable* if it is a sum of a completely positive and completely co-positive map.

$$\Phi = \Phi_1 + T \circ \Phi_2$$

where Φ_1, Φ_2 are *completely positive*.
Reduction. The reduction map [CAG97] $\Phi_r : \mathcal{M}_d \to \mathcal{M}_d$, defined as

$$\Phi_r(X) = \mathrm{Tr}(X)\mathbb{I}_d - X$$

is another positive not completely positive map, but is actually decomposable.

We can associate a *biquadratic* bihomogenous (degree $(1,1)$ in both $x, \bar{x}$ and $y, \bar{y}$ [3]) Hermitian polynomial to each such map,

$$p_\Phi(x,y) := \langle y|\Phi(|x\rangle\langle x|)|y\rangle\,.$$

3 Note that this is a special class of *bidegree* 2 Hermitian polynomials.

It is known that this map is positive if and only if this polynomial is positive [Cho75b].

Proposition 2.5 ([Faw21]). The decomposability of the map is characterized in terms of the *real* sum of squares property of the polynomial

$$\Phi \text{ is decomposable} \iff p_\Phi \text{ is r-SOS}$$

A decomposable map is positive, but the converse is not true in general. Surprisingly, only for linear maps from $\mathcal{M}_2 \to \mathcal{M}_2$ and from $\mathcal{M}_2 \to \mathcal{M}_3$, positivity ensures decomposability [Wor76]; in other words all corresponding polynomials are *real*-SOS.

Remark 2.6. In contrast to the complex case, a positive map $\Phi : \mathcal{M}_2(\mathbb{R}) \to \mathcal{M}_n(\mathbb{R})$ are sums of *congruence* maps, i.e, of the form $V^T X V$ [Cho75b, Cal73] which is equivalent to the corresponding real polynomial being SOS. For the analogous theory about positive maps on real matrices, see [J+21, Chapter 3.B].

Choi Polynomial. Choi provided the first example of a bi-quadratic *real* polynomial in $3+3$ variables which is not a sum of squares.

Theorem 2.7 ([Cho75b, CL77]). The following *real* biquadratic polynomial in $x, y \in \mathbb{R}^3$,

$$\begin{aligned} p(x,y) = x_1^2y_1^2 + x_2^2y_2^2 + x_3^2y_3^2 - 2x_1x_2y_1y_2 - 2x_2x_3y_2y_3 - 2x_3x_1y_3y_1 \\ + \mu x_1^2y_2^2 + \mu x_2^2y_3^2 + \mu x_3^2y_1^2 \end{aligned}$$

is positive for all $\mu \geq 1$ but *not* a sum of squares [CL77].

Later, he showed that this can be extended to show that the following map $\Phi : \mathcal{M}_3 \to \mathcal{M}_3$ is not decomposable [Cho80a, Appendix B], constructing the first example of a positive non-decomposable map.

$$\Phi \begin{pmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} X_{11} & -X_{12} & -X_{13} \\ -X_{21} & X_{22} & -X_{23} \\ -X_{31} & -X_{32} & X_{33} \end{pmatrix} + \mu \begin{pmatrix} X_{33} & 0 & 0 \\ 0 & X_{11} & 0 \\ 0 & 0 & X_{22} \end{pmatrix},$$

with $\mu \geq 1$ is positive but not decomposable.

Fejér-Riesz Theorem. A complex Laurent polynomial is of the form

$$p(z) = \sum_{k=-N}^{N} \lambda_k z^k$$

where $\lambda_k \in \mathbb{R}$. For such polynomials that are positive on the torus, $\mathbb{T}$, there exists a well known characterization as a square of another Laurent polynomial; this result is popularly known as the Fejér-Riesz theorem [Fej16, Rie16].

Theorem 2.8 ([Fej16, Rie16], Fejér-Riesz theorem)**.** Let $p(z) = \sum_{k=-N}^{N} \lambda_k z^k$ be a Laurent polynomial with real coefficients λ_k such that $p(z) \geq 0$ for all $z \in \mathbb{T}$. Then there exists a polynomial $q(z) = \sum_{k=0}^{N} b_k z^k$ such that

$$p(z) = |q(z)|^2$$

More details and generalizations of this result can be found in the review [HZ21] and the references therein.

2.2 POSITIVSTELLANSÄTZE

The sum of squares polynomial are a strict subset of positive polynomials. But can positive polynomials always be represented as a sum of squares of *rational* polynomials? This question was posed by Hilbert in 1900 at the International Congress of Mathematicians in Paris and listed in his list of problems. This was later affirmatively answered by Artin [Art27].

There have been a plethora of improvements of Artin's result, in form of representation results of positive polynomials that are positive on arbitrary semi-algebraic sets [Sch17, Put93], called Positivstellansätze. In this section, we focus primarily on the particular improvements by Pólya [Pól11] and Reznick [Rez95] to the positivity of polynomials on $\mathbb{R}^d$, the original question considered by Hilbert. For a more thorough introduction, we recommend the excellent notes by Reznick on this topic [Rez00]. Finally, we also discuss some results on positivity of complex Hermitian polynomials [Qui68, MHNR23].

Hilbert's 17th problem. Hilbert's 17th problem poses whether a positive polynomial instead has a decomposition as a sum of squares of *rational* functions. The modern rephrasing of this problem asks whether for any positive semidefinite polynomial $p \in P_{d,n}$ there exists a polynomial $0 \neq q \in \mathbb{H}[x]_d^m$ such that

$$p \cdot q^2 \in \Sigma_{d,n+2m}. \tag{2}$$

Note that if such a q exists, it also provides a certificate of the non-negativity of the polynomial p. This was answered in the affirmative by Artin [Art27]. Relatively recently, the quantitative version of the Artin's result was shown [LPR20]; for every d, n there exists a finite $l = l(d, n)$ such that there exists a $q \in \mathbb{H}[x]_d^l$ in Eq. (2) [4].

Pólya's Positivstellansatz. Although Artin's result solves Hilbert's question, it does not concretely specify the explicit form of the polynomial q. Pólya showed the following result about positive polynomials on $\mathbb{R}_+^d$.

Theorem 2.9. Let $p \in \mathbb{R}[x]$ be such that $\forall x \in \mathbb{R}_+^d \backslash \{0\}$, $p(x) > 0$. Then, there exists an $r \in \mathbb{N}$ such that the following polynomial

$$p(x) \cdot (\sum_{i=1}^{d} x_i)^r$$

has positive coefficients.

This theorem can also be made quantitative, by giving bounds on r for which the coefficients are non-negative [PR01].

Remark 2.10. The condition of p being strictly positive cannot be removed completely as there exist positive polynomials with non-trivial zeros (i.e. they are not strictly positive) such that $p \cdot (\sum_{i=1}^{d} x_i)^r$ does not have positive coefficients for any r. Later works also considered Pólya's Theorem for polynomials with finitely many zeros, and show that Polya's certificate works for such polynomials [CPR09, MT08].

Reznick's Positivstellansätze. Let $p \in \mathbb{R}[x]$ and $\tilde{p}(x) := p(x \odot x)$. Then, $\tilde{p}(x) > 0$ for all $x \in \mathbb{R}^d \backslash \{0\}$ if and only if $p(x) > 0$ for all $x \in \mathbb{R}_+^d \backslash \{0\}$. Then the Theorem 2.9 says that $\tilde{p}(x)(\sum_i x_i^2)^r$ has positive coefficients for sufficiently large r, and hence, in effect is also a *sum of squares*.

Reznick generalized this implication of Polya's result to all *strictly* positive polynomials. This is sometimes known as the theorem of *uniform denominators*.

4 The bound on l is a tower of 5 exponentials [LPR20]!

Theorem 2.11 ([Rez95]). Let $p \in \mathbb{R}[x]$ be such that $\forall x \in \mathbb{R}^d \backslash \{0\}$, $p(x) > 0$. Then, there exists an $r \in \mathbb{N}$ such that the following polynomial

$$p(x) \cdot (\sum_{i=1}^{d} x_i^2)^r$$

is a sum of squares.

Surprisingly, the strict positivity condition can be removed for $n = 3$ [Sch06]. The Motzkin polynomial $p_{\text{mot}}(x, y, z)(x^2 + y^2 + z^2)$ is a sum of squares [5], but it does not satisfy the hypothesis in Reznick's result since it has a non-trivial zero, $p(1, 1, 1) = 0$. In general, the strict positivity cannot be removed, as there exist positive polynomials that are not SOS for any r [VL23].

Refinements for the complex case. We finally consider the case of positive Hermitian polynomials, and the related refinements of Reznick's Positivstellansätze to the complex case [Qui68, TY06, MHNR23].

Theorem 2.12 ([Qui68, TY06, MHNR23]). Let $p \in \text{Herm}[z, \bar{z}]_d^n$ be such that $\forall z \in \mathbb{C}^d \backslash \{0\}$, $p(z) > 0$. Then, there exists an r such that the Hermitian polynomial

$$p(z) \cdot (\sum_{i=1}^{d} |z_i|^2)^r$$

is *complex* sum of squares. In fact, it is a sum of absolute squares of holomorphic functions.

The bounds for r were obtained in [MHNR23]. The r-SOS version of this theorem follows from the result in Theorem 2.11.

5 The exact sum of squares decomposition is

$$\begin{aligned}(x^2+y^2+z^2)\, p_{\text{mot}}(x,y,z) = {} & \tfrac{1}{4}\Big(xy(x^2-y^2)\Big)^2 + \tfrac{3}{4}\Big(xy(x^2+y^2-2z^2)\Big)^2 \\ & + (z^4 - x^2y^2)^2 + \Big(yz(x^2-z^2)\Big)^2 + \Big(xz(y^2-z^2)\Big)^2\end{aligned}$$

Corollary 2.13. Let $p \in \mathrm{Herm}[z, \bar{z}]_d^n$ be such that $\forall z \in \mathbb{C}^d \backslash \{0\}$, $p(z) > 0$. Then, there exists an r such that the Hermitian polynomial

$$p(z) \cdot (\sum_{i=1}^{d} |z_i|^2)^r$$

is *real* sum of squares.

Proof. Note that $p(x + iy) = p^{\mathrm{Re}}(x, y)$ and $\forall x, y \in \mathbb{R}^d \backslash \{0\}, p^{\mathrm{Re}}(x, y) > 0$. Then, by Theorem 2.11, it follows that the real polynomial

$$p^{\mathrm{Re}}(x, y) \cdot (\sum_{i=1}^{d} x_i^2 + \sum_{i=1}^{d} y_i^2)^r$$

is sum of squares for some $r \in \mathbb{N}$. Since this is the real part of the polynomial $p(z) \cdot (\sum_{i=1}^{d} |z_i|^2)^r$, this shows that the complex polynomial is r-SOS. ∎

We [he and Halmos] share a philosophy about linear algebra: we think basis-free, we write basis-free, but when the chips are down we close the office door and compute with matrices like fury.

Irving Kaplansky

3

Positivity of Matrices

The second chapter deals with positive properties of matrices and the corresponding convex cones. We begin with the discussion of positive semidefinite (PSD) matrices, and some constrained positive semidefinite matrices; with the analysis of their structures and applications to various fields. Later on, we provide a brief introduction to copositive and completely positive matrices.

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3.2 Completely Positive and Copositive Matrices 40

Notation	
PSD_d	Cone of $d \times d$ PSD matrices
CP_d	Completely positive matrices
NN_d	Non-negative matrices
DNN_d	Doubly nonnegative matrices: $\mathrm{PSD}_d \cap \mathrm{NN}_d$
Cop_d	Copositive matrices: $v^T M v \geq 0$ for all $v \geq 0$
SPN_d	Dual cone to DNN_d: $\mathrm{PSD}_d + \mathrm{NN}_d$
$\vartheta(G)$	Lovász theta number of a graph G
$\mathcal{E}_d$	The complex elliptope
$\mathcal{L}_d$	The real elliptope
$\mathcal{M}[H]$	Matrices with sparsity pattern given by a graph H
Δ	Standard simplex: $\{x \in \mathbb{R}^+_d \mid \sum_{i\in[d]} x_i = 1\}$

continued on next page

$\mathrm{R}_1[\mathcal{C}]$	Rank-one-generated part of a cone: $\mathrm{cone}\{\|v\rangle\langle v\| \in \mathcal{C}\}$
$\mathcal{M}_d^+[H]$	Sparse PSD matrices with sparsity pattern given by graph H
$\mathcal{K}_d^{(r)}$	Parrilo's r-th SOS hierarchy approximation of Cop_d
$\theta^{(r)}(G)$	r-th hierarchy approximation of the independence number $\alpha(G)$
$\mathcal{C}^{\odot}$	Schur (entry-wise) dual of a cone $\mathcal{C}$
$\mathrm{Sym}[\mathcal{M}_d(\mathbb{R}]$	Symmetric matrices in $\mathcal{M}_d(\mathbb{R}$

3.1 CONSTRAINED POSITIVE SEMIDEFINITE MATRICES

The positive semidefinite (PSD) cone is generated by its extremal rays that are rank-1 matrices, but the same is not true for its convex subsets. For any matrix cone $\mathcal{C} \subseteq \mathcal{M}_d^+$, we define

$$\mathrm{R}_1[\mathcal{C}] = \mathrm{cone}\{|v\rangle\langle v| \in \mathcal{C}\}.$$

Such a cone is *rank-one-generated* or ROG if

$$\mathrm{R}_1[\mathcal{C}] = \mathcal{C}.$$

For finite dimensional proper convex cones, this is equivalent to demanding that the extremal rays are rank 1. Deciding if a convex cone satisfies this property is a complex problem. We begin this section by presenting some general results about the ROG property when the positive semidefinite cone with at most 2 linear constraints is rank-1 generated. Later on, we discuss some of the popularly known examples of convex cones that are not rank-1 generated, complex correlation matrices, and sparse positive semidefinite matrices.

General results about ROG property. Firstly, we consider some general results about the rank-one-generated property for PSD cones with constraints, at-least in the case of real symmetric matrices. The more comprehensive analysis of this topic is available in [AKKW23, Hil16, KKW21]. Let $\mathcal{L} = \{Y_i \mid Y_i \in \mathrm{Sym}[\mathcal{M}_d(\mathbb{R})]\}_{i=1}^N$ be a collection of self-adjoint matrices. We define the constrained PSD set.

$$\mathcal{M}_d^+(\mathcal{L}) := \{X \in \mathcal{M}_d^+(\mathbb{R}) \mid \forall Y \in \mathcal{L},\, \mathrm{Tr}(XY) \geq 0\}.$$

Firstly, it was shown that for only 1 constraint, the rank-1 generated property of positive semidefinite matrices is retained [AKKW23].

Lemma 3.1 ([AKKW23]). Let $\mathcal{L} = \{Y\}$. Then, the constrained PSD convex cone $\mathcal{M}_d(\mathcal{L})$ is rank-1 generated.

For two constraints, a characterization of the rank-1 generated property was obtained [AKKW23].

Theorem 3.2 ([AKKW23]). Let $\mathcal{L} = \{Y_1, Y_2\}$. Then, the constrained PSD convex cone $\mathcal{M}_d(\mathcal{L})$ is rank-1 generated if and only if there exist either

- $(\alpha_1, \alpha_2) \neq 0$ such that $\alpha_1 Y_1 + \alpha_2 Y_2 \succeq 0$.
- $|a\rangle, |b\rangle, |c\rangle \in \mathbb{R}^d$ such that $Y_1 = |a\rangle\langle c| + |c\rangle\langle a|$ and $Y_2 = |b\rangle\langle c| + |c\rangle\langle b|$

Next, we present two famous examples of convex cones obtained by linearly constraining the positive semidefinite matrices $\mathcal{M}_d^+$. These are the convex cones of complex correlation matrices, and the sparse PSD matrices.

Complex Elliptope

Consider the linear space of matrices with equal diagonal entries.

$$\mathcal{E}_d := \{X \in \mathrm{Herm}[\mathcal{M}_d] \mid \forall i \in [d],\ X_{ii} = X_{11}\}$$

The *elliptope* (also called the correlation matrices) is the convex cone of PSD matrices with diagonal entries equal.

$$\mathcal{E}_d^+ := \mathrm{PSD}_d \cap \mathcal{E}_d.$$

Let $|x\rangle\langle x|$ be a general rank-1 matrix in the elliptope. This is equivalent to the condition that the diagonal entries $|x_i|^2$ are equal to 1, or $x \in \mathbb{T}^d$. Therefore, it follows that

$$\mathrm{R}_1[\mathcal{E}_d^+] = \mathrm{cone}\{|x\rangle\langle x| \mid |x\rangle \in \mathbb{T}^d\}.$$

The possible ranks of the extremal rays of the *elliptope* have been fully characterized [LT94], which is the content of the next theorem.

Theorem 3.3. (Ranks of extremal rays of complex elliptope [LT94]) The ranks of the extremal rays of the complex elliptope satisfy $r^2 \leq d$. For each r satisfying this condition, there exists a matrix $X \in \mathrm{ext}\, \mathcal{E}_d^+$ such that $\mathrm{rank}\, X = r$.

This result implies that the convex cone is rank-1 generated if and only if $d \leq 3$.

Theorem 3.4 (Algorithm, [LT94])**.** The following algorithm verifies if the correlation matrix $A \in \mathrm{Herm}[\mathcal{M}_d]$ is extremal.

1. Compute the rank of A and decompose the matrix into XX^* where $X \in \mathcal{M}_{d\times k}$.
2. Form a matrix Y consisting of the unique (upto unit multiples) rows of X. Consider $Y \in \mathcal{M}_{p\times k}$ where $p \leq d$. If $r^2 > p$, A is not extremal.
3. Compute $\dim(\mathrm{span}\{|y_j\rangle\langle y_j| \mid 1 \leq j \leq p\})$ where $|y_j\rangle$ is a row of Y. If it is r^2, the matrix is extreme.

The elliptope in the *real* case has been well studied as a relaxation of the max-cut problem on graphs [LP95].

$$\mathcal{L}_d := \{X \in \mathrm{Sym}[\mathcal{M}_d(\mathbb{R})] \mid \forall i \in [d],\ X_{ii} = X_{11}\}.$$

$$\mathrm{R}_1[\mathcal{L}_d] = \mathrm{cone}\{|x\rangle\langle x| \mid |x\rangle \in \{-1,1\}^d\}.$$

Let us briefly state the max-cut problem. Given a graph G, we want to partition the vertices V into two sets $V\backslash S$ and S such that the number of edges between them is maximum possible for all such partitions. This can be recast as the optimization problem.

$$\begin{aligned}\mathrm{maxcut}(G) = \max \quad & \frac{1}{2}\sum_{ij}(A_G)_{ij}(1 - x_i x_j) \\ & \text{such that } x_i \in \{-1,1\}.\end{aligned}$$

Note that $\sum_{i,j\in[d]}(A_G)_{ij}x_i x_j = \mathrm{Tr}(A_G\,|x\rangle\langle x|)$. Then, we can obtain a relaxation of the max-cut problem by replacing $|x\rangle \in \{-1,1\}^d$ by the *elliptope*.

$$\mathrm{maxcut}(G) \leq \sum_{ij} A_{ij} - \min \quad \frac{1}{2}\mathrm{Tr}(A_G \cdot X) \text{ such that } X \in \mathcal{L}_d.$$

This relaxes the max-cut, which is known to be NP-complete into a semidefinite program that can be solved efficiently. Similar techniques provide the best approximation algorithms for the max-cut problem in the case of weighted graphs [GW95]. For more results about the geometry of the elliptope and its dual, see [LP95].

Sparse PSD matrices

Recall that the graph of a matrix $G(X)$ is a graph on d vertices such that (i,j) is an edge if $X_{ij}X_{ji} > 0$. We define the following linear space of self-adjoint matrices whose sparsity pattern is described by subgraphs of a d-vertex graph H.

$$\mathcal{M}_d[H] := \{X \in \mathrm{Herm}[\mathcal{M}_d] \mid G(X) \subseteq H\}.$$

Consider the convex cone of H-sparse PSD matrices.

$$\mathcal{M}_d^+[H] := \mathcal{M}_d[H] \cap \mathrm{PSD}_d.$$

Theorem 3.5 ([PPS89]). The convex cone $\mathcal{M}_d^+[H]$ is rank-1 generated if and only if H is a *chordal* graph.

The sparse PSD matrices have a dual connection to the PSD completion problem. Consider an *incomplete* matrix $X \in \mathcal{M}_d$, i.e., only some of its entries are specified. Is there a completion of this matrix to a PSD matrix? A trivial necessary condition for such a matrix to exist is that all the *specified* principal sub-matrices have to be PSD. The PSD completion problem asks when this condition is also sufficient. The seminal result for this was obtained by [GJSW84], who showed that such a completion always exists if the graph corresponding to the specified entries is chordal.

To state the duality, we need to define the H-minor PSD matrices. Recall that $\mathrm{cliq}(H)$ denotes the set of cliques of the graph H, defined on the vertex set $[d]$, and for a matrix $X \in \mathcal{M}_d$, $X[I]$ denotes the principal $|I| \times |I|$ sub-matrix corresponding to the indices $I \subseteq [d]$. Consider the convex cone.

$$\mathcal{M}_d^{\boxplus}[H] := \{X \in \mathrm{Herm}[\mathcal{M}_d] \mid \forall I \in \mathrm{cliq}[H],\ X[I] \succeq 0\}.$$

Then, $X \in \mathcal{M}_d^{\boxplus}[H]$ will be called *completable* if there exists a matrix $Y \in \mathcal{M}_d^+$ such that $\forall I \in \mathrm{cliq}[H], Y[I] = X[I]$ denoted as $\mathcal{M}_d^{\mathrm{com}}[H]$. Note that the results in [GJSW84] imply that all matrices in $\mathcal{M}_d^{\boxplus}[H]$ are completable if the graph is chordal. Let us finally present the duality for the sparse PSD matrices [PPS89].

Theorem 3.6 (Rephrased from [PPS89]). Define the Schur-Dual cone

$$\mathcal{C}^{\odot} := \{Q \in \mathrm{Herm}[\mathcal{M}_d] \mid \forall Z \in \mathcal{C},\ Q \odot Z \succeq 0\}.$$

- $\mathrm{R}_1[\mathcal{M}_d^+[H]] = (\mathcal{M}_d^{\boxplus}[H])^{\odot}$

- $\mathcal{M}_d^+[H] = (\mathcal{M}_d^{\text{com}}[H])^\odot$

The maximum rank of the extremal element in $\mathcal{M}_d^+[H]$ is the called the order of the graph, and is not completely resolved for all graphs. We list the few examples of known orders for graphs, along with the references in Table 7.

Graph	Order	Reference
Chordal	1	[GJSW84, PPS89]
Complete Bipartite $K_{m,n}$	$\min(n, m^2 - m + 1)$	[GP90]
Cyclic C_n	$n - 2$	[AHMR88]

Table 7: Orders for various graphs

3.2 COMPLETELY POSITIVE AND COPOSITIVE MATRICES

This section will briefly introduce the notion of complete positive matrices, and its conic dual of copositive matrices. These concepts were first introduced by Diananda [Dia62], Hall-Neumann [HJN63], and can be traced to some possibly unpublished contributions from Motzkin [Shi21]. These matrices arise in different areas of mathematics, for example, block designs in combinatorial analysis and economic modelling. In recent years, these matrix cones have been abstractly studied in matrix analysis, and in optimization, since they provide a means to reformulate certain non-convex quadratic problems to copositive programs. We discuss some of the important results in this field from both perspectives; matrix analysis and combinatorial optimization.

Completely Positive Matrices. A matrix $X \in \text{Herm}[\mathcal{M}_d(\mathbb{R})]$ is completely positive [MM62, HJN63] if there is a *entrywise* non-negative matrix $C \in \mathcal{M}_{r\times d}(\mathbb{R}_+)$ such that X can be factored as

$$X = C^T C.$$

The minimum r such that such a factorization exists is called the CP-rank of the matrix. We denote the convex cone of completely positive matrices as CP_d. The extremal rays of completely positive matrices are rank-1 projectors with non-negative entries [HJN63].

$$\text{ext CP}_d = \{|v\rangle\langle v| \mid |v\rangle \in \mathbb{R}_+^d\}.$$

The membership problem in the completely positive matrices is NP-HARD [DG14].

Doubly Non-Negative Matrices. Note that the completely positive matrices are clearly non-negative and positive semidefinite. A matrix that is both positive semidefinite and has non-negative entries is called doubly non-negative.

$$\mathrm{DNN}_d := \mathrm{PSD}_d \cap \mathrm{NN}_d.$$

This is a relaxation of the completely positive matrices.

$$\mathrm{CP}_d \subseteq \mathrm{DNN}_d.$$

The equality holds if and only if $d \leq 4$ [MM62, HJN63]. Moreover, it is known that doubly non-negative matrices of rank 2 are completely positive [SMB21, Theorem 3.5]. For any matrix $X \in \mathcal{M}_d$, consider the comparison matrix,

$$M(X)_{ij} = \begin{cases} X_{ij} & \text{if } i = j \\ -|X_{ij}| & \text{if } i \neq j \end{cases}$$

This allows a non-trivial but efficient to check condition for the membership into CP matrices [SMB21, Theorem 3.5].

Theorem 3.7 (Comparison Matrix)**.** Let $X \in \mathrm{DNN}_d$. Then we have the following implication.

$$M(X) \succeq 0 \implies X \in \mathrm{CP}_d.$$

The converse of this theorem is not true, for example, the all-ones matrix $\mathbb{J}_d = \sum_{i,j\in[d]} |i\rangle\langle j|$ is completely positive, but $M(\mathbb{J}_d) \not\succeq 0$.

Extremal DNN Matrices. Recall that the doubly non-negative matrices are positive semidefinite and entrywise non-negative matrices (Section 3.2).

$$\mathrm{DNN}_d := \mathrm{PSD}_d \cap \mathrm{NN}_d\,.$$

The rank-1 generated version of this cone is exactly the set of completely positive matrices.

$$\mathrm{R}_1[\mathrm{DNN}_d] = \mathrm{CP}_d\,.$$

The possible ranks and constructions of the extremal DNN matrices has been researched in [HJL96], and we rephrase some of their results. It was shown that the ranks of the extremal matrices have some restrictions, which the next result quantifies.

Theorem 3.8 ([HJL96]). There exists an extremal DNN matrix with rank k if and only if $k \neq 2$ and

$$\begin{cases} k \leq n-2 & \text{if } n \text{ is even} \\ k \leq n-3 & \text{if } n \text{ is odd} \end{cases}$$

In [HJL96], the authors also provide an algorithm to verify if a given matrix is extremal in the doubly non-negative matrices.

Theorem 3.9 (Algorithm for extremal DNN rays, [HJL96]). The following algorithm verifies if the doubly non-negative matrix $A \in \mathrm{Sym}(\mathcal{M}_d(\mathbb{R}))$ is extremal.

1. Compute the rank of A and decompose the matrix into $X^T X$ where $X \in \mathcal{M}_{k \times d}$.
2. Compute the $d_{\text{span}} = \dim = \mathrm{span}\{X^T(|i\rangle\langle j| + |j\rangle\langle i|)X \mid i \leq j, A_{ij} = 0\}$.
3. $d_{\text{span}} = \frac{k(k+1)}{2} - 1 \implies A \in \mathrm{ext}\,\mathrm{DNN}_d$.

Graph-theoretic results. Let X be a matrix in $\mathcal{M}_d$. The graph of a matrix $G(X)$ is a graph on d vertices such that (i, j) is an edge if $X_{ij}X_{ji} > 0$. A graph is triangle-free if it contains no triangles. Then, for matrices that are triangle free, the positivity of the comparison matrix fully characterizes the complete positivity.

Theorem 3.10 (Triangle free matrices, [DJL94]). Let $X \in \mathrm{DNN}_d$ such that $G(X)$ is Δ-free. Then we have the following equivalence.

$$X \in \mathrm{CP}_d \iff M(X) \succeq 0.$$

A graph H is called completely positive if for all doubly non-negative matrices X such that $G(X) = H$ are completely positive [BH87]. The next result characterizes the completely positive graphs.

Theorem 3.11 (Long odd cycles, [BH87]). A graph G is completely positive if and only if it does not contain cycles of size ≥ 5.

For $d \leq 4$, any $G(X)$ does not have cycles of length ≥ 5 for any X, hence showing the equality of the completely positive and doubly non-negative cones.

Copositive Matrices. By conic duality, define the set of copositive matrices, $\mathrm{Cop}_d := (\mathrm{CP}_d)^\circ$. Since the extreme rays of completely positive matrices are rank 1 non-negative vectors, it follows that

$$\mathrm{Cop}_d = \{X \in \mathrm{Sym}[\mathcal{M}_d(\mathbb{R})] \mid \forall\, |v\rangle \in \mathbb{R}^d_+,\ \langle v|X|v\rangle \geq 0\}.$$

Note that the matrix polynomial is defined as

$$p_X(x) := \langle x|X|x\rangle = \sum_{i,j\in[d]} X_{ij}x_ix_j.$$

This provides a bijection between the symmetric matrices and homogenous polynomials of degree 2.

$$\mathrm{Sym}[\mathcal{M}_d(\mathbb{R})] \cong \mathbb{H}[x]_{2,d}.$$

The copositive property of a matrix X can be described by the positivity of the polynomial for all $x \in \mathbb{R}^+_d$ or equivalently,

$$\forall x \in \mathbb{R}^d,\ p_X(x \odot x) \geq 0.$$

Any matrix that is PSD or non-negative is clearly copositive. Moreover, the same is true of the sum of any PSD and non-negative matrix. This defines the convex cone of SPN [1],

$$\mathrm{SPN}_d := \mathrm{PSD}_d + \mathrm{NN}_d$$

Moreover, we have the following duality,

$$\mathrm{DNN}_d = (\mathrm{SPN}_d)^\circ.$$

Also, this cone has a description in terms of the sum of square polynomials.

$$X \in \mathrm{SPN}_d \iff \forall x \in \mathbb{R}^d,\ p_X(x \odot x) \in \Sigma_{d,4}.$$

A matrix that is copositive but not SPN is called *exceptional*. For $d \leq 4$, $\mathrm{SPN}_d = \mathrm{Cop}_d$ [Dia62] and the extremal rays of copositive matrices are just the extremal rays of PSD matrices and non-negative symmetric matrices

$$\mathrm{ext}\,\mathrm{Cop}_d = \mathrm{ext}\,\mathrm{SPN}_d = \{|v\rangle\langle v| \mid |v\rangle \in \mathbb{R}^d\} \cup \mathbb{R}_+\{|i\rangle\langle j| + |j\rangle\langle i|\}$$

1 The acronym SPN stands for the sum of Positive and Non-Negative matrices

The first example of any exceptional copositive matrix was the *Horn's* matrix in COP_5 [HJN63], that is also extremal in the copositive cone.

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

$\mathbf{COP}_5$. The first non-trivial case occurs when $d = 5$. The complete description of extremal rays in this case was obtained by Hildebrand [Hil12]. Firstly, note that that the convex cone of both completely positive matrices and copositive matrices are invariant under permutations and scalings, i.e for X copositive, $P_\pi X P_{\pi^{-1}}$ is copositive, and DXD is copositive for $D = \mathrm{diag}(d)$ where $d \geq 0$. This is also true for the extremal rays. Therefore, any matrix in the orbit (generated by permutations and scaling) of the Horn's matrix is extremal. Consider the following matrix parametrized by $\theta \in [0, 2\pi]^5$ introduced in [Hil12].

$$T(\theta) = \begin{pmatrix} 1 & -\cos\theta_4 & \cos(\theta_4+\theta_5) & \cos(\theta_2+\theta_3) & -\cos\theta_3 \\ -\cos\theta_4 & 1 & -\cos\theta_5 & \cos(\theta_5+\theta_1) & \cos(\theta_3+\theta_4) \\ \cos(\theta_4+\theta_5) & -\cos\theta_5 & 1 & -\cos\theta_1 & \cos(\theta_1+\theta_2) \\ \cos(\theta_2+\theta_3) & \cos(\theta_5+\theta_1) & -\cos\theta_1 & 1 & -\cos\theta_2 \\ -\cos\theta_3 & \cos(\theta_3+\theta_4) & \cos(\theta_1+\theta_2) & -\cos\theta_2 & 1 \end{pmatrix}.$$

Theorem 3.12 ([Hil12])**.** Let A be an extremal ray of the COP_5 cone. Then, if $A \notin \mathrm{SPN}_5$ and A is not in the orbit of the Horn's matrix, it is in the orbit of $T(\theta)$ where θ satisfies the two conditions

- $\forall j,\ \theta_j > 0$.
- $\sum_j \theta_j < \pi$.

The extremal rays of COP_6 have also been characterized recently [AHD21], and the high increase in complexity of such descriptions makes it very difficult to obtain such characterizations for any higher dimensions.

Copositive Programming. Consider the following standard quadratic optimization (SQP) problem over the simplex $\Delta := \{x \in \mathbb{R}_d^+ \mid \sum_{i\in[d]} x_i = 1\}$.

$$\gamma(A) := \min_{x\in\Delta} \langle x|A|x\rangle$$

If A is not a PSD matrix, this is a non-convex optimization problem. It has an equivalent formulation as a co-positive program [BDDK+00, DKP02, Bur09].

$$\Lambda(A) := \max\{\lambda \mid A - \lambda J_d \in \mathrm{Cop}_d\}.$$

Note that for any feasible λ, we have,

$$A - \lambda J_d \in \mathrm{COP}_d \iff \forall x \in \Delta, \langle x|A - \lambda J|x\rangle \geq 0.$$

Simplifying the right-hand side, we get, $\langle x|A|x\rangle - \lambda(\sum_i x_i)^2 \geq 0 \iff \langle x|A|x\rangle \geq \lambda$. This shows that $\gamma(A) \geq \Lambda(A)$. The reverse implication follows from the convex duality arguments [DKP02, Bur09].

Stable Set. Recall that for a graph G, a stable set is any induced graph that is empty. Then, $\alpha(G)$ is defined to be independence number of a graph G, i.e. the size of the largest stable set. From the adjacency matrix of the graph A_G, this problem can be recast as an optimization problem over the simplex, i.e the Motzkin-Strauss theorem [MS65].

$$\frac{1}{\alpha(G)} = \gamma(A_G + \mathbb{I}_d) = \min_{x\in\Delta} \langle x|A_G + \mathbb{I}_d|x\rangle .$$

Hence, by some simple computations, we obtain the following copositive program for $\alpha(G)$.

$$\alpha(G) = \max\{t \mid t(I_d + A_G) - J_d \in \mathrm{Cop}_d\}.$$

Since $\alpha(G)$ is NP-hard to compute [Kar09], this also shows that checking for copositivity of a given matrix is NP-hard. Finally, this implies that checking for polynomial positivity is NP-hard (copositivity being a special case of polynomial positivity).

Parillo's hierarchy. Since testing for copositivity is NP-hard, the apparatus of Reznick's and Polya's Positivestellansatz can be applied to have inner approximations of the copositive matrices. This idea was first introduced by Parillo [Par00] and applied to the independence number of the graph by de-Klerk-Paschenik [DKP02]. Consider the following convex cones labelled by $r \in \mathbb{N}$.

$$\mathcal{K}_d^{(r)} := \{X \in \mathrm{Herm}[\mathcal{M}_d] \mid p_X(x \odot x)||x||^{2r} \in \Sigma_d^{(2r+2)}\}.$$

The product of two polynomials $p \in \Sigma_d^{(n)}$ and $q \in \Sigma_d^{(m)}$ is also a sum of squares, implying that the hierarchy forms an increasing sequence of sets.

$$\mathrm{NN}_d + \mathrm{PSD}_d = \mathcal{K}_d^{(0)} \subsetneq \mathcal{K}_d^{(1)} \subseteq \cdots \subseteq \mathcal{K}_d^{(r)} \subseteq \mathrm{COP}_d$$

Testing if a matrix is in the r-th level of the hierarchy, $\mathcal{K}_d^{(r)}$ can be recast as a semidefinite program as it involves checking if a polynomial is sum of squares. By Reznick's theorem (see Theorem 2.11), these approximations satisfy the following inclusions.

$$\mathrm{int}(\mathrm{COP}_d) \subseteq \bigcup_{n=0}^{\infty} \mathcal{K}_d^{(n)} \subseteq \mathrm{COP}_d\,.$$

Both the inclusions in the previous statement are strict for the case of $d \geq 6$ [LV23]. For $d \leq 4$, the first level of the hierarchy $\mathcal{K}_d^{(0)}$ is equal to COP_d. For $d = 5$, it was shown in [LV22b] that $\bigcup_{n=0}^{\infty} \mathcal{K}_5^{(n)} = \mathrm{COP}_5$. Moreover, the Horn's matrix was shown to be in $\mathcal{K}_d^{(1)}$, i.e, the first level of the hierarchy [Par00].

Stability number hierarchy. The hierarchy by Parillo can be applied to the approximations of $\gamma(A)$. Consider the following approximations.

$$\gamma^{(r)}(A) = \max\{\lambda \mid A - \lambda J_d \in \mathcal{K}_d^{(r)}\}.$$

These form a sequence of decreasing approximations to $\gamma(A)$.

$$\gamma(A) \leq \ldots \leq \gamma^{(r)}(A) \leq \ldots \leq \gamma^{(0)}(A)$$

such that this converges to $\gamma(A)$.

$$\lim_{r\to\infty} \gamma^{(r)}(A) = \gamma(A).$$

For each r, the semidefinite program is efficiently solvable in polynomial time up to a fixed precision [PSVM25].

In particular, this approach can be applied to the copositive formulation of the independence number as well, leading to the lower bounds.

$$\theta^{(r)}(G) = \max\{t \mid t(I_d + A_G) - J_d \in \mathcal{K}_d^{(r)}\}.$$

The parameter $\theta^{(0)}$ coincides with the approximation introduced by Schrijver [Sch79a] as an improvement of the famous Lovász theta number [Lov79]. In their article, de Klerk and Paschenik [DKP02] conjecture that the hierarchy converges to the independence number for $r = \alpha(G) - 1$ and show its validity for all graphs with the number of vertices

$d \leq 8$. The properties and convergence of this hierarchy has been thoroughly analysed in [LV22a, LV23].

Permutation Symmetry. Consider A with some permutation symmetry, i.e $\forall \pi \in \mathcal{G} \subseteq S_n,\ A_{ij} = A_{\pi(i)\pi(j)}$. Then, define the twirling operation $\mathcal{T} : \mathcal{M}_d \to \mathcal{M}_d$.

$$\mathcal{T}(X) = \sum_{\pi \in \mathcal{G}} P_{\pi^{-1}} X P_\pi.$$

This is a projector into the matrix algebra with the permutation symmetry of the group $\mathcal{G}$. Consider the following quantity

$$\tilde{\gamma}(A) = \max\{\lambda \mid A - \lambda J_d \in \mathcal{T}(\mathrm{Cop}_d)\}.$$

The symmetrized optimization problem gives the same value, $\tilde{\gamma}(A) = \gamma(A)$. Note that in the second optimization, we have the optimization over the cone $\mathcal{T}(\mathrm{Cop}_d)$ that is possibly simpler to handle than the complete convex cone of co-positive matrices.

Semidefinite Representability. A spectrahedron is a shape that can be represented as a linear matrix inequality, i.e,

$$\{a \in \mathbb{R}^d \mid \sum_{i \in [d]} a_i A_i \succeq 0\}.$$

If there is an exact representation of a convex set as a spectrahedron or projected spectrahedron, the set is called semidefinite representable. The inclusion in a semidefinite representable set is solvable by a semidefinite program. The set of sum of square polynomials $\Sigma_d^{(2n)}$ is an example of a such a convex cone. The Helton-Nie conjecture asks if every *convex* semi-algebraic set can be written as a projection of a spectrahedron [HN09] (A set is semialgebraic set if it can be described using a finite boolean combinations of polynomial equations and inequalities). This was later disproved by Schreiderer in his seminal paper [Sch18]. He showed that the convex cone of positive polynomials is *not* semidefinite representable, except in the cases where it is equal to a sum of squares.

By Tarski-Seidenberg theorem on quantifier elimination, the convex cone of copositive matrices can be shown to *semi*-algebraic. It was recently shown that the copositive matrices is also not semidefinite representable for $d > 4$ [BKT22], implying the same for its dual of completely positive matrices.

Can you teleport only the body, or also the spirit [asking about quantum teleportation]?
– Only the spirit.

Asher Peres

4

Quantum Information Theory

The fourth chapter of the thesis deals with quantum information theory, with particular emphasis on separability and entanglement. The notion of PPT (Positivity under Partial Transposition) is central to this chapter, along with the associated PPT entangled states (or so-called bound entangled states). We end this section with some recent connections of quantum extendibility to SOS hierarchies.

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Notation	
$\mathrm{tr}_I(p)$	Marginal over random variable indexed by I and probability distribution p
$\mathrm{Tr}_I(X)$	Partial trace over subsystem(s) indexed by I
id_d	Identity map between matrix algebras
X^Γ	Partial transpose (on the second subsystem)
$C(\mathcal{L})$	Choi matrix of a linear map $\mathcal{L}$
$\mathbb{F}$	Flip (swap) operator: $\mathbb{F}(\lvert v\rangle \otimes \lvert w\rangle) = \lvert w\rangle \otimes \lvert v\rangle$
Sep_d	Separable states: $\mathrm{cone}\{\lvert v\rangle\langle v\rvert \otimes \lvert w\rangle\langle w\rvert \mid \lvert v\rangle, \lvert w\rangle \in \mathbb{C}^d\}$

continued on next page

BP_d	Block positive matrices; dual of Sep_d
PPT_d	Positive Partial Transpose States
Dec_d	Decomposable matrices/witnesses; dual of PPT_d
$\mathrm{DPS}_d^{(r)}$	Doherty-Parrilo-Spedalieri r-extendible states
$(\mathrm{PPT})\mathrm{BExt}_d^{(n,r)}$	(PPT) Bosonic r-extendible states on $\vee^n \mathbb{C}^d$
$\mathrm{SN}(X)$	Schmidt number of a mixed state X
$\mathrm{SR}(\lvert\psi\rangle)$	Schmidt rank of a pure state $\lvert\psi\rangle$
biSep_d	Biseparable states: conic hull of all bipartite separable states
biPPT_d	Biseparable PPT relaxation: conic hull of all bipartite PPT states
$\vee^n \mathbb{C}^d$	Symmetric subspace of $(\mathbb{C}^d)^{\otimes n}$
$\Pi_d^{(r)}$	Orthogonal projection onto $\vee^r \mathbb{C}^d$
$\mathcal{P}^{(n,r)}$	r-exchangeably extendible probability distributions on $[d]^n$
$\mathcal{S}^{(n,r)}$	r-exchangeably extendible (de-Finetti extendible) quantum states

4.1 QUANTUM POSTULATES

In this section, we give a brief mathematical introduction to some fundamental objects in quantum mechanics. For a thorough treatment of these topics, the reader should refer to the excellent introductory textbook in this subject by Nielsen and Chuang [NC10], or the one by Watrous [Wat18].

Quantum States. Let $\mathcal{H}$ be a finite dimensional complex Hilbert space $\mathcal{H}$ with $\dim(\mathcal{H}) = d$. The quantum states ρ are elements of the bounded (trace class) operators acting on this Hilbert space, $\mathcal{B}(\mathcal{H})$ which are positive semidefinite ($\rho \succeq 0$) and $\mathrm{Tr}(\rho) = 1$. Recall that a finite dimensional complex Hilbert space is isomorphic to $\mathbb{C}^d$ and hence, $\mathcal{B}(\mathbb{C}^d) \cong \mathcal{M}_d$, the algebra of $d \times d$ matrices. The quantum states can be also understood as a non-commutative generalization of finite classical probability distributions. The matrix algebra has a natural Euclidean inner product

$$\langle X, Y \rangle = \mathrm{Tr}(X^* Y)$$

which is also sometimes called the *Hilbert-Schmidt* inner product. Using this, we can define a 2-norm of the matrix

$$\|X\|_2^2 = \mathrm{Tr}(|X|^2) = \sum_{i=1}^{d} (\sigma_i(X))^2 = \sum_{i,j\in[d]} |X_{ij}|^2.$$

where $\sigma_i(X)$ are the singular values of the matrix X. For a quantum state $\rho \succeq 0$, $\|\rho\|_2^2 = \mathrm{Tr}(\rho^2)$ is called the *purity* of the state.

Pure and Mixed States. The rank-1 quantum states (which are of the form $|\varphi\rangle\langle\varphi|$ for some $|\varphi\rangle \in \mathbb{C}^d$) are called *pure states*, and satisfy $\|\rho\|_2^2 = 1$. The states not of this form are *mixed*, with $\|\rho\|_2^2 < 1$. Any state ρ, by the spectral decomposition, can be written as a convex sum of orthogonal pure states,

$$\rho = \sum_{k=1}^{K} \lambda_k |\psi_k\rangle \langle\psi_k|,$$

where $\lambda_k \geq 0$ satisfying $\sum_{k=1}^{K} \lambda_k = 1$. The purity of the state satisfies the following bounds.

$$1 \geq \|\rho\|_2^2 \geq \frac{1}{d}.$$

The minimum purity of a state is attained by the maximally mixed state $\frac{\mathbb{I}}{d}$.

Bloch Sphere. For $\mathcal{H} = \mathbb{C}^2$, the *Pauli matrices* are the following Hermitian matrices

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Together with the identity $\mathbb{I}_2$, they form an orthogonal basis for $\mathrm{Herm}[\mathcal{M}_2]$. The matrix algebra of Hermitian matrices, $\mathrm{Herm}[\mathcal{M}_2]$ has a bijective mapping to $\mathbb{R}^4$ as $X \mapsto (\mathrm{Tr}(X), r_x, r_y, r_z)$ where

$$\begin{aligned} r_x &:= \mathrm{Tr}(X\sigma_x) \\ r_y &:= \mathrm{Tr}(X\sigma_y) \\ r_z &:= \mathrm{Tr}(X\sigma_z) \end{aligned}$$

Any matrix has the following expansion in terms of the Pauli matrices

$$X = \mathrm{Tr}(X)\frac{\mathbb{I}}{2} + \frac{1}{2}(\sigma \cdot r).$$

The norm of a 2×2 matrix can be computed in terms of the components of the vector r.

$$\|X\|_2^2 = \frac{\mathrm{Tr}(X)^2}{2} + \frac{1}{2}(r_x^2 + r_y^2 + r_z^2).$$

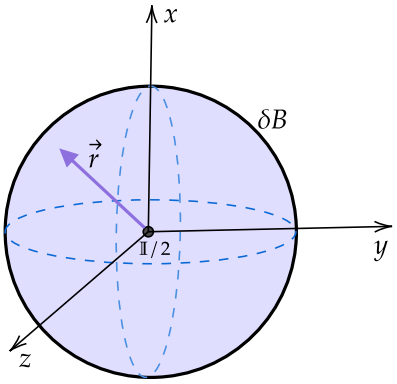


Figure 5: The Bloch ball

Therefore, this implies that the density matrices ($X \succeq 0$ and $\mathrm{Tr}(X) = 1$) are mapped to a unit ball $B^3 \subseteq \mathbb{R}^3$. This is colloquially called the *Bloch Ball* (whose boundary $\partial B^3 \cong S^2$ is called the Bloch Sphere). The pure states are located on the boundary of the ball ∂B, while the mixed states form the interior $\mathrm{int}(B)$. The state located in the center is $\frac{\mathbb{I}}{2}$ (the maximally mixed state).

Composite States. Two quantum systems can be thought of as "separate systems" if there are quantum operations acting on one system without affecting the other. In quantum mechanics, a composition of such systems is described using a tensor product Hilbert space, $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^{d'}$ which implies that the states of the system are positive semidefinite elements in the tensor product of matrix algebra.

$$\mathcal{M}_d \otimes \mathcal{M}_{d'} \cong \mathcal{B}(\mathbb{C}^d) \otimes \mathcal{B}(\mathbb{C}^{d'}) \cong \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^{d'}).$$

Quantum Channels. The process of evolution in quantum mechanics can be abstracted as performing a quantum *channel*. Since any such channel should map quantum states to states, it is a linear map that is positive and also trace preserving. A linear map $\mathcal{E} : \mathcal{M}_d \to \mathcal{M}_{d'}$ is called *completely positive* if for every $k \in \mathbb{N}$, the ampliated map $\mathcal{E} \otimes \mathbb{I}_k : \mathcal{M}_d \otimes \mathcal{M}_k \to \mathcal{M}_{d'} \otimes \mathcal{M}_k$ is positive. Since a channel can act locally on one part of a larger composite system, it should be completely positive. Such linear maps $\mathcal{E} : \mathcal{M}_d \to \mathcal{M}_d$ are called CPTP (completely positive and trace preserving) maps. Every such linear map has a Kraus decomposition, i.e., there exist operators $\{K_i\}_{i \in I} \in \mathcal{M}_d$ such that

$$\mathcal{E}(X) = \sum_{i \in I} K_i X K_i^* \quad \sum_{i \in I} K_i^* K_i = \mathbb{I}_d.$$

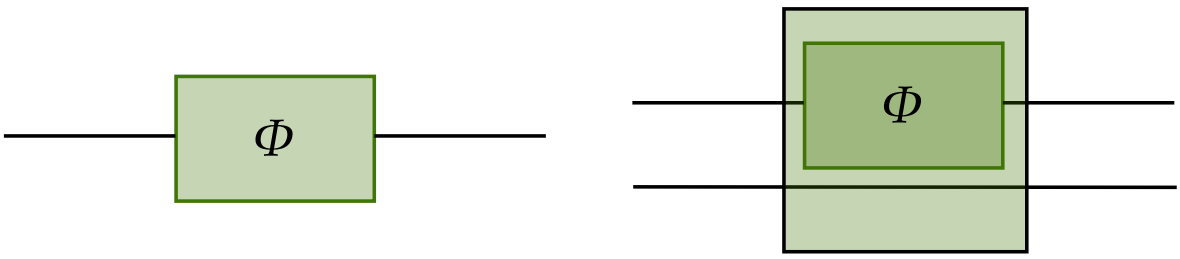


Figure 6: A quantum channel is completely positive, i.e any ampliation $\Phi \otimes \mathrm{id}_d$ is also completely positive.

Quantum Measurements. The measurement device in quantum mechanics outputs a *classical* value by taking in a quantum state. The quantum measurement device is modelled by Lüders rule that consists of a collection of operators $\mathcal{K} = \{K_i\}_{i \in I} \in \mathcal{M}_d$ such that $\sum_{i \in I} K_i^* K_i = \mathbb{I}_d$ that are assigned to any measurement. Then, any outcome i is obtained with the probability

$$p(i \,\|\, \text{State } X \text{ and Measurement } \mathcal{K}) = \mathrm{Tr}(X K_i^* K_i)$$

and the post measurement state after obtaining the outcome i is given as :

$$X \to \frac{K_i X K_i^*}{\mathrm{Tr}(X K_i^* K_i)}$$

4.2 QUANTUM ENTANGLEMENT

Entanglement is one of the essential feature of the quantum theory and has been a point of contention among physicists since the advent of quantum theory [EPR35]. Since the emergence of quantum information theory, the role of entanglement has shifted from a paradoxical concept into a *resource* which powers quantum protocols in quantum communication [SN96, BBC$^+$93], cryptography [Eke91], metrology [GLM11] and error correction [BDSW96]. Recently, it has found various connections in many-body quantum systems [AFOV08], and in fundamental physics, e.g., black hole thermodynamics [HP07]. Despite such importance, many fundamental facets of entanglement remain unsolved, particularly in mixed states. Even the membership problem for entanglement, that just involves deciding if a quantum state is entangled or not is a highly non-trivial problem [DSLS05] and an active area of research; moreover, it was also shown to be in the computational class of NP-HARD problems [Gur03, Gha10]. In this section, we provide a brief introduction to entanglement, and the quantum separability problem (QSep). A lot of excellent reviews of

these topics are available, we mention in particular the in-depth one by the Horodecki(s) [HHHH09]; also see [Ioa06] for the computational aspects of the separability problem.

Remark 4.1. Note that the set of positive semidefinite matrices is a convex cone, and the state space is a slice of the convex cone with $\mathrm{Tr}(\rho) = 1$. For this thesis, the normalization remains an unnecessary artifact of the physical world that will be done away with to make the analysis simpler. This in principle is done by defining the convex cone $\mathcal{C} \subseteq \mathcal{M}_d^+$ corresponding to the convex set $\mathcal{S}$ as

$$\mathcal{C} = \mathbb{R}_+ \mathcal{S}.$$

Separable States. A bipartite quantum state $X \in \mathcal{M}_d \otimes \mathcal{M}_d$ is called product (or uncorrelated) if it is of the form $X = \rho \otimes \sigma$ for $\rho, \sigma \succeq 0$. If two parties have access to such a state, and both parties (usually called Alice and Bob) is allowed to only perform measurements *locally* cannot generate *any* shared correlations.

$$p(i,j) = \mathrm{Tr}\left(M_i^A \otimes M_j^B(\rho \otimes \sigma)\right) = \mathrm{Tr}(M_i^A \rho) \cdot \mathrm{Tr}(M_j^B \sigma)$$

The notion of a state not being entangled can be formally generalized in the following fashion; a quantum state is called separable if it can be prepared using local operations and *classical* communications (LOCC). The separable states are of the form

$$\sum_{k=1}^{K} p_k(\rho_k \otimes \sigma_k) \quad \text{for} \quad p_k \geq 0, \sum_{k=1}^{K} p_k = 1.$$

Any state not of the above form is called to be *entangled*. For example, it can be shown that the Bell state, $\Phi := \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11| + |01\rangle\langle 10| + |10\rangle\langle 01|)$ is an entangled state.

This is also motivated by the fact that by performing only local measurements on a separable state, the generated correlations between two parties have a classical interpretation (in form of a shared classical random variable) [1]

$$p(i,j) = \mathrm{Tr}\left(M_i^A \otimes M_j^B(\sum_{k=1}^{K} \rho_k \otimes \sigma_k)\right) = \sum_{k=1}^{K} p_k \,\mathrm{Tr}(M_i^A \rho_k) \cdot \mathrm{Tr}(M_j^B \sigma_k).$$

To make the analysis easier, it is useful to define the convex *cone* of separable states (see Remark 4.1).

$$\mathrm{Sep}_d := \{\sum_{k=1}^{K} |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k| \mid |v_k\rangle, |w_k\rangle \in \mathbb{C}^d\}.$$

1 On the other hand, there exist states that are *not* separable, but all correlations generated by such states are amenable to an explanation with classical correlations [Wer89].

The extremal rays of the separable cone are the pure product states.

$$\operatorname{ext} \operatorname{Sep}_d = \{|v\rangle\langle v| \otimes |w\rangle\langle w| \mid |v\rangle, |w\rangle \in \mathbb{C}^d\}.$$

This is a proper convex cone (i.e closed, pointed and has a non-empty interior).

Quantum Separability Problem. Let $K \subseteq \mathbb{R}^d$ be a convex set. Then, we define for $\beta \in \mathbb{R}_+$, the following outer β-approximation of the set K.

$$B(K, \beta) := \{x \in \mathbb{R}^d \mid \exists y \in K, \|x - y\| \leq \beta\}.$$

Also, we define the points at-least β distance away from the boundary of the set K.

$$B(K, -\beta) = \{x \in \mathbb{R}^d \mid B(\{x\}, \beta) \subseteq K\}.$$

Any convex set is well-bounded p-centered if there exists a $\alpha_{\text{in}}, \alpha_{\text{out}} \in \mathbb{R}_+$ and $p \in K$ such that

$$B(\{p\}, \alpha_{\text{in}}) \subseteq K \subseteq B(\{0\}, \alpha_{\text{out}}).$$

Definition 4.2 (Weak Membership Problem)**.** Let $K \subseteq \mathbb{R}^d$ be a convex, compact and well bounded p-centered set. Then, given $y \in \mathbb{R}^d$ and error parameter $\beta \in \mathbb{Q}$, output

- NO if $y \notin B(K, \beta)$.
- YES if $y \in B(K, -\beta)$.

It was shown that the weak membership problem for separability is strongly NP-HARD [Gha10] following an earlier work by Gurvits [Gur03]. A problem is called strongly NP-hard if it is NP-hard even if the magnitudes of its numerical parameters (here β) are polynomially bounded in the length of its input (here d). Intuitively, this means that deciding if a state is approximately separable by tolerating a *polynomially decreasing error* in d is NP-HARD. The exact complexity of the separability problem is still an open question [IQO], or whether it stays NP-HARD with β constant.

Separable Balls. The geometry of separable states is highly non-trivial to describe fully; it is a convex set with $d^4 - 1$ parameters. A key aspect of the geometry of a convex set is the size of the largest ball that fits entirely inside it. The size of this ball (which is centered around $\mathbb{I}$) in the l_2 norm, and also other norms has been considered in [GB02]. We consider the following result from [GB02].

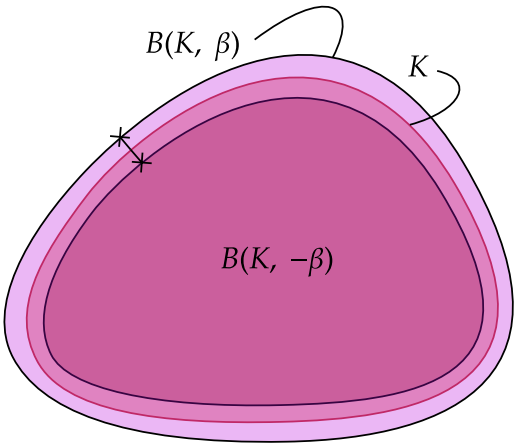


Figure 7: The weak separability problem asks whether a given point is inside or outside with error β.

Theorem 4.3 ([GB02])**.** Let $\rho \in \mathrm{Herm}[\mathcal{M}_d^{\otimes 2}]$ such that

$$\|\rho\|_2^2 = \mathrm{Tr}(\rho^2) \leq \frac{1}{d^2 - 1}.$$

Then, ρ is separable.

Moreover, it can be shown that this is the largest separable ball centered around the maximally mixed state [GB02]. This is one of the few sufficient criteria for separability of ρ. Intuitively, this implies that the quantum states that are *sufficiently* mixed are separable.

Choi-Jamiołkowski Isomorphism [Cho75a, Jam72]. The set of bipartite matrices $\mathcal{M}_d \otimes \mathcal{M}_d$ has a natural isomorphism to linear maps $\mathcal{M}_d \to \mathcal{M}_d$. For every linear map $\mathcal{L}$, there is an associated matrix $C_{\mathcal{L}}$ defined as

$$C_{\mathcal{L}} := [\mathcal{L} \otimes \mathrm{id}_d](|\varphi\rangle\langle\varphi|)$$

where $|\varphi\rangle = \sum_{i \in [d]} |ii\rangle$. This matrix is called its Choi Matrix. A given map $\mathcal{L}$ is completely positive if and only if $C(\mathcal{L}) \succeq 0$.

Entanglement Breaking (EB) Maps. A linear map is entanglement breaking [HSR03] if for all $\rho \in \mathcal{M}_d^{\otimes 2}$, $\rho \succeq 0$, we have,

$$[\mathcal{L} \otimes \mathrm{id}_d](\rho) \in \mathrm{Sep}_d.$$

This implies that this map *breaks* entanglement for any state by acting locally on one system. By the Choi-Jamiołkowski Isomorphism, this property is in correspondence with the separability of the Choi state.

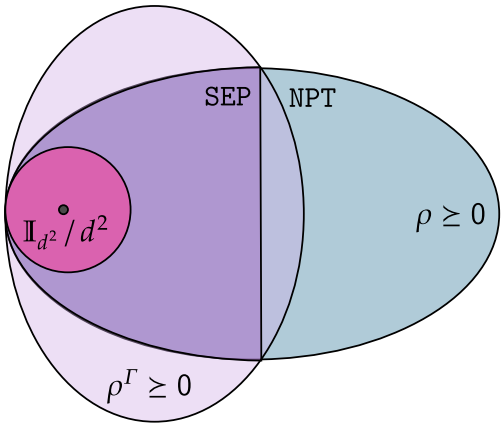


Figure 8: The separable ball inside the positive semidefinite matrices. Surprisingly, the separable ball touches the boundary of the PSD matrices as well

Proposition 4.4 ([HSR03]). $\mathcal{L}$ is entanglement breaking $\iff$ $C(\mathcal{L})$ is separable.

Block Positivity. Another useful strategy to study the separability problem is to study its conic dual, which are the *block positive matrices*.

$$\mathrm{BP}_d := (\mathrm{Sep}_d)^\circ.$$

Another equivalent description of this convex cone is in terms of positivity of the corresponding Hermitian matrix polynomial :

$$\mathrm{BP}_d = \{X \in \mathrm{Herm}[\mathcal{M}_d \otimes \mathcal{M}_d] \mid \forall v, w \in \mathbb{C}^d,\ \langle v \otimes w | X | v \otimes w \rangle \geq 0\}.$$

This follows from noting that extremal rays of separable states are the rank-1 matrices of the form $|v \otimes w\rangle\langle v \otimes w|$. Also, the block positive matrices have a natural correspondence to positive maps [HHH01] :

Theorem 4.5 (Duality [HHH01]).

- $\Phi \in \mathrm{Pos}_d \iff C(\Phi) \in \mathrm{BP}_d$.
- $\rho \in \mathrm{Sep}_d$ if and only if $(\Phi \otimes \mathrm{id}_d)(\rho) \succeq 0$ for all $\Phi \in \mathrm{Pos}_d$.

We here sketch a proof of this theorem, based on [HHH01]. Consider the following identity

$$\langle x|\Phi(|y\rangle\langle y|)|x\rangle = \langle x \otimes \overline{y}|C(\Phi)|x \otimes \overline{y}\rangle \, .$$

The map Φ is positive if and only if for $x, y \in \mathbb{C}^d$, $\langle x|\Phi(|y\rangle\langle y|)|x\rangle \geq 0$. This implies the first assertion. For the second assertion, note that

Peres-Horodecki criterion. The transposition map acts as an entanglement criterion as it is positive but not completely positive [HHH96, Per96]. By computing the eigenvalues, we can check if the matrix

$$\mathrm{id}_d \otimes T(X) := X^\Gamma \not\succeq 0$$

which implies that the state is entangled. Moreover, there are efficient algorithms to apply this test, as checking eigenvalues is poly-time in the size of the matrix. Surprisingly, this test is also sufficient if $d \cdot d' \leq 6$ [HHH96]. We consider the convex cone of PPT matrices.

$$\mathrm{PPT}_d := \{X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes 2}] \mid X, X^\Gamma \succeq 0\}.$$

We also define the convex cone of *decomposable* matrices as :

$$\mathrm{DEC}_d := \{X \in \mathrm{Herm}[\mathcal{M}_d \otimes \mathcal{M}_d],\ X = X_1 + X_2^\Gamma \mid X_1, X_2 \succeq 0\}.$$

This is dual to the cone of bipartite PPT matrices $\mathrm{PPT}_d.s$

Theorem 4.6 (Duality with PPT [HHH01])**.**

- $\Phi \in \mathrm{Dec}_d \iff C(\Phi) \in \mathrm{DEC}_d$.
- $\rho \in \mathrm{PPT}_d$ if and only if $(\Phi \otimes \mathrm{id}_d)(\rho) \succeq 0$ for all $\Phi \in \mathrm{Dec}_d$.

The first example of non-decomposable (or indecomposable) maps occurred in [Cho80a], with the first example of PPT entangled state presented much later in [Hor97] [2] The analysis of this duality in the quantum information literature began in early 2000s [BCH+02, LKHC01]. This led to some new examples of positive indecomposable maps [Ter01] and PPT entangled states [DMS+03].

Range criterion and Horodecki State. Since there exist non-decomposable maps $\mathcal{M}_3 \to \mathcal{M}_3$, the duality of PPT and decomposable maps implies the existence of PPT entangled state in $\mathcal{M}_3 \otimes \mathcal{M}_3$. The first example of such a state was constructed by Horodecki [Hor97]

2 Although, a construction of a PPT entangled state was already accomplished in 1982 by Stormer, but it was not called as such [Stø82].

$$\rho_a^{3\otimes 3} = \frac{1}{8a+1}\begin{pmatrix} a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1+a) & 0 & \frac{1}{2}\sqrt{1-a^2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 \\ a & 0 & 0 & 0 & a & 0 & \frac{1}{2}\sqrt{1-a^2} & 0 & \frac{1}{2}(1+a) \end{pmatrix}.$$

Figure 9: The Horodecki's state [Hor97] is PPT entangled for $0 < a < 1$.

which can be shown to be entangled by the range criterion which is a useful necessary condition on the range of a separable state, and can be applied to detect entanglement.

Proposition 4.7 ([Hor97])**.** Let $X \in \mathrm{Sep}_d$. Then, all the product vectors $|\varphi_1\rangle \otimes |\varphi_2\rangle$ in the $\mathrm{Ran}(X)$ span $\mathrm{Ran}(X)$. And the vectors $|\varphi_1\rangle \otimes |\varphi_2\rangle$ such that $|\varphi_1\rangle \otimes |\overline{\varphi_2}\rangle \in \mathrm{Ran}(X)$ span $\mathrm{Ran}(X^\Gamma)$.

The application of this criterion is to find all product vectors $|\varphi_1\rangle \otimes |\varphi_2\rangle$ in the range, and to find an *orthogonal vector* to all $|\varphi_1\rangle \otimes |\overline{\varphi_2}\rangle$ in the range of the partial transpose.

PPT Extremal and Edge States. Recall that an element A of a convex cone is extremal if decomposing $A = X + Y$ where $X, Y \in \mathcal{C}$ implies that there exists $\lambda \in [0, 1]$ such that $X = \lambda A$ and $Y = (1-\lambda)A$. These states are important from the perspective of convex cones as any state can be written as a conic sum of extremal states.

The *pure* separable states are extremal in the PPT cone, as they are extremal in PSD matrices. The extremality in the PPT cone can be studied by defining a slightly weaker notion of *edge*-states. A PPT entangled quantum state is called edge if there is no product vector $|x, y\rangle$ in its range such that $|x, \overline{y}\rangle$ is in the range of the partial transpose. If $|x, y\rangle \in \mathrm{Ran}(X)$ and $|x, \overline{y}\rangle \in \mathrm{Ran}(X)$, for some $\varepsilon > 0$ the following state is again PPT,

$$X - \varepsilon\, |x, y\rangle\langle x, y|$$

and hence cannot be extremal. Therefore the extremality (and edge) property constrains the possible ranks of the state and its partial transpose, as for states with high enough ranks, there always exist product states in their range. These ideas can be used to constrain

the ranks of extremal PPT states in low dimensions $3 \otimes 3$ and $2 \otimes 4$ [AGKL10]. It was also shown in [HLVC00] that all $X \in \mathrm{PPT}_d$ such that $\mathrm{rank}(X) \leq d$ are separable. We refer the reader to the articles [CĐ13, Sko11, Kye13] for more in-depth details about extremal (and edge) PPT entangled states from a convex geometry perspective.

4.3 PPT ENTANGLED STATES AND DISTILLABILITY

In this section, we discuss some different questions connected to PPT states, PPT entanglement and decomposability of linear maps.

Semidefinite Representability of Separable States. Recall that a convex cone is semidefinite representable if it can be written as a projection of a spectrahedron. The convex cone of separable states in $\mathcal{M}_d \otimes \mathcal{M}_{d'}$ is equal to PPT if $d \cdot d' \leq 6$ and hence has a semidefinite representation. For any other fixed dimensions d, d', the set of separable states is not semi-definite representable [Faw21], providing new counterexamples to the Helton-Nie conjecture [HN09]. This provides more indication of the highly non-trivial structure of the separable cone, even in low dimensions.

PPT squared conjecture. A linear map $\Phi : \mathcal{M}_d \to \mathcal{M}_d$ is called completely copositive if $T \circ \Phi$ is completely positive. Such a map is called PPT if it is both completely positive and completely copositive. Φ is PPT if and only if $C(\Phi)$ is PPT. Therefore all entanglement breaking maps are PPT, but the converse is not true in $d \geq 3$. It was conjectured by Christandl [RJK+12] that the composition of PPT maps is always entanglement breaking.

> **Conjecture 4.8** ([RJK+12])**.** The composition of two PPT maps is entanglement breaking.

The motivation for this conjecture is whether the PPT entangled states are useful as a resource in quantum *repeaters*, in particular it is equivalent to the following statement [BCHW15], "If Alice and Charlie share a PPT state and that Bob and Charlie share a PPT state; then the state of Alice and Bob, conditioned on any measurement by Charlie, is always separable". A counterexample of such a conjecture would imply the existence of resourceful PPT states for this protocol. This conjecture can also be formulated in terms of the dual objects as:

Conjecture 4.9 ([CMHW19]). For any PPT map $\Lambda : \mathcal{M}_d \to \mathcal{M}_d$ and any positive map $P : \mathcal{M}_d \to \mathcal{M}_d$ the composition $\Lambda \circ P$ is decomposable.

Schmidt number of PPT entangled states. The Schmidt *rank* (SR) of a pure bipartite state is its number of non-zero Schmidt coefficients in the state, or equivalently the rank of the partial trace of X, $\mathrm{rank}(\mathrm{Tr}_1(X))$. This is a measure of entanglement for pure states, which intuitively quantifies how many effective degrees of freedom are entangled in X. This notion has a natural extension to *mixed* states through the convex roof construction, called in the general case as the Schmidt *number* [TH00].

$$\mathrm{SN}(X) = \min_{X=\sum_{k=1}^{K}|v_k\rangle\langle v_k|} \left\{ \max_k \mathrm{SR}(|v_k\rangle) \right\}.$$

The PPT entangled states are considered to be noisy, and hence close to separable. There has been a recent interest in understanding the Schmidt numbers possible for PPT entangled states. It is conjectured that the Schmidt number for PPT states cannot be maximal, i.e, it is strictly less than d for $d \otimes d$ states. It was shown that all PPT entangled states $X \in \mathcal{M}_3 \otimes \mathcal{M}_3$ have $\mathrm{SN}(X) \leq 2$ [SBL01, YLT16]. This was used to show the PPT squared conjecture for linear maps $\mathcal{M}_3 \to \mathcal{M}_3$ [CYT19]. Recently, some classes of PPT entangled states $\mathcal{M}_d \otimes \mathcal{M}_d$ have been constructed that achieve linear SN in d, for such constructions, see [HLLMH18] (achieving $\lfloor \frac{d}{4} \rfloor$) [PV19, Par26, KG24] (achieving $\lfloor \frac{d}{2} \rfloor$). For low dimensional cases, PPT states with Schmidt number 3 were constructed in a $5 \otimes 5$ system [KG24].

Absolute Separability. A quantum state $X \in \mathrm{Herm}[\mathcal{M}_d \otimes \mathcal{M}_d]$ is called absolutely *separable* if the matrix

$$UXU^*$$

is separable for all bipartite unitary matrices, $U \in \mathcal{U}(d \otimes d)$. These states remain unentangled even if a *global* "entangling" unitary is applied to the system, i.e, they have a much stronger form of separability. The (un-normalised) maximally mixed state $\mathbb{I} \otimes \mathbb{I}$ is absolute separable as it is fixed under all global unitaries. Also, the states in the Gurvits-Barnum ball [GB02], the separable ball around the maximally mixed state are also absolutely separable (as the purity is unchanged by unitary matrices). In general, the absolutely separable states are completely characterized by their *spectrum*. For 2×2 systems, the conditions on the spectrum ($\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0$.) that are equivalent absolute separability is [Joh13]:

$$\lambda_1 \leq \lambda_3 + 2\sqrt{\lambda_4 \cdot \lambda_2}.$$

Similarly to ASep, we can consider absolutely PPT state, i.e., a state X such that

$$UXU^*$$

is PPT for all $U \in \mathcal{U}(d \otimes d)$. This property also depends only on the spectrum, in fact, the property can be characterized in terms of semidefinite conditions on the spectrum [Hil07]. The absolute PPT and absolute Sep sets are conjectured to coincide , and are known to coincide for systems of size $2 \times d$ [Joh13].

Distillability and Tensor Stable Positivity. A quantum state ρ is called to be distillable if we can perform a conversion

$$\rho^{\otimes n} \underset{\text{LOCC}}{\longrightarrow} |\psi\rangle\langle\psi|^{\otimes \lfloor rn \rfloor}$$

for $r > 0$ as $n \to \infty$. This can be reduced to a matrix-theoretic condition on the state : a state ρ is distillable if there exists an $n \in \mathbb{N}$ and ψ with Schmidt rank 2 such that

$$\langle\psi|(\rho^\Gamma)^{\otimes n}|\psi\rangle < 0.$$

Since for any PPT state $\rho^\Gamma \succeq 0$, it implies that PPT entangled states are *not* distillable. Whether undistillability implies PPT is unsolved: which is the famous NPT distillability conjecture. The main breakthrough in this conjecture came by the results of [DSS+00], where they reduced the problem of distillability of all NPT states to a *two* parameter family of states called *canonical* NPT states.

> **Question 4.10** ([MHRW16])**.** Is there a positive map Λ that is not CP or co-CP such that $\Lambda^{\otimes n}$ is positive for all n?

This question has been decided in the negative for qubit maps [MH21]. In particular, the existence of such a map implies that both the *NPT distillability* and *PPT squared conjecture* are false [MHRW16, MH18]. It was shown that instead of positive, if we demand a much stronger condition of decomposability, the question can be answered in the negative [MH18].

4.4 MULTIPARTITE ENTANGLEMENT

In this section, we discuss the separability problem for more than two parties. Although the entanglement is already complicated to describe in the bipartite setting, the multipartite setting brings new facets to entanglement; even for pure states.

Genuine Multipartite Entanglement. We first consider the following examples of different 3-qubit quantum states.

1. $|000\rangle$
2. $|000\rangle + |110\rangle = (|00\rangle + |11\rangle) \otimes |0\rangle$.
3. $|000\rangle + |111\rangle$
4. $|001\rangle + |010\rangle + |100\rangle$

The state (1) is a product state in 3 parties, while the remaining states cannot be factorized as such. Although all the states are entangled; the (2) state is only product across the bi-partition $12|3$. For the (3) and (4), it is not separable across *any* bipartition. Such states are called *genuinely* multipartite entangled. In particular, the states of the form (3) are called GHZ (Greenberger-Horne-Zeilinger) states [GHZ89], and they are inequivalent (by LOCC or even probabilistic LOCC) to the states in the family (4), which are W states. Although, it can be shown that the states in W-class can be approximated by the states in the GHZ-class (where this equivalence class is defined by SLOCC operations).

Mixed states. The notion of multipartite entanglement can be generalized to mixed states can be obtained taking conic mixtures. We define the following convex cone of states separable across the bipartition $1|23$,

$$\mathrm{Sep}_{1|23} := \mathrm{cone}\{|\psi\rangle\langle\psi| \mid |\psi\rangle = |\psi_1\rangle \otimes |\psi_{23}\rangle\}$$

and similarly, $\mathrm{Sep}_{1|32}$ and $\mathrm{Sep}_{12|3}$ can be defined. We also define the convex cone of *fully separable* states.

$$\mathrm{Sep}_{1|2|3} := \mathrm{cone}\{|\psi\rangle\langle\psi| \mid |\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes |\psi_3\rangle\}.$$

Clearly, we have the following inclusions between these sets.

$$\mathrm{Sep}_{1|2|3} \subseteq \mathrm{Sep}_{2|31} \cap \mathrm{Sep}_{1|32} \cap \mathrm{Sep}_{12|3}\,.$$

The counter-intuitive fact is that this inclusion is strict; there exist states which are separable across all bipartitions but not fully separable [BDM+99]. The bi-separable states lie in the conic mixtures of these sets.

$$\mathrm{biSep}_d := \mathrm{cone}\{\mathrm{Sep}_{12|3}, \mathrm{Sep}_{13|2}, \mathrm{Sep}_{32|1}\}.$$

Finally, the states that are not bi-separable are *genuinely* multipartite entangled mixed states. The relaxations of separability can be obtained by the following sets.

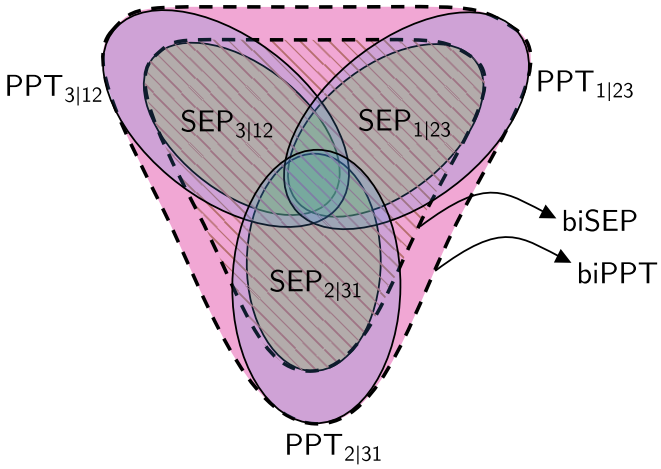


Figure 10: The notions of tripartite entangled states. The convex set of biseparable states is the convex hull of all the sets $\mathrm{Sep}_{12|3}, \mathrm{Sep}_{13|2}, \mathrm{Sep}_{32|1}$. The fully separable states lie strictly inside the intersection $\mathrm{Sep}_{12|3} \cap \mathrm{Sep}_{13|2} \cap \mathrm{Sep}_{32|1}$.

$$\mathrm{Sep}_{1|23} \subsetneq \mathrm{PPT}_{1|23} := \{X \in \mathrm{Herm}[\mathcal{M}_d] \mid X \succeq 0, X^{\Gamma_{1|23}} \succeq 0\}$$

and similarly, we can define $\mathrm{PPT}_{1|32}$ and $\mathrm{PPT}_{12|3}$. Moreover, we have the following relaxation of *biseparable* states.

$$\mathrm{biSep}_d \subseteq \mathrm{biPPT}_d := \mathrm{cone}\{\mathrm{PPT}_{12|3}, \mathrm{PPT}_{13|2}, \mathrm{PPT}_{32|1}\}.$$

Hence, any tripartite state not in biPPT_d is genuinely multipartite entangled. These properties are represented pictorially in the next figure.

An example witness for genuine multipartite entanglement can be constructed in the projective way by using the GHZ state [ABLS01],

$$|\mathrm{GHZ}\rangle := \frac{|000\rangle + |111\rangle}{\sqrt{2}} \qquad W_{\mathrm{GHZ}} := \frac{\mathbb{I}}{2} - |\mathrm{GHZ}\rangle\langle\mathrm{GHZ}|\,.$$

This witness detects multipartite entangled states in the vicinity of the GHZ state.

The concept of biseparability can be generalized to multipartite systems. We introduce the notion of k-producible states, that are mixtures of quantum states entangled on a maximum of k-systems.

Definition 4.11 ([ISTY08, MMRRP+25]). Let $\mathcal{H} = \bigotimes_{i=1}^{n} \mathcal{H}_i$ be the Hilbert space of an n-partite quantum system. A pure state $|\psi\rangle \in \mathcal{H}$ is called *k-producible* if there exists a partition of $[n]$ into disjoint subsets $S_1, \ldots, S_m$ such that $|S_j| \leq k$ for all j and

$$|\psi\rangle = \bigotimes_{j=1}^{m} |\varphi_j\rangle,$$

where $|\varphi_j\rangle$ is a pure state on the subsystems indexed by S_j. A mixed state $X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$ is called *k-producible* if,

$$X \in \mathrm{cone}\{|\psi\rangle\langle\psi| \mid |\psi\rangle \text{ is } k\text{-producible}\}.$$

The entanglement depth of a state ρ is the smallest k such that ρ is k-producible. A state is *genuinely $(k+1)$-partite entangled* if it is $(k+1)$-producible but not k-producible.

The state ρ is called *genuinely multipartite entangled* if it has the maximum entanglement depth n. In this setting, *genuine entanglement* underpins protocols such as secret sharing and multiparty teleportation [HBB99, CZG06].

Qubits. The separability problem for bipartite qubit mixed states is essentially solved: PPT provides a necessary and sufficient condition for separability and just involves checking PSD of a 4×4 matrix [Hor97]. Surprisingly, even for the first non-trivial case of 3 qubits, this problem is highly complex and no such semidefinite characterization exists; moreover there exist entangled states with positive partial transposition across all bi-partitions [BDM+99] (and even separable across all bipartitions). Moreover, the hierarchy of states can be considered [DC00].

- Fully separable, i.e $\mathrm{Sep}_{1|1|1}$.
- 3 qubit biseparable, i.e, in $\mathrm{Sep}_{1|23} \cap \mathrm{Sep}_{1|32} \cap \mathrm{Sep}_{12|3}$
- 2 qubit biseparable, i.e, in $\mathrm{Sep}_{1|23} \cap \mathrm{Sep}_{1|32}$ but *not* in $\mathrm{Sep}_{12|3}$.
- 1 qubit biseparable, i.e in $\mathrm{Sep}_{1|23}$ but *not* in $\mathrm{Sep}_{12|3} \cup \mathrm{Sep}_{13|2}$.
- Fully inseparable states, states that are *not* in $\mathrm{Sep}_{12|3} \cup \mathrm{Sep}_{13|2} \cup \mathrm{Sep}_{23|1}$.

Modulo system permutations, this gives five different increasing classes for entanglement, each of which is non-empty [DC00]. Note the fully inseparable states are a subset of *genuinely* multipartite entangled states (the states that are not biseparable).

4.5 QUANTUM EXTENDIBILITY

In this section, we consider the property of extendibility of quantum states. This property is concerned with the existence of quantum *extensions*, which are states in larger number of parties whose marginals correspond to the original state. There exist various notions of the extendibility of quantum states, see [DPS04, NOP09, ACG+26, SJZ24, GNP25b]. First, we consider the classical and quantum de-Finetti theorem (in both the finite and asymptotic regimes). Then, we consider the different hierarchies from the literature, the DPS hierarchy, and the graph extendibility. We consider then the conic duals of these hierarchies, that are connected to entanglement witnesses and sum of squares.

Classical De-Finetti Theorem. Let $p : [d]^n \to [0,1]$ be a discrete variable probability distribution, i.e $\sum_{i\in[d]^n} p(i) = 1$. Such a distribution is called exchangeable if

$$\forall \sigma \in S_n, \quad p(i_1, i_2 \dots i_n) = p(i_{\sigma(1)}, i_{\sigma(2)} \dots i_{\sigma(n)}).$$

We define the marginal of any exchangeable probability distribution

$$\mathrm{tr}_{[r]}(p)(i_1, i_2 \dots i_{n-r}) := \sum_{j\in[d]^r} p(i_1, i_2 \dots i_{n-r}, j_1, j_2 \dots j_r).$$

Since this distribution is exchangeable, it does not matter which r variables parties we marginalize over. We define the class of r-variable exchangeably extendible probability distributions.

$$\mathcal{P}^{(n,r)} := \{\mathrm{tr}_{[n-r]}(p) \mid p : [d]^n \to [0,1], \sum_{i\in[d]^n} p_i = 1, p \text{ is exchangeable } \}$$

These form a sequence of decreasing sets for each r,

$$\mathcal{P}^{(n,r)} \subseteq \mathcal{P}^{(n+1,r)}.$$

The classical de Finetti theorem shows that the limit of this sequence is the class of conditionally independent and identically distributed probability distribution, i.e,

$$p(i_1, i_2 \dots i_r) = \sum_{k=1}^{K} \lambda(k) v(i_1, k) v(i_2, k) \dots v(i_n, k)$$

where v is a probability distribution from $[d] \times [K] \to [0,1]$, and $\lambda(k) : [K] \to [0,1]$ be a finite probability distribution. Then, the following finite version of the De-Finetti theorem was shown by Diaconis and Freedman [DF80].

Theorem 4.12 (Finite de-Finetti theorem [DF80])**.** Let $p : [d]^n \to [0,1]$ be an n-exchangeable probability distribution. Then, there exist probability distributions $\alpha_k : [d] \to [0,1]$ and $\lambda : [K] \to [0,1]$ such that

$$\forall r \leq n, \quad \| \operatorname{tr}_{[n-r]}(p) - \sum_{k=1}^{K} \lambda_k \alpha_k^{\otimes r} \| \leq 2 \cdot \frac{dr}{n}$$

In fact, it can be shown that the dependence of $O(\frac{r}{n})$ is optimal, and examples of probability distributions achieving them have been constructed [DF80]. There is a dimension independent bound of a tight order as well, i.e, $\frac{(r(r-1))}{n}$, that also works for the case of infinite outcome random variables [DF80].

Quantum De Finetti Theorem. Let $X \in \operatorname{Herm}[\mathcal{M}_d^{\otimes n}]$ be a quantum state which is exchangeable (or permutation symmetric).

$$\forall \pi \in S_n, \quad [P_\pi, X] = 0.$$

Then, we proceed analogously to the classical case and define the decreasing sequence of sets

$$\mathcal{S}^{(n,r)} := \{\operatorname{Tr}_{[n-r]}(\rho) \mid \operatorname{Tr}(\rho) = 1, \forall \pi \in S_n, \quad [P_\pi, X] = 0\}$$

$$\mathcal{S}^{(n,r)} \subseteq \mathcal{S}^{(n+1,r)}.$$

The quantum de Finetti theorem [FS04] shows that the limit of this sequence is the class of conditionally independent product states, i.e,

$$X = \sum_{k=1}^{K} \lambda(k) \rho^{\otimes k}$$

where ρ is a density matrix ($\rho \succeq 0, \operatorname{Tr}(\rho) = 1$), and $\lambda(k) : [K] \to [0,1]$ be a finite probability distribution. Analogous to the classical case, a finite version of the quantum de-Finetti version was also shown [CKMR07].

Theorem 4.13 ([CKMR07])**.** Let $X \in \operatorname{Herm}[\mathcal{M}_d^{\otimes n}]$ be an exchangeable operator such that $X \succeq 0, \operatorname{Tr}(X) = 1$. Then, there exist a finite set of density matrices $\{\alpha_k\}_{k=1}^K \in \operatorname{Herm}[\mathcal{M}_d^{\otimes r}]$ such that $\operatorname{Tr}(\alpha_k) = 1$ and $\lambda_k : [K] \to [0,1]$ be a finite probability distribution such that

$$\forall r \leq n, \quad \| \operatorname{Tr}_{[n]\setminus[r]}(X) - \sum_{k=1}^{K} \lambda_k \alpha_k^{\otimes r} \|_1 \leq 2\frac{d^2 r}{n}$$

This means that *sufficiently* small marginals of exchangeable density matrices are close to mixtures of i.i.d quantum states. In the quantum case, we gain a factor of d compared to the classical case.

Question 4.14. Let $X \in \operatorname{Herm}[\mathcal{M}_d^{\otimes n}]$ be an exchangeable operator such that $X \succeq 0, \operatorname{Tr}(X) = 1$ and satisfies the PPT across all bi-partitions. How close are the marginals of this operator to the case of i.i.d product states?

Let $X \in \operatorname{Herm}[\mathcal{M}_d \otimes \mathcal{M}_d]$ such that $X \succeq 0$. Then, X is K_r- extendible if there exists a matrix $\tilde{X} \in \operatorname{Herm}[\mathcal{M}_d^{\otimes r}]$ satisfying $\tilde{X} \succeq 0$ such that

$$\forall i, j, \quad \operatorname{Tr}_{[r]\setminus\{i,j\}}(\tilde{X}) = X.$$

It is called K_r- PPT extendible if this $\tilde{X}$ can be chosen to be PPT across all bipartitions.

Note that to have a graph extension, the state ρ must be symmetric under the flip operator, i.e $F\rho = \rho F$. If $X = \sum_{k=1}^{K} \alpha_k \otimes \alpha_k$, then, we have the canonical K_n-extension,

$$\tilde{X} = \sum_{k=1}^{K} \alpha_k^{\otimes n} \subseteq \operatorname{Herm}[\mathcal{M}_d^{\otimes n}].$$

Remark 4.15. It has been shown in [BL26] that a similar approach to de-Finetti theorems (finite and infinite) fails in the analogous real case, since there exists states *not* of the form

$$\sum_{k=1}^{K} p_k \alpha_k^{\otimes n} \qquad \alpha_k \in \operatorname{Herm}[\mathcal{M}_d(\mathbb{R})]$$

which can be infinitely extended. Such a state can be constructed by noting that $u = \frac{1}{\sqrt{2}}(1, i)$,

$$|u\rangle\langle u|^{\otimes n} + |\overline{u}\rangle\langle\overline{u}|^{\otimes n} \in \mathcal{M}_d[\vee^n(\mathbb{R})]$$

and is an extension of $|u\rangle\langle u|^{\otimes 2} + |\overline{u}\rangle\langle\overline{u}|^{\otimes 2}$ and is not of the form $\sum_{k=1}^{K} p_k \alpha_k^{\otimes 2}$, see [BL26].

DPS hierarchy. The extendibility hierarchy by Doherty, Parillo and Spedalieri provides semidefinite outer approximations of the set of separable states, by using ideas from the De-Finetti theorem [DPS04]. We define the notion of DPS extendible states.

Definition 4.16 (DPS extendibility [DPS04])**.** Let $X \in \mathrm{Herm}[\mathcal{M}_d \otimes \mathcal{M}_d]$ such that $X \succeq 0$. Then, X is r-PPT extendible if there exists a matrix $\tilde{X} \in \mathrm{Herm}[\mathcal{M}_d \otimes \vee^{r+1}\mathcal{M}_d]$ satisfying $\tilde{X} \succeq 0$ such that

$$\mathrm{Tr}_{[r+1]\setminus\{1,2\}}(\tilde{X}) = X.$$

and $\tilde{X}$ is PPT across all bi-partitions.

The convex cones of DPS r-extendible states is denoted as $\mathrm{DPS}_d^{(r)}$. If

$$X = \sum_{k=1}^{K} |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k|,$$

then, we have the state extension

$$\tilde{X} = \sum_{k=1}^{K} \frac{1}{||w_k||^{2r}} |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k|^{\otimes r+1} \subseteq \mathrm{Herm}[\mathcal{M}_d \otimes \vee^{r+1}\mathcal{M}_d].$$

Moreover, we have the following sequence of inclusions between the sets,

$$\mathrm{Sep}_d \subseteq \cdots \subseteq \mathrm{DPS}_d^{(r)} \subseteq \cdots \subseteq \mathrm{DPS}_d^{(2)} \subseteq \mathrm{DPS}_d^{(1)} = \mathrm{PPT}_d$$

such that it converges to the set of separable states, which follows from the De-Finetti theorem

$$\bigcap_{r=1}^{\infty} \mathrm{DPS}_d^{(r)} = \mathrm{Sep}_d.$$

We finish by mentioning the result in [FF21], which outlines a rigorous connection of the dual of the DPS hierarchy to the *real* sum of squares, although this dual connection to the "sum-of-squares" has been mentioned several times in the literature, and seems to be colloquial knowledge.

Theorem 4.17 ([FF21])**.** Let $F_X(v, w) = \langle v \otimes w|X|v \otimes w\rangle$ be a Hermitian complex polynomial in $\mathbb{C}[v, w, \bar{v}, \bar{w}]$. Then, the following statements are equivalent.

1. $X \in (\mathrm{DPS}_d^{(r)})^\circ$

2. There exist $\forall i \in [d], W_i \succeq 0$ such that

$$(\mathbb{I}_d \otimes \Pi_d^{(r)})(X \otimes \mathbb{I}_d^{r-1})\mathbb{I}_d \otimes \Pi_d^{(r)} = (\mathbb{I}_d \otimes \Pi_d^{(r)})W_0 + \sum_{i=1}^{d-1} W_i^{\Gamma_i}(\mathbb{I}_d \otimes \Pi_d^{(r)})$$

3. $F_X(v, w)||w||^{2m}$ is r-SOS.

Convergence of the DPS hierarchy. The closeness of approximation of the set of separable states by the DPS hierarchy *without* the PPT constraint is exactly the same as that of Theorem 5.14, i.e, of the order $O(\frac{1}{r})$. The power of the PPT constraint on the DPS hierarchy has been analyzed in [NOP09], and it can be shown that the approximation is quadratically better with the PPT constraint, i.e, $O(\frac{1}{r^2})$ for the best separable problem (BSS). Similar results have been obtained in [FF21], even for more general class of optimization problems that can be approximated using real SOS. Of course, for practical computations, this gain is partly offset by checking the PPT constraint for the extension.

Extendibility in Quantum Information. Although extendibility plays an important role in the separability problem, we mention here some other areas where extendibility plays a more physical or information-theoretic role. In [KDWW19, SMW25], a resource theory of extendibility was defined analogously to the resource theory of entanglement, which has the free states as the k-extendible states, and was used to give bounds on some tasks in quantum communication. The symmetric extendibility is also shown to have cryptographic applications connected to the generation of secret private keys [MCL06, Now16]. Moreover, a measure of entanglement called *Squashed Entanglement* is intimately connected to extendibility [LW18]; it was shown that it is small values for highly extendible states. Moreover, the extendibility and the de-Finetti type results display one of the essential features of entanglement, the inability of a system to share entanglement with multiple parties, or the *monogamy* of entanglement.

"Symmetry, as wide or as narrow as you may define its meaning, is one idea by which man through the ages has tried to comprehend and create order, beauty and perfection.

Herman Weyl

5

Symmetry and Entanglement

Symmetry has always played a central role in quantum mechanics, as it enables exact solutions to some complex problems, like calculation of atomic spectra or ground states of Hamiltonians. Also, the physical systems under consideration sometimes naturally display some symmetries. In this chapter, we discuss the aspects of quantum separability problem with symmetries. We first review the entanglement properties of quantum states with the full unitary and orthogonal group invariance, which are the popularly known Werner and Isotropic states. The rest of the discussion in this chapter will be centered around the entanglement in quantum states with local diagonal unitary and orthogonal symmetries. We finish this chapter with a review of entanglement in Bose-Symmetric states, and the Mixtures of Dicke states.

Notation	
$\mathcal{U}(d)$, $\mathcal{O}(d)$	Unitary and orthogonal groups of $d \times d$ matrices
$D\mathcal{U}_d$	Diagonal unitary group: $\{\mathrm{diag}(x) \mid x \in \mathbb{T}^d\}$
$D\mathcal{O}_d$	Diagonal orthogonal group: $\{\mathrm{diag}(x) \mid x \in \{-1,1\}^d\}$
S_n	Symmetric group of permutations on $[n]$
P_σ	Permutation operator on $(\mathbb{C}^d)^{\otimes n}$ associated to $\sigma \in S_n$
$\mathbb{F}_{d^2}$	Flip (swap) operator: $\mathbb{F}_{d^2}(\lvert v\rangle \otimes \lvert w\rangle) = \lvert w\rangle \otimes \lvert v\rangle$
$\mathbb{W}_{d^2}$	(Unnormalized) projector onto the maximally entangled state; $\mathbb{W}_{d^2} = \sum_{i,j\in[d]} \lvert ii\rangle\langle jj\rvert$
$X^{\mathrm{wer}}_{a,b}$	Werner states: two-parameter family of $\mathcal{U}(d)$-invariant states
$X^{\mathrm{iso}}_{a,b}$	Isotropic states: two-parameter family of $(U \otimes \overline{U})$-invariant states

continued on next page

$X^{\mathrm{bra}}_{a,b,c}$	Brauer states: three-parameter family of $\mathcal{O}(d)$-invariant states
Π_Φ, $\Pi_{\ydiagram{1,1}}$, $\Pi_{\ydiagram{2}}$	Orthogonal projectors onto the maximally entangled, antisymmetric, and symmetric subspaces
LDUI_d	Local Diagonal Unitary Invariant states
CLDUI_d	Conjugate Local Diagonal Unitary Invariant states
LDOI_d	Local Diagonal Orthogonal Invariant states
$X^{\mathrm{LDOI}}_{(A,B,C)}$	LDOI state parametrized by matrix triple (A, B, C)
$X^{\mathrm{LDUI}}_{(A,C)}$, $X^{\mathrm{CLDUI}}_{(A,B)}$	LDUI and CLDUI state parametrizations
$\mathcal{M}^{\times 3}_{\mathbb{C}^d}$	Linear space of matrix triples (A, B, C) with common diagonal
TCP_d	Triplewise Completely Positive matrix triples; separability cone for LDOI states
PCP_d	Pairwise Completely Positive matrix pairs; separability cone for (C)LDUI states
DUC	Diagonal Unitary Covariant linear maps
CDUC	Conjugate Diagonal Unitary Covariant linear maps
DOC	Diagonal Orthogonal Covariant linear maps
$\Phi_{A,B,C}$	DOC map parametrized by matrix triple (A, B, C)
$\vee^n \mathbb{C}^d$	Symmetric subspace of $(\mathbb{C}^d)^{\otimes n}$
$\Pi^{(n)}_d$	Orthogonal projection onto $\vee^n \mathbb{C}^d$; $\Pi^{(n)}_d = \frac{1}{n!}\sum_{\pi\in S_n} P_\pi$
$\lvert D_\alpha\rangle$	Qudit Dicke state labeled by occupation vector $\alpha \in \mathbb{N}^{(n)}_d$
$\mathsf{BosSep}^{(n)}_d$	Fully separable bosonic states: $\mathrm{cone}\{\lvert v\rangle\langle v\rvert^{\otimes n} \mid \lvert v\rangle \in \mathbb{C}^d\}$
$\mathsf{BosEW}^{(n)}_d$	Bosonic entanglement witnesses; conic dual of $\mathsf{BosSep}^{(n)}_d$
$\mathsf{BosPPT}^{(n,k)}_d$	Bosonic states with PPT across the $k:(n-k)$ bipartition

continued on next page

$\mathsf{BosDec}_d^{(n,k)}$	Decomposable bosonic matrices; conic dual of $\mathsf{BosPPT}_d^{(n,k)}$
$\mathsf{BExt}_d^{(n,r)}$	(n,r)-hypergraph bosonic extendible states
$\mathsf{PPTBExt}_d^{(n,r)}$	(n,r)-hypergraph PPT bosonic extendible states

5.1 UNITARY AND ORTHOGONAL SYMMETRIES

Werner, Isotropic and Brauer states. Recall that $\mathcal{U}(d)$ and $\mathcal{O}(d)$ are respectively the groups of unitary and orthogonal matrices. For $\rho \in \mathrm{Herm}[\mathcal{M}_d \otimes \mathcal{M}_d]$, we have the following families of symmetric states.

State	Invariance condition
Werner [Wer89]	$\forall U \in \mathcal{U}(d) : (U \otimes U)\, \rho\, (U \otimes U)^* = \rho$
Isotropic [HH99]	$\forall U \in \mathcal{U}(d) : (U \otimes \overline{U})\, \rho\, (U \otimes \overline{U})^* = \rho$
Brauer [Key02]	$\forall O \in \mathcal{O}(d) : (O \otimes O)\, \rho\, (O \otimes O)^T = \rho$

Observe that every Werner and every isotropic state is automatically a Brauer state: Since the Werner and isotropic states are invariant to a larger set of group elements that also contain every orthogonal group element. Let $\mathbb{I}_{d^2}$ and $\mathbb{F}_{d^2}$ denote the identity and the flip matrix. Then, the Brauer states are parametrized by three parameters.

$$X^{\mathrm{bra}}_{a,b,c} := a\frac{\mathbb{I}_{d^2}}{d^2} + b\frac{\mathbb{F}_{d^2}}{d} + c\frac{\mathbb{W}_{d^2}}{d}.$$

Moreover, the Werner and the Isotropic states are the two parameter subsets of Brauer states, by setting $c = 0$ and $b = 0$ respectively.

$$X^{\mathrm{wer}}_{a,b} := a\,\frac{\mathbb{I}_{d^2}}{d^2} + b\,\frac{\mathbb{F}_{d^2}}{d} \qquad X^{\mathrm{iso}}_{a,b} := a\,\mathbb{I}_d + b\,\frac{\mathbb{W}_{d^2}}{d}.$$

Theorem 5.1 ([VW01, PJPY24]). For the class of Brauer states, and the subclasses of Werner states and Isotropic states, the separability property is equivalent to the PPT for all dimensions.

$$X^{\mathrm{iso/wer/bra}}_{a,b,c} \in \mathrm{Sep}_d \iff X^{\mathrm{iso/wer/bra}}_{a,b,c} \in \mathrm{PPT}_d$$

Sometimes, it is convenient to parametrize these states differently to characterize separability. We define the following orthogonal projectors.

$$\Pi_{\varnothing} := \frac{\mathbb{W}_{d^2}}{d}, \quad \Pi_{\square\atop\square} := \frac{\mathbb{I}_{d^2} - \mathbb{F}_{d^2}}{2}, \quad \Pi_{\square\square} := \frac{\mathbb{I}_{d^2} + \mathbb{F}_{d^2}}{2} - \frac{\mathbb{W}_{d^2}}{d} \tag{3}$$

The three classes of states can also be parameterized as follows:

1. The Werner states form a one-parameter family, parameterized by $q \in [0,1]$, given by a convex combination of the normalised antisymmetric and symmetric projectors:

$$q \cdot \frac{\Pi_{\square\atop\square}}{\mathrm{Tr}[\Pi_{\square\atop\square}]} + (1-q) \cdot \frac{I - \Pi_{\square\atop\square}}{\mathrm{Tr}[I - \Pi_{\square\atop\square}]}. \tag{4}$$

   This is separable if and only if $q \leq \frac{1}{2}$ [Wer89].

2. The isotropic states form a one-parameter family, parameterized by $p \in [0,1]$, given by a convex combination of the maximally entangled state and the normalized projection onto its orthogonal complement:

$$p \cdot \Pi_{\Phi} + (1-p) \cdot \frac{I - \Pi_{\Phi}}{\mathrm{Tr}[I - \Pi_{\Phi}]}. \tag{5}$$

   This is separable if and only if $p \leq \frac{1}{d}$ [HH99].

3. The Brauer states form a two-parameter family, parameterized by $p, q \in [0,1]$ with $p + q \leq 1$, given by a convex combination of all three normalized orthogonal projectors:

$$p \cdot \Pi_{\Phi} + q \cdot \frac{\Pi_{\square\atop\square}}{\mathrm{Tr}[\Pi_{\square\atop\square}]} + (1-p-q) \cdot \frac{\Pi_{\square\square}}{\mathrm{Tr}[\Pi_{\square\square}]}. \tag{6}$$

   This is separable if and only if $p \leq \frac{1}{d}$ and $q \leq \frac{1}{2}$[Key02].

Extendibility of Werner, Isotropic and Brauer states. We present here a few known results about the de-Finetti (or graph) extendibility of these states [SJZ24, ACG+26]. Firstly, note that the class of Brauer states is invariant under the conjugation by the Flip operator.

$$\mathbb{F}_{d^2} X^{\mathrm{bra}}_{a,b,c} \mathbb{F}_{d^2} = X^{\mathrm{bra}}_{a,b,c}.$$

This is necessary for de-Finetti extendibility of any state. The quantum states that are completely *graph* extendible are separable, but they form *strict* subset of all separable Brauer states. For the parametrization in Eq. (4), Eq. (26) and Eq. (6), the following results about extendibility was shown in [ACG+26]; see also [SJZ24].

States	Parameter ranges for n-extendibility
Werner	$q \leq \frac{d-1}{2d} \cdot \frac{(n+k+d)(n-k)}{n(n-1)} + \frac{k(k-1)}{n(n-1)}, \quad k = n \bmod d$
Brauer	$p \leq \frac{1}{d} + \left(1 - \frac{1}{d}\right) \frac{1}{n + n \bmod 2 - 1}, \quad q \leq q_W(n,d)$
Isotropic	$p \leq \begin{cases} \frac{1}{d^2} + \left(1 - \frac{1}{d^2}\right) \frac{1}{n + n \bmod 2 - 1} & \text{if } d > n \text{ or } d \text{ or } n \text{ even}, \\ \frac{1}{d^2} + \left(1 - \frac{1}{d^2}\right) \min\left\{\frac{2d+1}{2dn+1}, \frac{1}{n-1}\right\} & \text{if } n \geq d \text{ and both odd} \end{cases}$

Table 10: de-Finetti Extendibility of Werner, Isotropic and Brauer states [ACG+26].

Family	**Limiting set ($n \to \infty$)**
Werner	$q \leq \frac{d-1}{2d}$
Brauer	$p \leq \frac{1}{d}, \quad q \leq \frac{d-1}{2d}$
Isotropic	$p \leq \frac{1}{d^2}$

Table 11: Limiting separability bounds as $n \to \infty$.

5.2 DIAGONAL UNITARY AND ORTHOGONAL SYMMETRY

LDUI, CLDUI and LDOI states. Let $D\mathcal{U}_d := \{\mathrm{diag}(x) \mid x \in \mathbb{T}^d\}$ be the group of diagonal unitary matrices, and $D\mathcal{O}_d := \{\mathrm{diag}(x) \mid x \in \{-1,1\}^d\}$ be the group of diagonal orthogonal matrices. Then, we have the following families of invariant states [SN21, JM19].

Acronym	Name	Invariance condition
LDUI	Local Diagonal Unitary Invariant	$\forall U \in D\mathcal{U}(d) : (U \otimes U)\,\rho\,(U \otimes U)^* = \rho$
CLDUI	Conjugate Local Diagonal Unitary Invariant	$\forall U \in D\mathcal{U}(d) : (U \otimes \overline{U})\,\rho\,(U \otimes \overline{U})^* = \rho$
LDOI	Local Diagonal Orthogonal Invariant	$\forall O \in D\mathcal{O}(d) : (O \otimes O)\,\rho\,(O \otimes O)^T = \rho$

We denote the linear spaces corresponding to the LDUI, CLDUI, and LDOI states as LDUI_d, CLDUI_d and LDOI_d respectively. Note that $\mathrm{LDUI}_d \cup \mathrm{CLDUI}_d \subseteq \mathrm{LDOI}_d$. Due to the symmetry properties, these matrices are highly sparse, hence, it is useful to re-parametrize them.

Sparsity Pattern and Linear Structure. We define the following sets of matrix triples with common diagonals.

$$\mathcal{M}_{\mathbb{C}^d}^{\times 3} := \{(A, B, C) \in \mathcal{M}_d^{\times 3} \mid \mathrm{diag}(A) = \mathrm{diag}(B) = \mathrm{diag}(C)\}.$$

This forms a linear space (with element-wise addition) over the complex numbers. By counting the number of parameters, it is easy to see that the dimension of this space is $3d^2 - 2d$, as each matrix has d^2 elements and we subtract $2d$ because of the common diagonals. Then, we have the following isomorphism $\mathrm{LDOI}_d \cong \mathcal{M}_{\mathbb{C}^d}^{\times 3}$.

$$X_{(A,B,C)}^{\mathrm{LDOI}} := \sum_{i,j\in[d]} A_{ij}\,|ij\rangle\langle ij| + \sum_{i\neq j\in[d]} B_{ij}\,|ii\rangle\langle jj| + \sum_{i\neq j\in[d]} C_{ij}\,|ij\rangle\langle ji|\,.$$

Moreover, we have, $\mathrm{LDUI}_d \cong \mathrm{CLDUI}_d \cong \mathcal{M}_{\mathbb{C}^d}^{\times 2}$ with the respective parametrization.

$$X_{(A,C)}^{\mathrm{LDUI}} := \sum_{i,j\in[d]} A_{ij}\,|ij\rangle\langle ij| + \sum_{i\neq j\in[d]} C_{ij}\,|ij\rangle\langle ji|\,.$$

$$X_{(A,B)}^{\mathrm{CLDUI}} := \sum_{i,j\in[d]} A_{ij}\,|ij\rangle\langle ij| + \sum_{i\neq j\in[d]} B_{ij}\,|ii\rangle\langle jj|\,.$$

These matrices also have a block-diagonal structure in the computational basis, which is state in the next theorem [SN21].

Theorem 5.2 (LDOI spectrum [SN21]). The LDOI state $X^{\mathrm{LDOI}}_{(A,B,C)}$ can be block diagonalized as

$$X^{\mathrm{LDOI}}_{(A,B,C)} \cong B \bigoplus \oplus_{i<j} \begin{pmatrix} A_{ij} & C_{ij} \\ C_{ji} & A_{ji} \end{pmatrix}.$$

From this, we can obtain the block-diagonalization of LDUI and CLDUI matrices,

$$X^{\mathrm{LDUI}}_{(A,C)} \cong \oplus_{i\leq j} \begin{pmatrix} A_{ij} & C_{ij} \\ C_{ji} & A_{ji} \end{pmatrix} \quad X^{\mathrm{CLDUI}}_{(A,B)} \cong B \bigoplus \oplus_{i\neq j\in[d]} \{A_{ij}\}.$$

Moreover, we can construct the HS inner product of LDOI states in terms of the matrix triples. We use $\tilde{L} := L - \mathrm{diag}(L)$ to denote the matrix without its diagonal.

$$\mathrm{Tr}\left((X^{\mathrm{LDOI}}_{(A,B,C)})^* X^{\mathrm{LDOI}}_{(P,Q,R)}\right) = \mathrm{Tr}(A^*P) + \mathrm{Tr}(\tilde{B}^*\tilde{Q}) + \mathrm{Tr}(\tilde{C}^*\tilde{R}).$$

Let us finally define the real vector space

$$\mathcal{M}^{\times 3}_{\mathbb{R}^d} := \{(A,B,C) \in \mathcal{M}^{\times 3}_{\mathbb{C}^d} \mid A \in \mathcal{M}_d(\mathbb{R}) \text{ and } B, C \in \mathrm{Herm}[\mathcal{M}_d]\}.$$

For any $X^{\mathrm{LDOI}}_{(A,B,C)}$ is self-adjoint if and only if $(A,B,C) \in \mathcal{M}^{\times 3}_{\mathbb{R}^d}$.

LDOI under Permutations. The vector subspaces $\mathrm{CLDUI}_d, \mathrm{LDUI}_d, \mathrm{LDOI}_d \subseteq \mathcal{M}_d \otimes \mathcal{M}_d$ are invariant under pairwise leg permutations [SN21]:

$$\begin{aligned} F X^{(3)}_{(A,B,C)} F &= X^{(3)}_{(A^\top,B,C^\top)}, \\ \left(X^{(3)}_{(A,B,C)}\right)^\top &= X^{(3)}_{(A,B^\top,C^\top)}, \\ \left(X^{(3)}_{(A,B,C)}\right)^\times &= X^{(3)}_{(A^\top,B^\top,C)}, \\ \left(X^{(3)}_{(A,B,C)}\right)^R &= X^{(3)}_{(B,A,C)}, \end{aligned}$$

where F is the flip operator ($F|ab\rangle = |ba\rangle$), $\times$ permutes the legs of a 4-tensor diagonally and R is the realignment operation. Moreover, the space LDOI_d has the following additional symmetries:

$$\begin{aligned} \left(X^{(3)}_{(A,B,C)}\right)^\Gamma &= X^{(3)}_{(A,C,B)}, \\ F X^{(3)}_{(A,B,C)} &= X^{(3)}_{(C^\top,B,A^\top)}, \\ \left(X^{(3)}_{(A,B,C)}\right)^\top &= X^{(3)}_{(A,C^\top,B^\top)}, \\ X^{(3)}_{(A,B,C)} F &= X^{(3)}_{(C,B,A)}. \end{aligned}$$

Separability of LDOI states. In this section, we analyze the separability of LDOI states in terms of conditions on the matrix triple. To do this, the convex cone of Triplewise Completely Positive (TCP) matrices was introduced in [SN21].

Definition 5.3 (TCP)**.** A matrix triple $(A, B, C) \in \mathcal{M}_{\mathbb{R}^d}^{\times 3}$ is called Triplewise Completely Positive (TCP) if there exists a finite set of vectors $\{|v_k\rangle\}_{k=1}^K, \{|w_k\rangle\}_{k=1}^K$ such that

$$A = \sum_{k=1}^{K} |v_k \odot v_k\rangle\langle w_k \odot w_k| \quad B = \sum_{k=1}^{K} |v_k \odot w_k\rangle\langle v_k \odot w_k| \tag{7}$$

$$C = \sum_{k=1}^{K} |\overline{v_k} \odot w_k\rangle\langle \overline{v_k} \odot w_k| \tag{8}$$

The separability of LDOI states is equivalent to the TCP property of the parametrizing matrix triple [SN21].

$$X_{(A,B,C)}^{\text{LDOI}} \in \text{Sep}_d \iff (A, B, C) \in \text{TCP}_d.$$

Moreover, we can define the convex cone of Pairwise Completely Positive (PCP) Matrices as

$$\begin{aligned} \text{PCP}_d :&= \left\{(A, B) \in \mathcal{M}_{\mathbb{R}^d}^{\times 2} \;\middle|\; (A, B, \text{diag}(A)) \in \text{TCP}_d\right\} \\ &= \text{cone}(|v_k \odot v_k\rangle\langle w_k \odot w_k|, |v_k \odot w_k\rangle\langle v_k \odot w_k|) . \end{aligned}$$

For $A = B = C$, these convex cones reduce to the familiar completely positive matrices, $(A, A, A) \in \text{TCP}_d \iff (A, A) \in \text{PCP}_d \iff A \in \text{CP}_d$. Hence, these can be considered as a generalization of completely positive matrices to matrix pairs and triples [1]. Finally, generalizing the comparison matrix based sufficient condition for complete positivity, a similar condition for PCP was also identified.

Theorem 5.4 ([JM19, SN21])**.** Let (X, Y) such that it satisfies the following conditions

- $Y \succeq 0$
- $\forall i, j,\ X_{ij}X_{ji} \geq |Y_{ij}|^2$.

1 This also justifies the naming conventions of PCP and TCP.

Then, we have the following implication.

$$M(Y) \succeq 0 \implies (X, Y) \in \mathrm{PCP}_d$$

The previous result provides a non-trivial sufficient criterion for separability for (C)LDUI states. The converse of the previous theorem is false, as the condition $M(Y) \succeq 0$ is equivalent to the $Y \in \mathrm{PCP}_d$ cone of *factor-width* 2, strictly smaller than the PCP_d cone. Since CP membership is NP-hard, this also implies a similar hardness for PCP and TCP. Moreover, for $d > 4$, the non-existence of any semidefinite representation of CP matrices implies the same for these convex cones. The remaining case is that of PCP_3 matrices.

PPT relaxation. The conditions for which an LDOI state is PPT can be easily identified from its block diagonalization. Moreover, the partial transpose just "flips" the matrix arguments B and C for the LDOI state. Recall that the notation ≥ 0 corresponds to entrywise non-negativity of the matrix while $\succeq 0$ means positive semidefinite.

Proposition 5.5 ([SN21]). We have the following equivalences for the LDOI states.

- $X^{\mathrm{LDOI}}_{(A,B,C)} \succeq 0 \iff A \geq 0, B \succeq 0, A_{ij}A_{ji} \geq |C_{ij}|^2$.
- $(X^{\mathrm{LDOI}}_{(A,B,C)})^\Gamma \succeq 0 \iff A \geq 0, C \succeq 0, A_{ij}A_{ji} \geq |B_{ij}|^2$.
- $(X^{\mathrm{LDOI}}_{(A,B,C)})$ is PPT iff $A \geq 0$ and $B, C \succeq 0, A_{ij}A_{ji} \geq |B_{ij}|^2, |C_{ij}|^2$.

Diagonally Covariant Channels. We consider the diagonal unitary covariance conditions of linear maps. The covariance of the map has an exact correspondence with the symmetry of the Choi-matrix, that allow us to rephrase the results about the states in this language. The following classes of linear maps were introduced and studied in [SN21].

By $\delta_X : \mathcal{M}_d \to \mathcal{M}_d$, we denote the following "classical" map.

$$\delta_X(A) := \sum_{i\in[d]} \sum_{j\in[d]} X_{ij}A_{jj} \left|i\right\rangle\!\left\langle i\right| .$$

Then, every DOC map has the following form [SN21].

$$\forall A \in \mathcal{M}_d, \quad \Phi_{X,Y,Z}(A) = \delta_X(A) + \mathring{Y} \odot \mathring{A} + \mathring{Z} \odot \mathring{A}^T$$

The Choi-matrix of a DOC map is exactly the LDOI state with the same parameters,

$$C(\Phi_{A,B,C}) = X^{\mathrm{LDOI}}_{A,B,C}.$$

Acronym	Name	Covariance condition
DUC	Diagonal Unitary Covariant	$\forall U \in D\mathcal{U}(d):\ U\Phi(X)U^* = \Phi(UXU^*)$
CDUC	Conjugate Diagonal Unitary Covariant	$\forall U \in D\mathcal{U}(d):\ U\Phi(X)U^* = \Phi(\overline{U}XU)$
DOC	Diagonal Orthogonal Covariant	$\forall O \in D\mathcal{O}(d):\ O\Phi(X)O = \Phi(OXO)$

Permutation symmetries. In general, the membership in TCP is complex, and sometimes it is beneficial to impose further permutation symmetries on the matrices A, B and C. Let G be a subgroup of permutations S_d. Then, we define the linear space of G-invariant triples,

$$\mathcal{M}^{\times 3}_{\mathbb{R}^d}[G] := \{(A_1, A_2, A_3) \in \mathcal{M}^{\times 3}_{\mathbb{C}^d} \mid \forall i, \pi \in G, [P_\pi, A_i] = 0\}.$$

If G is the group of all permutations S_d, these matrices have equal entries on the off-diagonal and on the diagonals.

$$A_i = \lambda_i \mathbb{I}_d + \mu_i \tilde{\mathbb{J}}_d$$

where $\lambda_1 = \lambda_2 = \lambda_3$. These are the hyper-octahedral states that were studied in [PJPY24]. For this class of states, it was shown that PPT=Sep for *all* d. Note that the Werner, Isotropic and Brauer states also belong to this class, hence this generalizes the result in Theorem 5.1.

$\triangle$-free LDOI states and PPT entanglement. The LDOI states can be used to generate some high dimensional examples of PPT entangled states. This was accomplished in [Sin21], by using the comparison matrix criterion, and the graph of the matrix A. Let $X^{\text{LDOI}}_{(A,B,C)}$ be an LDOI state such that the graph $G(A)$ is triangle-free. Then, it can be shown that for all separable states $M(B)$ and $M(C)$ are positive semidefinite matrices thus providing a necessary criterion for separability. This can be used to show that the following PPT LDOI state $\mathcal{M}_4 \otimes \mathcal{M}_4$ is PPT entangled.

Schur Product Maps. Consider the following linear map $\Phi : \mathcal{M}_d \to \mathcal{M}_d$ defined as

$$\Phi(X) = B \odot X.$$

This is known as the Schur Multipliers [HLP+18]. Moreover, some of the entanglement-theoretic properties of this map are easy to characterize. From the Schur-Product theorem, it follows that this map is positive iff $B \succeq 0$ and trace preserving if $\text{diag}(B) = \mathbb{I}_d$. Moreover, positivity of this map also implies complete positivity. Also, it can be shown

that this map is PPT if and only if B is diagonal, which implies that it is also entanglement breaking.

In [KMP17], the following modifications of the Schur-Product Maps were considered, labelled by a parameter t and the adjacency matrix of a graph G.

$$\Phi_{t,G}(X) = t\,\mathrm{Tr}(X)\frac{\mathbb{I}_d}{d} + A_G \odot X.$$

Then, it was shown that this map is completely positive if and only if it is PPT, which is iff $t \geq \lambda_{\min}(A_G)$ [KMP17]. Moreover, the minimum value of t such that the map is positive satisfies [KMP17].

$$t_{\mathrm{pos}} \geq \max\left\{1,\ -\lambda_{\min}(A_G),\ \frac{-d\,\lambda_{\min}(A_G)}{|E|},\ \frac{\lambda_{\max}(A_G)}{\vartheta(G)-1}\right\}.$$

Here $\vartheta(G)$ is the *Lovasz* theta number of the graph [Lov79].

Generalized Choi Maps. The famous Choi map $\Phi_c : \mathcal{M}_3 \to \mathcal{M}_3$ was the first example of a positive *indecomposable map* [Cho82, Cho80b]. The Choi map is a DUC linear map with the following parametrization,

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \quad B = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}.$$

Many generalizations of the Choi-Map have been introduced in the literature, and most of them still preserve the LDOI structure. One such generalization [CKL92] is obtained by replacing A by a general circulant 3×3 matrix.

$$A = \begin{pmatrix} a & b & c \\ c & a & b \\ b & c & a \end{pmatrix} \quad B = \begin{pmatrix} a & -1 & -1 \\ -1 & a & -1 \\ -1 & -1 & a \end{pmatrix}.$$

Theorem 5.6 ([CKL92])**.** The linear map $\Phi[a, b, c]$ is positive if and only if the following three conditions are satisfied:

$$a \geq 1, \tag{9}$$

$$a + b + c \geq 3, \tag{10}$$

$$bc \geq (2-a)^2 \quad \text{if } 1 \leq a \leq 2. \tag{11}$$

The linear map $\Phi[a, b, c]$ is decomposable if and only if the following two conditions are satisfied:

$$a \geq 1, \tag{12}$$

$$bc \geq \left(\frac{3-a}{2}\right)^2 \quad \text{if } 1 \leq a \leq 3. \tag{13}$$

A generalization of the Choi map to $d > 3$ was considered in [TT88, Ha03]. For more generalizations of Choi-type map beyond the circulant scenario, see [CMR18, BSSC25]. For other known classes of positive linear maps that have the diagonal symmetry, see also [SN21, Example 7.5].

PPT squared conjecture. The class of DOC maps are preserved under composition. Moreover, the composition condition can be also understood in terms of the parametrizing matrix triples [SN21],

$$\Phi_{A_1,B_1,C_1} \circ \Phi_{A_2,B_2,C_2} = \Phi_{A,B,C} \tag{14}$$

$$A = A_1 A_2, \quad B = B_1 \odot B_2 + C_1 \odot C_2^T - \operatorname{diag}\Big(B_1 \odot B_2 + C_1 \odot C_2^T - A_1 \odot A_2\Big),$$
$$C = B_1 \odot C_2 + C_1 \odot B_2^T - \operatorname{diag}\Big(B_1 \odot C_2 + C_1 \odot B_2^T - A_1 \odot A_2\Big).$$

Recall that the PPT squared conjecture posits that the composition of two PPT maps is entanglement breaking. This conjecture holds for the DOC maps Φ_{A_1,B_1,C_1} and Φ_{A_1,B_1,C_2} if either C_1 or C_2 is diagonal [NP25, SN22a], while the methods employed do not extend to the general DOC channels. It was also shown that it holds *generically* for two random (but even correlated) PPT DOC channels [NP25].

5.3 BOSE SYMMETRY AND MIXTURES OF DICKE STATES

In this section, we consider the separability problem in the class of quantum states with permutation symmetry [ISTY08, TG09]. This symmetry acts on the states by leaving it invariant under exchange of particles, and provides some interesting aspects to the separability problem. For bipartite systems, some of the known entanglement criterion are equivalent to just PPT, while for *multi*-partite systems, either the states are *genuinely* multipartite entangled, or fully separable. We finally discuss the class of *mixtures* of Dicke states, the class of bosonic states with diagonal symmetries, and discuss the correspondence with completely positive, and doubly non-negative matrices.

Symmetric Subspace. We first recall some facts about the symmetric subspace. Let $\sigma \in S_n$ be a bijection from $[n] \to [n]$ and $P_\sigma \in \mathcal{M}_d^{\otimes n}$ be the permutation matrix defined as :

$$P_\sigma := \sum_{i \in [d]^n} |i_1 i_2 \dots i_n\rangle\langle i_{\sigma^{-1}(1)} i_{\sigma^{-1}(2)} \dots i_{\sigma^{-1}(n)}|.$$

For $n = 2$, we have only two possible permutation operators, corresponding to the identity permutation, $P_{\mathsf{id}} =: \mathbb{I}_d \otimes \mathbb{I}_d$ and the flip permutation, $P_{(12)} := F$.

The symmetric subspace of order n and local dimension d is the linear space of vectors $|\psi\rangle \in (\mathbb{C}^d)^{\otimes n}$ that are invariant under all permutations.

$$\vee^n \mathbb{C}^d := \{|\psi\rangle \in (\mathbb{C}^d)^{\otimes n} \mid \forall \pi \in S_n,\ P_\pi |\psi\rangle = |\psi\rangle\}.$$

The symmetric subspace has an equivalent description as the following span [Har13, Theorem 3]:

$$\vee^n \mathbb{C}^d = \mathrm{span}_{\mathbb{C}}\{|\psi\rangle^{\otimes n} \mid |\psi\rangle \in \mathbb{C}^d\}. \tag{15}$$

Moreover, the orthogonal projection into the symmetric subspace $\Pi_d^{(n)} : (\mathbb{C}^d)^{\otimes n} \to \vee^n \mathbb{C}^d$ can be explicitly constructed by the sum of the permutation operators,

$$\Pi_d^{(n)} := \frac{1}{n!} \sum_{\pi \in S_n} P_\pi.$$

Let $\alpha \in \mathbb{N}^d$ be a vector of natural numbers, such that $|\alpha| := \sum_{i \in [d]} \alpha_i = n$. We will denote the set of all such vectors as $\mathbb{N}_d^{(n)}$. We define the counting function, $\gamma : [d]^n \to \mathbb{N}_d^{(n)}$ with the components $\gamma(i)_j := |\{k \in [n] \mid i_k = j\}|$ that count the number of elements of the multi-index that get mapped to the value j. For all occupation vectors $\alpha \in \mathbb{N}_d^{(n)}$, there is a *unique* canonical multi-index (α) in $\gamma^{-1}(\alpha)$ that satisfies the ordering, $(\alpha)_1 \leq (\alpha)_2 \dots \leq (\alpha)_n$.

We define the following pure quantum states labeled by $\alpha \in \mathbb{N}_d^{(n)}$,

$$|D_\alpha\rangle := \frac{1}{\sqrt{\binom{n}{\alpha}}} \sum_{i \in [d]^n : \gamma(i) = \alpha} |i\rangle \in (\mathbb{C}^d)^{\otimes n},$$

where $\binom{n}{\alpha} = \frac{n!}{\alpha_1! \alpha_2! \dots \alpha_d!}$ is the multinomial coefficient. These states are known as *qudit Dicke states*, and vector α is called the *occupation vector*.

It is easy to verify that $\Pi_d^{(n)} |D_\alpha\rangle = |D_\alpha\rangle$ for all $\alpha \in \mathbb{N}_d^{(n)}$, hence the Dicke states are symmetric. These states form an ortho-*normal* basis for the symmetric subspace $\vee^n \mathbb{C}^d$. This also implies that the cardinality of the set $\mathbb{N}_d^{(n)}$ is equal to the dimension of the symmetric subspace,

$$d_{\mathsf{sym}} = \dim(\vee^n \mathbb{C}^d) = |\mathbb{N}_d^{(n)}| = \binom{d+n-1}{d-1} = \binom{d+n-1}{n}.$$

For $n = 1$, the Dicke states are just equal to the computational basis:

$$|D_{(0,\ldots,1_i,\ldots,0)}\rangle = |i\rangle\,.$$

Bosonic States. The matrices that are supported only on the symmetric subspace are called Bose-Symmetric, or Bosonic. We have some equivalent characterizations of Bosonic matrix $X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$.

(1) $X = \Pi_d^{(n)} X \Pi_d^{(n)}$.

(2) $\mathrm{ran}(X), \mathrm{ran}(X^*) \subseteq \vee^n \mathbb{C}^d$.

(3) $\forall \sigma \in S_n, \quad X = P_\sigma X = X P_\sigma$.

Proof. We show that all the above definitions are equivalent.

(1) $\implies$ (2). We observe that, $\mathrm{ran}(\Pi_d^{(n)} X \Pi_d^{(n)}) \subseteq \mathrm{ran}(\Pi_d^{(n)}) = \vee^n \mathbb{C}^d$, and the same for the adjoint.

(2) $\implies$ (3). Let $|\psi\rangle \in \mathbb{C}^d$. We have, $X|\psi\rangle \in \vee^n \mathbb{C}^d$ as $\mathrm{ran}(X) \in \vee^n \mathbb{C}^d$. This shows,

$$\forall \sigma, |\psi\rangle \in \mathbb{C}^d, \quad P_\sigma X |\psi\rangle = X |\psi\rangle\,.$$

Also, by a similar argument, we have,

$$\forall \sigma, |\psi\rangle \in \mathbb{C}^d, \quad P_\sigma X^* |\psi\rangle = X^* |\psi\rangle \implies (X P_\sigma)^* = X^* \implies X P_\sigma = X.$$

(3) $\implies$ (1). $X = P_\sigma X \implies X = \frac{1}{n!} \sum_{\sigma \in S_n} P_\sigma X = \Pi_d^{(n)} X$. Similarly, we have, $X = X \Pi_d^{(n)}$. This completes the proof.

■

We denote the linear space of bosonic matrices as

$$\mathcal{M}[\vee^n \mathbb{C}^d] := \{X \in \mathcal{M}_d^{\otimes n} \mid X = \Pi_d^{(n)} X \Pi_d^{(n)}\}$$

and the real linear space of hermitian bosonic matrices as

$$\mathrm{Herm}[\vee^n \mathbb{C}^d] := \{X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid X = \Pi_d^{(n)} X \Pi_d^{(n)}\}.$$

From [Har13, Section 1.1], we also have the following descriptions of these spaces.

$$\mathcal{M}[\vee^n \mathbb{C}^d] = \mathrm{span}_{\mathbb{C}} \left\{ |\psi\rangle\langle\psi|^{\otimes n} \;\middle|\; |\psi\rangle \in \mathbb{C}^d \right\}, \tag{16}$$

$$\mathrm{Herm}[\vee^n \mathbb{C}^d] = \mathrm{span}_{\mathbb{R}} \left\{ |\psi\rangle\langle\psi|^{\otimes n} \;\middle|\; |\psi\rangle \in \mathbb{C}^d \right\}. \tag{17}$$

Entanglement in Bosonic States. Firstly, we set up the general theory of entanglement for bosonic states in multipartite systems. In contrast to general states, for *multipartite* bosonic states, the permutation symmetry leads to a simplification of the entanglement structure.

Theorem 5.7 ([ISTY08, Theorem 1])**.** Let $X \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$. Then, the state has entanglement depth 1 or n. Particularly, if it has entanglement depth 1, there exist $\{|v_k\rangle\}_{k=1}^K$ such that,

$$X = \sum_{k=1}^{K} |v_k\rangle\langle v_k|^{\otimes n}.$$

We denote all *fully* separable bosonic states (entanglement depth = 1) as

$$\mathsf{BosSep}_d^{(n)} := \mathrm{cone}\{|v_k\rangle\langle v_k|^{\otimes n} \mid |v_k\rangle \in \mathbb{C}^d\}, \tag{18}$$

which forms a proper convex cone. The dual to this the set of Bosonic entanglement witness (EW).

$$\mathsf{BosEW}_d^{(n)} := \left(\mathsf{BosSep}_d^{(n)}\right)^\circ.$$

It is easy to see that $O \in \mathsf{BosEW}_d^{(n)}$ if and only if

$$\forall\, |v\rangle \in \mathbb{C}^d \quad \langle v^{\otimes n}|O|v^{\otimes n}\rangle \geq 0.$$

Recall that all *bipartite* separable states satisfy the PPT (Positivity under Partial Transposition) property, i.e, PPT is a necessary condition for separability. The separable bosonic states (ref. Theorem 5.7) are separable across any bipartitions; hence, they also satisfy the PPT property across *each* such partition. In general, a bosonic state might only satisfy the PPT property across some bipartitions, and not all. Let I be a subset of $[n]$. We use Γ_I to denote the partial transpose of the systems indexed by I. We can use bosonic symmetry to show that the PPT property only depends on the size of the bipartition we consider while applying the partial transpose, and not on the particular systems that are transposed.

Proposition 5.8. (PPT in symmetric states) Let $\rho \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$ be a bosonic matrix. Let I and J be arbitrary subsets of $[n]$ such that $|I| = |J|$. Then,

$$\rho^{\Gamma_I} \geq 0 \iff \rho^{\Gamma_J} \geq 0.$$

Proof. For a bosonic state, we have,

$$\forall \pi \in S_n \; P_\pi \rho P_{\pi^{-1}} = \rho.$$

Let π be a permutation that maps the elements of the set I to J. Then,

$$\rho^{\Gamma_I} = (P_\pi \rho P_{\pi^{-1}})^{\Gamma_I} = (P_\pi \rho^{\Gamma_J} P_{\pi^{-1}}). \quad \blacksquare$$

Therefore, following the previous Proposition 5.8, consider the following convex cones.

Definition 5.9. BosPPT cones Let $0 \leq k \leq \lfloor n/2 \rfloor$. We define the following convex cones,

$$\mathsf{BosPPT}_d^{(n,0)} := \{\rho \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \rho \geq 0\}$$
$$\mathsf{BosPPT}_d^{(n,k)} := \{\rho \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \rho^{\Gamma_{[k]}} \geq 0\}.$$

Note that $\mathsf{BosPPT}^{(n,0)}$ is the bosonic PSD matrices, and $\mathsf{BosPPT}^{(n,k)}$ is the set of bosonic matrices having the PPT property across the bipartition $[k] : [n]\backslash[k]$. Clearly, all the separable states (see Eq. (18), Theorem 5.7) satisfy the following inclusion.

$$\mathsf{BosSep}_d^{(n)} \subseteq \bigcap_{k=0}^{\lfloor n/2 \rfloor} \mathsf{BosPPT}_d^{(n,k)} =: \mathsf{BosPPT}_d^{(n)}. \tag{19}$$

This means that the separable states satisfy the PPT property across all the bipartitions.

We now introduce the conic dual of the PPT sets. Note that we will consider the conic dual in the ambient space of $\mathrm{Herm}[\vee^n \mathbb{C}^d] \subseteq \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$. We define the following convex cone of decomposable bosonic matrices,

$$\mathsf{BosDec}_d^{(n,k)} := \left(\mathsf{BosPPT}_d^{(n,k)}\right)^\circ.$$

We also have the following characterization of the $\mathsf{BosDec}_d^{(n,k)}$.

Theorem 5.10. $O \in \mathsf{BosDec}_d^{(n,k)}$ if and only if there exist positive semi-definite operators, $P \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$ such that,

$$O \;=\; \Pi_d^{(n)} (P^{\Gamma_{[k]}}) \Pi_d^{(n)}. \tag{20}$$

Corollary 5.11. We have the following conic-duality:

$$\left(\bigcap_{k=0}^{\lfloor n/2\rfloor} \mathsf{BosPPT}_d^{(n,k)}\right)^\circ = \mathrm{cl}\left(\sum_{k=0}^{\lfloor n/2\rfloor} \mathsf{BosDec}_d^{(n,k)}\right) =: \mathsf{BosDec}_d^{(n)},$$

The latter set can be described explicitly as

$$\mathsf{BosDec}_d^{(n)} = \left\{O \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid \exists\{P_k \succeq 0\}_{k=0}^{\lfloor n/2\rfloor}, O = \Pi_d^{(n)}\left(\sum_{k=0}^{\lfloor n/2\rfloor} P_k^{\Gamma_{[k]}}\right)\Pi_d^{(n)}\right\}.$$

We have the following inclusions and dualities of convex cones in the Bosonic subspace.

$$\mathrm{BosSep}_d^{(n)} \subseteq \mathrm{BosPPT}_d^{(n,k)} \subseteq \mathrm{BosPPT}_d^{(n,0)} \subseteq \mathrm{BosDec}_d^{(n,k)} \subseteq \mathrm{BosEW}_d^{(n,0)}$$

For $n = 2$ and $d = 2$, i.e, in 2 qubits, the sets $\mathrm{BosPPT}_2^{(2)}$ and $\mathrm{BosSep}_2^{(2)}$ coincide, this follows from the sufficiency of the PPT criterion for general two qubit separability. This is also true for 3 qubit bosonic states [ESBL02], while for $n \geq 4$ qubits, some explicit constructions of PPT entangled states are known [TAH+12, ATSL12]; see also [TAQ+18, Section 5, Section E.1]. For bipartite states, it was shown that the CCNR, and covariance matrix tests are equivalent to PPT [TG09]; generally the CCNR and correlation matrix tests are complementary to the PPT test, and also detect some classes of PPT entangled states. In particular, we have the following equivalent descriptions of $X \in \mathrm{BosPPT}_d^{(2)}$ [TG09].

1. $\mathrm{Tr}(X(A \otimes A)) \geq 0$ for all $A \in \mathrm{Herm}[\mathcal{M}_d]$.
2. X satisfies the CCNR criterion, $\|X^{\mathrm{re}}\|_1 \leq 1$, where X^{re} denotes the realignment map and $\|\cdot\|_1$ denotes the trace norm.
3. The correlation matrix, defined via the matrix elements as

$$C_{kl} := \langle M_k \otimes M_l\rangle - \langle M_k \otimes \mathbb{1}\rangle\langle \mathbb{1} \otimes M_l\rangle \tag{21}$$

is positive semidefinite.

Moreover, to construct the PPT entangled state for 3×3 bosonic systems, [TG09] adopt a clever approach, which we describe briefly. In general, a n-qudit bosonic state has associated $\lfloor n/2\rfloor$ bipartitions. In particular, it might satisfy the PPT condition across one bipartition but not the other. Moreover, consider the basis of $\vee^4\mathbb{C}^2$,

$$\mathrm{sym}(|0000\rangle), \mathrm{sym}(|0001\rangle), \mathrm{sym}(|0011\rangle), \mathrm{sym}(|0111\rangle), \mathrm{sym}(|1111\rangle).$$

By using the mapping $|00\rangle \to |\tilde{0}\rangle\,, |01\rangle + |10\rangle \to |\tilde{1}\rangle\,, |11\rangle \to |\tilde{2}\rangle$, we can represent the basis as,

$$|\tilde{0}\tilde{0}\rangle\,, |\tilde{0}\tilde{1}\rangle + |\tilde{1}\tilde{0}\rangle\,, |\tilde{0}\tilde{2}\rangle + |\tilde{1}\tilde{1}\rangle + |\tilde{2}\tilde{0}\rangle\,, |\tilde{1}\tilde{2}\rangle + |\tilde{2}\tilde{1}\rangle\,, |\tilde{2}\tilde{2}\rangle$$

which are elements of the $\mathbb{C}^3 \vee \mathbb{C}^3$.

Moreover, this mapping also preserves separability and the PPT property, i.e a separable state in $\vee^4\mathbb{C}^2$ only if it is separable state in $\mathbb{C}^3 \vee \mathbb{C}^3$ and PPT across the bipartition $2:2$ iff PPT in the bipartite system. Therefore, any quantum state in $\mathrm{Herm}[\vee^4\mathbb{C}^2]$ that is PPT across $2:2$ bipartition, but is NPT across $3:1$ bipartition can be mapped to a PPT entangled $\mathbb{C}^3 \vee \mathbb{C}^3$ state. Such states were numerically constructed in [TG09]. For a more comprehensive review of entanglement in bosonic states, see the recent review [MMRRP$^+$25, Section 3]

Bosonic Extendibility. We finally discuss the extendibility property of Bosonic states. [DPS04, Ter04, CKMR07]. This property is concerned with the existence of an extension, i.e, a state supported on a larger number of systems, such that some chosen reductions of such a state are equal to the original quantum state. Here, we discuss the notion is well-suited to bosonic states, which we call the *hypergraph extendibility* (see also [CKMR07]), which is connected to the de-Finetti/graph extendibility [CKMR07, ACG$^+$26]. Let us begin by defining this notion.

Definition 5.12. Let $r, n \in \mathbb{N}$ be non-negative integers. A matrix $\tilde{X} \in \mathrm{Herm}[\vee^{n+r}\mathbb{C}^d]$ is called a (n,r)-*hypergraph bosonic extension* of a matrix $X \in \mathrm{Herm}[\vee^n\mathbb{C}^d]$ if both of the following conditions hold:

(1) $\tilde{X} \succeq 0$

(2) $\forall\big(A \subseteq [n+r],\ |A| = r\big) \quad \mathrm{Tr}_A(\tilde{X}) = X.$

We call such an extension a (n,r)-*hypergraph PPT bosonic extension* if the extension $\tilde{X}$ is also PPT across all bipartitions. Note that, thanks to the symmetry property, one could have replace the "$\forall$" in the second point above by an "$\exists$".

If X, Y have a (n,r)-hypergraph (PPT) bosonic extension $\tilde{X}, \tilde{Y}$ (resp.), then $\tilde{X} + \tilde{Y}$ is the (n,r)-hypergraph (PPT) bosonic extension of $X + Y$. Similarly, $\tilde{X}$ is a (n,r)-hypergraph (PPT) bosonic extension of X , then, $\lambda\tilde{X}$ is the (n,r)-hypergraph (PPT) bosonic extension

of λX. We denote these cones of (n, r)-hypergraph bosonic extendable states as $\mathsf{BExt}_d^{(n,r)}$ and (n, r)-hypergraph PPT bosonic extendable states as $\mathsf{PPTBExt}_d^{(n,r)}$, where $r \geq 0$:

$$\mathsf{BExt}_d^{(n,r)} := \{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \exists \tilde{X} \in \mathsf{PSD}_d^{(n+r)} \text{ s.t. } \mathrm{Tr}_{[r]} \tilde{X} = X\} \tag{22}$$

$$\mathsf{PPTBExt}_d^{(n,r)} := \{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \exists \tilde{X} \in \mathsf{BosPPT}_d^{(n+r)} \text{ s.t. } \mathrm{Tr}_{[r]} \tilde{X} = X\}. \tag{23}$$

Remark 5.13. Note that for $r = 0$, $\mathsf{BExt}_d^{(n,0)}$ reduces to the set of all n-partite bosonic states, while $\mathsf{PPTBExt}_d^{(n,0)}$ reduces to the set of n-partite bosonic states with all bipartitions PPT:

$$\mathsf{BExt}_d^{(n,0)} = \mathsf{PSD}_d^{(n)}$$
$$\mathsf{PPTBExt}_d^{(n,0)} = \mathsf{BosPPT}_d^{(n)}.$$

Recall that any separable state in the bosonic subspace, $X \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$ is of the form

$$X = \sum_{k=1}^{K} |v_k\rangle\langle v_k|^{\otimes n} \text{ for } |v_k\rangle \in \mathbb{C}^d.$$

Consider, for any $r \geq 0$, the following operator $\tilde{X} \in \mathrm{Herm}[\mathcal{M}_d^{\otimes(n+r)}]$:

$$\tilde{X} := \sum_{k=1}^{K} \frac{1}{||v_k||^{2r}} |v_k\rangle\langle v_k|^{\otimes(n+r)}.$$

It is easy to verify that $\tilde{X}$ is an (n, r)-hypergraph bosonic extension of X. Moreover, this extension is also PPT across all bipartitions. Hence, we have the following inclusions, showing that the newly introduced sets form a decreasing hierarchy of outer approximations of the separable set:

$$\begin{array}{ccccccccccc}
\mathsf{BosSep}_d^{(n)} & \subseteq \cdots \subseteq & \mathsf{BExt}_d^{(n,r)} & \subseteq \cdots \subseteq & \mathsf{BExt}_d^{(n,1)} & \subseteq & \mathsf{BExt}_d^{(n,0)} & = & \mathsf{PSD}_d^{(n)} \\
\| & \cdots & \cup\mathsf{I} & \cdots & \cup\mathsf{I} & & \cup\mathsf{I} & & \cup\mathsf{I} \\
\mathsf{BosSep}_d^{(n)} & \subseteq \cdots \subseteq & \mathsf{PPTBExt}_d^{(n,r)} & \subseteq \cdots \subseteq & \mathsf{PPTBExt}_d^{(n,1)} & \subseteq & \mathsf{PPTBExt}_d^{(n,0)} & = & \mathsf{BosPPT}_d^{(n)}
\end{array}$$

We have the following de-Finetti type result for bosonic extendibility (without the PPT).

Theorem 5.14. (Bosonic De-Finetti [CKMR07]) Let $X \in \mathrm{Herm}[\vee^n \mathcal{M}_d]$ be a Bosonic state such that $X \succeq 0, \mathrm{Tr}(X) = 1$. Then, there exist a finite set vec-

tors $|v_k\rangle_{k=1}^K \in \mathbb{C}^d$, with norm $\|v_k\| = 1$ and p_k be a finite probability distribution such that

$$\| \operatorname{Tr}_{[n]\setminus[m]}(X) - \sum_{k=1}^{K} p_k \, |v_k\rangle\langle v_k|^{\otimes m} \|_1 \leq 2\frac{dm}{n}$$

Note that the bound in the bosonic case is the same as for the classical case from Theorem 4.12.

Mixtures of Dicke States. Recall that the Dicke states $|D_\alpha\rangle$ form a basis of the symmetric subspace, hence for any $X \in \operatorname{Herm}[\vee^n \mathbb{C}^d]$, we have the following expansion in the Dicke basis.

$$X = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} \lambda_{\alpha,\beta} \left|D_\alpha\right\rangle\!\left\langle D_\beta\right| .$$

If we also demand that X has the diagonal unitary symmetry, it removes the off-diagonal coherence terms in the Dicke basis. To see this, note that the following

$$\forall U \in D\mathcal{U}_d \quad U^{\otimes n} X \overline{U}^{\otimes n} = X$$

implies that for all $\theta \in [0, 2\pi]^d$, we have

$$\sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} \lambda_{\alpha,\beta} \left|D_\alpha\right\rangle\!\left\langle D_\beta\right| = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} e^{i\theta\cdot(\alpha-\beta)} \lambda_{\alpha,\beta} \left|D_\alpha\right\rangle\!\left\langle D_\beta\right| .$$

Hence, this shows that $\forall \alpha, \beta \in \mathbb{N}_d^{(n)} \lambda_{\alpha,\beta} = e^{i\theta\cdot(\alpha-\beta)}\lambda_{\alpha,\beta}$. This holds for all θ if and only if $\alpha = \beta$. which shows that X is diagonal in the Dicke basis, or is a mixture of Dicke states. In the bipartite case, X has the following expression.

$$X = \sum_{i \leq j} p_{ij} \, |D_{ij}\rangle\langle D_{ij}| .$$

This class has $\frac{d(d+1)}{2}$ parameters p_{ij}. Consider the following matrix $A \in \mathcal{M}_d$ defined as

$$A_{ij} := \begin{cases} p_{ii}, & \text{if } i = j, \\ \dfrac{p_{ij}}{2}, & \text{if } i \neq j. \end{cases}$$

This allows us to write X in the LDUI/LDOI parametrization,

$$X = X_{A,A}^{\text{LDUI}} = X_{A,\operatorname{diag}(A),A}^{\text{LDOI}}.$$

Hence, by the Proposition 5.5, it is evident that the state $X^{\mathrm{LDUI}}_{A,A}$ is PPT if and only if

$$A \in \mathrm{PSD} \cap \mathrm{NN}_d = \mathrm{DNN}_d.$$

Recall the state $X^{\mathrm{LDUI}}_{A,A}$ is separable if and only if $(A, A) \in \mathrm{PCP}_d$. This is actually equivalent to the *complete positivity* of the matrix A. Since $\mathrm{DNN}_d = \mathrm{CP}_d$ for $d \leq 4$, it implies that a mixture of Dicke states is PPT if and only if it is separable [Yu16, TAQ+18].

In the multipartite case, it was shown in [QRS17, Yu16] that PPT across the most *balanced* bipartition is necessary and sufficient for the state to be separable. The general case of qudits was analysed recently in [RPAR+25], where the conditions for PPT were analysed and it was conjectured that for $d = 3, 4$, the situation is analogous to the bipartite case, i.e, there is no PPT entanglement. In the remaining cases, i.e for $d \geq 5$, any multipartite PPT state, that has any entangled bipartite state as its marginal, is automatically entangled. In Chapter 9, we discuss the extension of these results to the qudit case, and resolve the conjectures in [RPAR+25].

	$n = 2$	$n = 3$	$n \geq 4$
$d = 2$	No	No	No
$d = 3$	No	??	??
$d = 4$	No	??	??
$d \geq 5$	Yes	Yes	Yes

[TAQ+18, Yu16]

[RPAR+25]

Table 12: Is there PPT entanglement in mixtures of Dicke states of n parties and local dimension d?

Part II

PRESENTATION OF ARTICLES

6

Entanglement in cyclic sign invariant quantum states

This is the reproduction of the article **Entanglement in cyclic sign invariant quantum states**, Aabhas Gulati, Ion Nechita and Satvik Singh. J. Math. Phys. 66, 122202 (2025) [GNS25].

6.1 INTRODUCTION

With the significant advent of quantum information science over the past few decades, entanglement has emerged as a fundamental resource, with practical applications in cryptography [Eke91], communication [BBC$^+$93], and computation [RB01]. However, entanglement theory has inherent computational complexity: it is NP-hard to decide whether a given bipartite quantum state is entangled or not [Gur03]. Consequently, several sufficient conditions to detect the presence of entanglement have been developed [HHHH09]. Among them, perhaps the simplest one is the so-called positivity under partial transpose (PPT) criterion [Per96]: any unentangled (or separable) bipartite state remains positive after transposition is applied to either one of the subfactors. In low dimensions, this criterion is necessary and sufficient to detect entanglement: any qubit-qubit or qubit-qutrit quantum state is separable if and only if it is PPT [Stø63, HHH96]. However, in higher dimensions, there exist quantum states that are PPT but still entangled [Hor97]. Curiously, one cannot distill any pure entanglement from such PPT entangled states by using local operations and classical communication (LOCC) [HHH98], even though the entanglement cost of preparing such states under LOCC is non-zero [VC01, YHHSR05]. Consequently, the existence of PPT entangled states is closely related to the irreversibility of the resource theory of entanglement [VC01, LR23].

Another perspective on the complexity of entanglement is of a geometric nature. The sets of separable and PPT states in a $d \otimes d$ system are convex bodies in a high-dimensional

($d^4 - 1$) space. Consequently, these sets are difficult to characterize geometrically. One way to tackle this problem is by imposing symmetries to reduce the dimension of the state space, which makes the problem more tractable [Wer89, HH99, VW01]. The maximal (local) symmetry one can impose on a $d \otimes d$ system is that of invariance under the full unitary group $\mathcal{U}(d)$:

$$\forall U \in \mathcal{U}(d): \quad (U \otimes U)\rho(U \otimes U)^* = \rho \quad \text{or} \quad (U \otimes \bar{U})\rho(U \otimes \bar{U})^* = \rho.$$

Quantum states with this symmetry are known as *Werner* [Wer89] and *isotropic* [HH99] states, respectively. These states can be described by a single real parameter. Crucially, the convex sets of PPT and separable states coincide under this symmetry and can be characterized completely (see [VW01, Fig 1]). In other words, the constraint of full local unitary invariance is too severe to accommodate the existence of PPT entanglement. Similar results also hold for the class of states that are invariant under the full orthogonal group $\mathcal{O}(d)$ [VW01, Key02]. It is then natural to relax the symmetry constraints by considering subgroups $G \subseteq \mathcal{U}(d)$ and $H \subseteq \mathcal{O}(d)$ that are large enough to keep the dimension of the corresponding invariant spaces tractable, but not too large, lest the problem becomes trivial as above.

In recent work [NS21, SN21, Sin21], some of the authors of this work have considered the subgroups of diagonal unitary and diagonal orthogonal matrices: $G = D\mathcal{U}(d)$ and $H = D\mathcal{O}(d)$, respectively. States that are invariant under the local action of these groups (called Local Diagonal Unitary/Orthogonal Invariant or LDUI/LDOI) can be parametrized by a triple of $d \times d$ matrices (A, B, C) with a common diagonal, and the convex sets of PPT and separable states can be described by imposing suitable positivity conditions on these matrices. Except for $d = 2$, PPT is not equivalent to separability, and many examples of PPT entangled states can be constructed with this symmetry [Sin21]. A well known class of LDOI states are mixtures of the so-called *Dicke* states [Yu16] [TAQ+18], which correspond to matrix triples of the form $(A, \mathrm{diag}(A), A)$ in the LDOI parametrization. The problem of detecting entanglement for these states is equivalent to the well known complete positivity problem from optimization theory [BSM03], which is also known to be NP-hard [TAQ+18].

6.1.1 *Summary of results*

In this paper, we interpolate between the full unitary/orthogonal groups and their diagonal counterparts by considering the *cyclic phase* and *cyclic sign* subgroups: $G = \mathfrak{C}\mathcal{DU}(d) := \mathrm{Cyc}(d) \ltimes \mathcal{DU}(d)$ and $H = \mathfrak{C}\mathcal{DO}(d) := \mathrm{Cyc}(d) \ltimes \mathcal{DO}(d)$, respectively. Here, $\mathrm{Cyc}(d)$ is the abelian group of *cyclic permutations* of d elements and $\ltimes$ denotes the semi-direct

product. States that are locally invariant under these groups are called *Local Cyclic Phase Invariant* (LCPI) and *Local Cyclic Sign Invariant* (LCSI), respectively. These states lie in between the classes discussed above, satisfying reverse inclusion relations to those satisfied by the symmetry groups (see Eqs (24),(25)). The cyclic symmetry forces the (A, B, C) matrices in the LDOI parameterization of these states to be *circulant*. Consequently, these states can be parameterized by a triple of vectors (a, b, c) with a common first entry, allowing them to be expressed by $3d - 2$ parameters for a given local dimension d. Despite the highly symmetric form of these states, we will see that PPT entanglement still exists in this class for all $d \geq 3$.

$$D\mathcal{U}(d) \text{ (LDUI states)} \leq \mathfrak{C}\mathcal{D}\mathcal{U}(d) \text{ (\textbf{LCPI states})} \leq \mathcal{U}(d) \text{ (Werner/isotropic states)} \tag{24}$$

$$D\mathcal{O}(d) \text{ (LDOI states)} \leq \mathfrak{C}\mathcal{D}\mathcal{O}(d) \text{ (\textbf{LCSI states})} \leq \mathcal{O}(d) \text{ (Brauer states)} \tag{25}$$

We study the convex structure of several cones with cyclic symmetry that are relevant from the perspective of quantum information, such as the cones of positive semidefinite, PPT, and separable matrices. Each of these cones can be characterized simply by imposing some positivity conditions on the vector triples (a, b, c). In particular, we introduce the notion of *Circulant* Triplewise Completely Positive vector triples that characterizes separability for LCPI/LCSI states. This is inspired by the results in [SN21]. Crucially, the circulant structure makes the *Fourier transform* a critical tool to analyze the positivity properties of LCPI/LCSI states.

We study mixtures of Dicke states with cyclic symmetry in detail. We analyze PPT and separable states of this form, providing explicit results in low dimensions and emphasizing PPT entanglement when present. The problem of determining separability or PPT in this class reduce to a circulant version of deciding if a given matrix is completely positive or doubly non-negative, respectively [TAQ+18] [BSM03]. For all $d \geq 5$, we prove the existence of PPT entangled states in this class. Importantly, the PPT cone restricted to this family is *polyhedral*; we enumerate the extremal rays in small dimension ($d \leq 7$) and relate the general case to that of computing the *semi-positive cone* [ST18] of the Fourier matrix. We explicitly compute *all* the extremal rays of the separable cone and its dual in the first non-trivial case ($d = 5$) and provide some partial results for $d = 6, 7$, showing the presence of PPT entanglement. Finally, we study the corresponding cyclic sign *covariant linear maps* that are defined using three vector parameters, in the same fashion as the

Group	Inv. Q. States	Dim. Inv.	Abelian	∃ PPT ent.	References
$\{\mathrm{id}\}$	all states	d^4	Y	Y	-
$\mathcal{DO}(d)$	LDOI	$3d^2-2d$	Y	Y	[SN21]
$\mathcal{DU}(d)$	(C)LDUI	$2d^2-d$	Y	Y	
$\mathrm{Cyc(d)} \ltimes \mathcal{DO}(d)$	LCSI	$3d-2$	N	Y	this paper
$\mathrm{Cyc(d)} \ltimes \mathcal{DU}(d)$	LCPI	$2d-1$	N	Y	
$\mathrm{Sym(d)} \ltimes \mathcal{DO}(d)$	hyperoctahedral	4	N	N	[PJPY24]
$\mathcal{O}(d)$	Brauer	3	N	N	[VW01, Key02]
$\mathcal{U}(d)$	Werner (UU) isotropic ($U\bar{U}$)	2	N	N	[Wer89, HH99]

Table 13: Families of symmetric bipartite quantum states and their invariance groups. In the third column we list the dimension of the (real) vector space of invariant bipartite self-adjoint *matrices*. The fourth and fifth columns list the commutativity property of the invariance group and respectively whether the family of invariant matrices contains PPT entangled states.

states. Using results from [SN21], we can characterize the property of complete positivity and entanglement breaking in terms of the vector triples. Notably, we show that some classes of covariant maps satisfy the PPT^2 conjecture [Chr12].

In Table 13, we present all the classes of symmetric states introduced above, emphasizing the existence of PPT entanglement; see Section 6.3 for more details. Let us mention here that circulant symmetry has received some attention in the literature, in particular with respect to the *Quantum Fourier Transform* [ZLIW17, IV20, YHaJ23].

6.1.2 *Outline of the paper*

We provide some background on the separability problem, convex geometry and circulant matrices in Section 6.2. In Section 6.3, we describe some known families of symmetric states, as presented in Table 13. In Section 6.4, we introduce the families of LCPI/LCSI states and explore some of their basic properties. The linear and convex structure of LCPI/LCSI states is explored in Section 6.4.1 and Section 6.4.2, respectively. Some special

classes of LCSI states are discussed in Section 6.5. Section 6.6 contains results about an important subclass of LCSI states: *cyclic mixture of Dicke states*. Finally, Section 6.7 contains results about the corresponding cyclic sign *covariant linear maps* and the PPT^2 conjecture [Chr12].

6.2 PRELIMINARIES

6.2.1 *Notation*

We start by defining the notation used throughout this paper. A vector v is an element in either $\mathbb{C}^d$ or $\mathbb{R}^d$, and is labelled using vector components starting from index 0. We sometimes also use Dirac's *bra-ket* notation to write vectors. In this notation, column vectors $v \in \mathbb{C}^d$ are written as kets $|v\rangle$ and their dual row vectors (conjugate transposes) $v^* \in (\mathbb{C}^d)^*$ are written as bras $\langle v|$. The standard *inner product* $v^* w = \langle v, w\rangle$ on $\mathbb{C}^d$ is denoted by $\langle v|w\rangle$ and the rank one matrix vw^* is denoted by the *outer product* $|v\rangle\langle w|$. The standard basis in $\mathbb{C}^d$ is denoted by $\{|i\rangle\}_{i\in[d]}$, where $[d] := \{0, 1, \ldots, d-1\}$.

We define $\mathcal{M}_d(\mathbb{C})$ as the set of $d \times d$ complex matrices and $\mathcal{M}_d^{\mathrm{sa}}(\mathbb{C}) := \{A \in \mathcal{M}_d(\mathbb{C}) : A = A^*\}$ as the set of $d \times d$ self-adjoint complex matrices, where the conjugate transpose of $A \in \mathcal{M}_d(\mathbb{C})$ is denoted by A^*. $\mathcal{M}_d(\mathbb{R})$ and $\mathcal{M}_d^{\mathrm{sa}}(\mathbb{R})$ are defined similarly for real matrices. The cone of positive semi-definite matrices in $\mathcal{M}_d(\mathbb{C})$ is denoted by PSD_d, and the cone of entry-wise non-negative matrices by EWP_d. The set of all linear maps $\Phi : \mathcal{M}_d(\mathbb{C}) \to \mathcal{M}_d(\mathbb{C})$ is denoted by $\mathcal{T}_d(\mathbb{C})$. A map $\mathcal{E} \in \mathcal{T}_d(\mathbb{C})$ is called *positive* if $\mathcal{E}(X) \in \mathsf{PSD}_d$ for all $X \in \mathsf{PSD}_d$. We say that a map $\mathcal{E}$ is *k-positive* if the map $\mathrm{id}_n \otimes \mathcal{E} : \mathcal{M}_n \otimes \mathcal{M}_d \to \mathcal{M}_n \otimes \mathcal{M}_d$ is positive for all $1 \leq n \leq k$, where $\mathrm{id}_n : \mathcal{M}_n(\mathbb{C}) \to \mathcal{M}_n(\mathbb{C})$ is the identity map. A map that is k-positive for all $k \in \mathbb{N}$ is called *completely positive*. The linear transposition map $\mathsf{T} : \mathcal{M}_d(\mathbb{C}) \to \mathcal{M}_d(\mathbb{C})$ is positive but not 2-positive. Finally, we denote by $\mathcal{F} : \mathbb{C}^d \to \mathbb{C}^d$ the discrete Fourier transform, which maps

$$x \mapsto \mathcal{F}x = \left(\frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} x_j \omega^{jk}\right)_{k=0}^{d-1}$$

where $\omega = e^{2\pi \mathrm{i}/d}$ is a primitive d-th root of unity.

6.2.2 *Separability and PPT entanglement*

Definition 6.1. A bipartite positive matrix $\rho \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ is said to be separable if

$$\rho = \sum_{i=1}^{N} |v_i\rangle\langle v_i| \otimes |w_i\rangle\langle w_i|$$

for some finite set of vectors $|v_i\rangle, |w_i\rangle \in \mathbb{C}^d$, and it is said to be entangled otherwise.

We denote the convex cone of all separable matrices in $\mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ by SEP_d. By the Hahn-Banach hyperplane theorem, it is possible to separate this set from every entangled state using a hyperplane. For any *entangled state* ρ we can find a Hermitian operator W such that

- $\mathrm{Tr}(\sigma W) \geq 0$ for all σ in SEP_d
- $\mathrm{Tr}(\rho W) < 0$

This Hermitian operator is called an entanglement witness. Horodecki's criterion [HHH96] gives us a operational way to detect entanglement, by finding a positive map Φ such that $(\mathrm{id}_d \otimes \Phi)(\rho)$ is not positive semi-definite. One important positive map in this regard is the transposition map T. The states which are not positive under transposition are entangled, while the rest of the states are called PPT states, which also includes the set of SEP states. This criterion to verify entanglement is called the PPT (Positivity under Partial Transpose) criterion. In the case of $d = 2$, the reverse implication is also true, i.e. any state that is PPT is also separable [Stø63, HHH96]. This is not true for $d \geq 3$. The states that satisfy the PPT condition but are still entangled (for $d \geq 3$) are called PPT entangled states [Hor97].

Definition 6.2 (Separability Problem)**.** Given a bipartite density matrix $\rho \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$, decide whether $\rho \in \mathsf{SEP}$ or not.

It is well known that the membership problem (and the weak membership problem) for SEP is NP-hard [Gur03, Gha10]. Unless P = NP, there is no computationally efficient criterion to decide if a state is separable or entangled. In later sections, we will study the SEP problem for the class of symmetric states.

6.2.3 *Circulant Matrices*

Circulant matrices are highly symmetric matrices that appear naturally in many areas of mathematics [Dav79]. We start with their basic definition.

Definition 6.3. The *circulant* matrix $A \in \mathcal{M}_d(\mathbb{C})$ associated with a vector $a \in \mathbb{C}^d$, denoted $A = \mathsf{circ}(a)$, is defined entrywise as follows

$$A_{ij} = a_{(j-i) \bmod d}.$$

A matrix $A \in \mathcal{M}_d(\mathbb{C})$ is said to be *circulant* if $A = \mathsf{circ}(a)$ for some $a \in \mathbb{C}^d$. We denote the set of all circulant matrices in $\mathcal{M}_d(\mathbb{C})$ by Circ_d.

If we define the right cyclic shift $S : \mathbb{C}^d \to \mathbb{C}^d$ as $S : (a_0, a_1, \ldots a_{d-1}) \to (a_{d-1}, a_0, \ldots a_{d-2})$, it is clear that the rows of the matrix $A = \mathsf{circ}(a)$ are $a, S(a), S^2(a) \ldots S^{d-1}(a)$:

$$A = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_{d-2} & a_{d-1} \\ a_{d-1} & a_0 & a_1 & \cdots & a_{d-3} & a_{d-2} \\ a_{d-2} & a_{d-1} & a_0 & \cdots & a_{d-2} & a_{d-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ a_2 & a_3 & a_4 & \cdots & a_0 & a_1 \\ a_1 & a_2 & a_3 & \cdots & a_{d-1} & a_0 \end{pmatrix}.$$

Remark 6.4. $\mathsf{Circ}_d \subseteq \mathcal{M}_d(\mathbb{C})$ forms a d-dimensional commutative algebra with the standard operations of matrix addition and matrix multiplication. Recall that $|1\rangle = (0\,1\,0 \cdots 0)^\top$ is the second canonical basis vector and let $P = \mathsf{circ}(|1\rangle) \in \mathcal{M}_d(\mathbb{C})$ be a shift permutation. Then, any circulant matrix $A \in \mathcal{M}_d(\mathbb{C})$ can be written as

$$A = \sum_{i=0}^{d-1} a_i P^i, \quad \text{where } a_i = A_{0,i}.$$

Recall that the Fourier transform matrix $\mathcal{F} \in \mathcal{M}_d(\mathbb{C})$ is defined entrywise as $\mathcal{F}_{jk} = \omega^{jk}/\sqrt{d}$, where $\omega = e^{2\pi \mathrm{i}/d}$ is the d^{th} primitive root of unity. The $1/\sqrt{d}$ factor ensures that $\mathcal{F}$ is unitary. The inverse Fourier transform $\mathcal{F}^{-1} = \mathcal{F}^*$ is given by $(\mathcal{F}^{-1})_{jk} = \omega^{-jk}/\sqrt{d}$.

Proposition 6.5 ([Dav79, Chapter 3.2])**.** The eigenvalues $\{\lambda_i\}_{i=0}^{d-1}$ of a circulant matrix $A = \mathsf{circ}(a) \in \mathcal{M}_d(\mathbb{C})$ are obtained by taking the Fourier transform of a:

$$\forall j \in [d], \qquad \lambda_j = (\sqrt{d}\mathcal{F}a)_j = \sum_k a_k \omega^{jk},$$

where $\omega = e^{2\pi i/d}$ is the d^{th} primitive root of unity.

Proof. This follows from the fact that the Fourier matrix diagonalizes circulant matrices:

$$\mathcal{F}^* \cdot \mathrm{circ}(a) \cdot \mathcal{F} = \mathrm{diag}(\sqrt{d}\mathcal{F}a)$$

■

Remark 6.6. A circulant matrix $A = \mathsf{circ}(a) \in \mathcal{M}_d(\mathbb{C})$ is Hermitian iff $a_i = \overline{a_i}^{\mathsf{R}} = \overline{a_{d-i}}$. The *reversal* operation $a \to a^{\mathsf{R}}$, is defined as

$$\forall i \in [d] \qquad (a^{\mathsf{R}})_i := a_{(-i) \bmod d}.$$

In the case of circulant matrices, we have: $\mathsf{circ}(a^{\mathsf{R}}) = \mathsf{circ}(a)^\top$.

Definition 6.7. The bilinear circular convolution map $* : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C}^d$ is defined as

$$\forall k \in [d], \qquad (a * b)_k = \sum_{j=0}^{d-1} a_j b_{k-j} = \langle \bar{a}| P^{-k} |b^{\mathsf{R}}\rangle$$

The circular convolution corresponds exactly to the multiplication of two circulant matrices:

$$\forall a, b \in \mathbb{C}^d : \qquad \mathsf{circ}(a)\mathsf{circ}(b) = \mathsf{circ}(a * b) = \mathsf{circ}(b * a) = \mathsf{circ}(b)\mathsf{circ}(a).$$

Finally, the Hilbert-Schmidt inner product of circulant matrices corresponds to the euclidean inner product of vectors,

$$\mathrm{Tr}(\mathsf{circ}(a)^*\mathsf{circ}(b)) = d\,\langle a|b\rangle$$

6.2.4 *Convexity*

In this section, we introduce some basic notions from convex analysis.

Definition 6.8. Let V be a real vector space. A *convex cone* $\mathcal{C}$ is a subset of V having the following two properties:

- if $x \in \mathcal{C}$ and $\lambda \in \mathbb{R}^+ = [0, \infty)$, then $\lambda x \in \mathcal{C}$.
- if $x, y \in \mathcal{C}$, then $x + y \in \mathcal{C}$.

In particular, $0 \in \mathcal{C}$. The cone $\mathcal{C}$ is said to be *pointed* if $\mathcal{C} \cap (-\mathcal{C}) = \{0\}$; in other words, $\mathcal{C}$ is pointed if it does not contain any line.
For a vector $v \neq 0$, the half-line $\mathbb{R}_+ v := \{\lambda v : \lambda \in \mathbb{R}_+\} \subseteq \mathcal{C}$ is called an *extremal ray* of $\mathcal{C}$ (we write $\mathbb{R}_+ v \in \operatorname{ext} \mathcal{C}$) if

$$v = x + y \quad \text{with } x, y \in \mathcal{C} \implies x, y \in \mathbb{R}_+ v.$$

Definition 6.9. Given a cone $\mathcal{C}$, we define its *dual cone* by

$$\mathcal{C}^* = \{\alpha \in V^* : \alpha(x) \geq 0, \forall x \in \mathcal{C}\} \subseteq V^*,$$

where V^* is the vector space dual to V. If V has an inner product structure, then the elements of the dual are of the form $\alpha(x) = \langle v_\alpha, x \rangle$ for some $v_\alpha \in V$.

Definition 6.10. For convex cones $C_1 \subseteq V$ and $C_2 \subseteq V$ in the real vector space V, we define have the sum of cones,

$$C_1 + C_2 := \{x + y : x \in C_1, y \in C_2\}$$

This is again a convex cone.

The next theorem is a well known theorem about dual cones and sum of cones in convex geometry. We give the proof for completeness.

Theorem 6.11. For any closed convex cones C_1 and C_2, we have,

$$(C_1 + C_2)^\circ = C_1^\circ \cap C_2^\circ$$

Proof. Let $x \in (C_1 + C_2)^\circ$. Then, by definition, $x \in (C_1 + C_2)^\circ$ implies that $x \cdot (y_1 + y_2) \geq 0$ for all $y_1 \in C_1$ and $y_2 \in C_2$. Setting $y_2 = 0$ gives $x \cdot y_1 \geq 0$ for all $y_1 \in C_1$. Similarly, setting $y_1 = 0$ gives $x \cdot y_2 \geq 0$ for all $y_2 \in C_2$. Therefore, $x \in C_1^\circ \cap C_2^\circ$.

To show the converse, assume $x \in C_1^\circ \cap C_2^\circ$. Then $x \cdot y_1 \geq 0$ for all $y_1 \in C_1$ and $x \cdot y_2 \geq 0$ for all $y_2 \in C_2$. For any $y_1 \in C_1$ and $y_2 \in C_2$, we have $x \cdot (y_1 + y_2) = x \cdot y_1 + x \cdot y_2 \geq 0$. Thus, $x \in (C_1 + C_2)^\circ$. ■

Example 6.12. The cone of *entrywise non-negative* $d \times d$ matrices is defined as

$$\mathsf{EWP}_d := \{A \in \mathcal{M}_d(\mathbb{R}) : A_{ij} \geq 0 \ \forall i, j \in [d]\},$$

and the cone of *positive semidefinite* $d \times d$ matrices is defined as

$$\mathsf{PSD}_d := \{B \in \mathcal{M}_d^{\mathrm{sa}}(\mathbb{C}) : \langle x|B|x\rangle \geq 0 \ \forall x \in \mathbb{C}^d\}$$

play a fundamental role in this work. The two cones $\mathsf{EWP}_d \subseteq \mathcal{M}_d(\mathbb{R})$ and $\mathsf{PSD}_d \subseteq \mathcal{M}_d^{sa}(\mathbb{C})$ are self-dual. Their extremal rays are

$$\operatorname{ext} \mathsf{EWP}_d = \{\mathbb{R}_+ |i\rangle\langle j|\}_{i,j\in[d]} \quad \text{and} \quad \operatorname{ext} \mathsf{PSD}_d = \{\mathbb{R}_+ |x\rangle\langle x|\}_{|x\rangle\in\mathbb{C}^d, |x\rangle\neq 0}.$$

In this article, we will deal with some important cones in $\mathcal{M}_d(\mathbb{C})$ as their sections in the circulant subspace, $\mathsf{Circ}_d \subseteq \mathcal{M}_d(\mathbb{C})$. Therefore we use the notation

$$\overrightarrow{\mathcal{K}} = \mathsf{circ}^{-1}(\mathcal{K} \cap \mathsf{Circ}_d),$$

where the cone $\mathcal{K}$ is a cone in $\mathcal{M}_d(\mathbb{C})$. From the last section we also know that Circ_d is isomorphic to the space $\mathbb{C}^d$ by the map $\mathsf{circ}(d) : \mathbb{C}^d \ni a \mapsto \mathsf{circ}(a) \in \mathsf{Circ}_d$.

Definition 6.13. Consider the following two cones

$$\overrightarrow{\mathsf{EWP}}_d := \mathsf{circ}^{-1}(\mathsf{Circ}_d \cap \mathsf{EWP}_d)$$
$$\overrightarrow{\mathsf{PSD}}_d := \mathsf{circ}^{-1}(\mathsf{Circ}_d \cap \mathsf{PSD}_d)$$

seen as subsets of $\mathbb{C}^d$.

Proposition 6.14. For the cones $\overrightarrow{\mathsf{EWP}}_d$ and $\overrightarrow{\mathsf{PSD}}_d$ the following are true.

- $\operatorname{ext}(\overrightarrow{\mathsf{EWP}}_d) = \{\mathbb{R}^+ |k\rangle\}_{k=0}^{d-1}$

- $\mathrm{ext}(\overrightarrow{\mathsf{PSD}}_d) = \{\mathbb{R}^+\mathcal{F}^{-1}\,|k\rangle\}_{k=0}^{d-1}$

Proof. The first statement is obvious. For the second part, we observe that $\overrightarrow{\mathsf{PSD}}_d = \mathcal{F}^{-1}(\overrightarrow{\mathsf{EWP}}_d)$, so that $\mathrm{ext}(\overrightarrow{\mathsf{PSD}}_d) = \{\mathbb{R}^+\mathcal{F}^{-1}\,|k\rangle\}_{k=0}^{d-1}$. ■

Remark 6.15. The extremal rays of the $\overrightarrow{\mathsf{PSD}}_d$ cone $\mathbb{R}_+ f_k = \mathbb{R}_+\mathcal{F}^{-1}\,|k\rangle$, for $k = 0, 1, \ldots, d-1$, are just multiples of the columns of the inverse fourier matrix:

$$(f_k)_i = \frac{1}{\sqrt{d}}\omega^{-ik} = \frac{1}{\sqrt{d}}(f_k * (\overline{f_k})^{\mathsf{R}})_i$$

6.3 FAMILIES OF SYMMETRIC STATES

In this section, we explore different classes of symmetric states that have been previously considered in the literature. Our classification starts from the symmetry group that leaves invariant the bipartite quantum states. We consider unitary representations of a group G

$$G \ni g \mapsto U_g \in \mathcal{U}(d)$$

and the corresponding families of bipartite quantum states $\rho \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ that are invariant under the following actions:

$$\rho = (U_g \otimes U_g)\rho(U_g \otimes U_g)^* \quad \text{or} \quad \rho = (U_g \otimes \bar{U}_g)\rho(U_g \otimes \bar{U}_g)^*.$$

6.3.1 *Unitary and orthogonal invariance*

The unitary group $G = \mathcal{U}(d)$ with its standard representation gives rise to the *isotropic states*

$$\rho \in \mathrm{span}\{I_d \otimes I_d, \omega_d\}, \tag{26}$$

where ω_d is the *maximally entangled state*

$$\omega_d := \frac{1}{d}\sum_{i,j=1}^{d} |ii\rangle\langle jj| \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}),$$

in the case of the $U - U$ representation [HH99]. For the conjugate representation $U - \bar{U}$, one obtains the *Werner states* [Wer89]

$$\rho \in \mathrm{span}\{P_s, P_a\} = \mathrm{span}\{I_d \otimes I_d, F_d\}, \tag{27}$$

where $P_{s,a}$ are, respectively, the orthogonal projections on the symmetric and anti-symmetric subspaces of $\mathbb{C}^d \otimes \mathbb{C}^d$:

$$P_s = \frac{I_{d^2} + F_d}{2} \qquad P_a = \frac{I_{d^2} - F_d}{2},$$

with $F_d \in \mathcal{U}(d^2)$ being the *flip* (or *swap*) operator:

$$F_d = \sum_{i,j=1}^{d} |ji\rangle\langle ij| \,.$$

For the orthogonal group $G = \mathcal{O}(d)$, the normal and conjugate representations are identical and give rise to the *Brauer states* [VW01, Key02], which generalize isotropic and Werner states:

$$\rho \in \mathrm{span}\{I_d \otimes I_d, \omega_d, F_d\}, \tag{28}$$

The separable (or equivalently the PPT) states in these classes have been completely characterized [Wer89] [HH99] [Key02] ; there are no PPT entangled states.

6.3.2 *Local diagonal orthogonal invariance*

Consider now the subgroup $\mathcal{DU}(d) \leq \mathcal{U}(d)$ of *diagonal unitary matrices* and its orthogonal counterpart $\mathcal{DO}(d) \leq \mathcal{O}(d)$. The corresponding invariant states are called respectively local diagonal unitary invariant (LDUI), conjugate local diagonal unitary invariant (CLDUI), and local diagonal orthogonal invariant (LDOI) [SN21]. Since the invariance group is smaller that the full unitary (resp. orthogonal) group, these families are larger then the ones in Eqs. (26), (27), and (28).

Acronym	Symmetry	Condition
LDUI	local diagonal unitary invariant	$(U \otimes U)X(U \otimes U)^* = X$
CLDUI	conjugate local diagonal unitary invariant	$(U \otimes \bar{U})X(U \otimes \bar{U})^* = X$
LDOI	local diagonal orthogonal invariant	$(O \otimes O)X(O \otimes O)^* = X$

The conditions above hold for all diagonal $d \times d$ unitary matrices $U \in \mathcal{DU}_d$ and all diagonal orthogonal $d \times d$ matrices $O \in \mathcal{DO}_d$. Any LDOI matrix is of the form [SN21]

$$X_{(A,B,C)} = \sum_{i,j} A_{ij}|ij\rangle\langle ij| + \sum_{i \neq j} B_{ij}|ii\rangle\langle jj| + \sum_{i \neq j} C_{ij}|ij\rangle\langle ji|, \tag{29}$$

where $A, B, C \in \mathcal{M}_d(\mathbb{C})$, and $\operatorname{diag} A = \operatorname{diag} B = \operatorname{diag} C$. If B (resp. C) here is diagonal, then the resulting family of matrices form the LDUI (resp. CLDUI) subspace. These two subspaces are linked via the operation of partial transpose, and hence the separability results for one class apply identically to the other class as well. CLDUI matrices are of the form:

$$X_{(A,B)} = \sum_{i,j} A_{ij}|ij\rangle\langle ij| + \sum_{i \neq j} B_{ij}|ii\rangle\langle jj| \tag{30}$$

It turns out that separability of these matrices is closely linked with the cones of pairwise and triplewise completely positive matrices, which we introduce now. We denote the entrywise (or Hadamard) product between vectors $v, w \in \mathbb{C}^d$ by $v \odot w$ or $|v \odot w\rangle$.

Definition 6.16. [SN21] Let $A, B, C \in \mathcal{M}_d(\mathbb{C})$.

- The pair (A, B) is called *pairwise completely positive* (PCP) if there exist a finite set of vectors $\{|v_k\rangle, |w_k\rangle\}_{k \in I} \subset \mathbb{C}^d$ such that

$$A = \sum_{k \in I} |v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}|, \quad B = \sum_{k \in I} |v_k \odot w_k\rangle\langle v_k \odot w_k| .$$

- The triple (A, B, C) is called *triplewise completely positive* (TCP) if there exist a finite set of vectors $\{|v_k\rangle, |w_k\rangle\}_{k \in I} \subset \mathbb{C}^d$ such that

$$A = \sum_{k \in I} |v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}|, \quad B = \sum_{k \in I} |v_k \odot w_k\rangle\langle v_k \odot w_k| ,$$
$$C = \sum_{k \in I} |v_k \odot \overline{w_k}\rangle\langle v_k \odot \overline{w_k}| .$$

Theorem 6.17. [SN21] Let $A, B, C \in \mathcal{M}_d(\mathbb{C})$. Then,

- $X_{(A,B)}$ is separable $\iff$ (A, B) is PCP.
- $X_{(A,B,C)}$ is separable $\iff$ (A, B, C) is TCP.

The set of all $d \times d$ PCP and TCP matrix pairs and triples form convex cones [SN21, Proposition 5.6], which we denote by PCP_d and TCP_d, respectively.

6.3.3 *Semi-direct product constructions*

We now consider *intermediate* subgroups

$$\mathcal{DU}(d) \leq G \leq \mathcal{U}(d)$$

that would give rise to intermediate families of invariant states. To do so, we shall consider semi-direct products of the diagonal unitary group $\mathcal{DU}(d)$ (resp. the diagonal unitary group $\mathcal{DU}(d)$) with a subgroup H of the symmetric (permutation) group $\mathrm{Sym}(d)$:

$$G := H \ltimes \mathcal{DU}(d) \quad \text{with } H \leq \mathrm{Sym}(d). \tag{31}$$

Recall that the semi-direct product $H \ltimes \mathcal{DU}(d)$ group endows the cartesian product $H \times \mathcal{DU}(d) = H \times \mathbb{T}^d$ with the product rule

$$(\sigma, u) \cdot (\pi, v) := (\sigma\pi, u \odot (\sigma.v)),$$

where the action of symmetric group on vectors reads

$$\forall i \in [d] : \qquad (\sigma.v)_i = v_{\sigma^{-1}(i)}.$$

The unitary representation U_g of G is given by permutation matrices with phases. Concretely, for $\sigma \in H$ and $u \in \mathbb{T}^d$, we have

$$\left[U_{\sigma,u}\right]_{ij} = \mathbb{1}_{i=\sigma(j)} u_i.$$

The same notions can be defined for the diagonal orthogonal group $\mathcal{DO}(d)$. Importantly, one recovers the *hyperoctahedral group* as $\mathrm{Hyp}(d) := \mathrm{Sym}(d) \ltimes \mathcal{DO}(d)$.

The table below shows the states invariant under the action of classical groups that are relevant to our study, using the construction above. For the permutation group H, we consider either the full group $\mathrm{Sym}(d)$ or the (abelian) subgroup of *cyclic permutations* $\mathrm{Cyc}(d)$.

$\ltimes$	$\mathrm{Sym}(d)$	$\mathrm{Cyc}(d)$
$\mathcal{D}U(d)$	axisymmetric states [SES16]	generalized axisymmetric states [SBSGS22]
$\mathcal{D}O(d)$	hyperoctahedral states [PJPY24]	LCSI states (*this paper*)

Let us consider in more detail the hyperoctahedral group which can be defined as a semi-direct product of group of permutation matrices with diagonal orthogonal group,

$\mathrm{Hyp}(d) = \mathrm{Sym(d)} \ltimes D\mathcal{O}(d)$. A bipartite matrix X is said to be hyperoctahedral if it satisfies $(O \otimes O)X(O \otimes O)^\top = X$ for all orthogonal matrices in the group $\mathrm{Hyp}(d)$. This class of highly symmetric states were considered in the recent paper [PJPY24] where they were shown to have the form

$$X^{\mathsf{Hyp}}_{a,a',b,c} = a \sum_i |ii\rangle\langle ii| + a' \sum_{i\neq j} |ij\rangle\langle ij| + b \sum_{i\neq j} |ii\rangle\langle jj| + c \sum_{i\neq j} |ij\rangle\langle ji|\,,$$

for complex parameters $a, a', b, c \in \mathbb{C}$. This class reduces to the well-known Werner states when $a = a'$ and $b = 0$ (resp. isotropic states when $a = a'$ and $c = 0$).

In [PJPY24] it was also shown that all the PPT states in this class are also separable.

Theorem 6.18 ([PJPY24, Theorem 4.1])**.** A hyperoctahedral quantum state that is PPT is necessarily separable:

$$X^{\mathsf{Hyp}}_{a,a',b,c} \text{ is SEP} \iff X^{\mathsf{Hyp}}_{a,a',b,c} \text{ is PPT}$$

Remark 6.19. Instead of taking the complete group of permutation matrices, we can restrict to subgroups that are 2-transitive (i.e if the orbit of $(\pi(i), \pi(j)) = \{(l, m), l \neq m\ \forall l, m\}$), we get the same class of states.

Given the lack of PPT entanglement in the set of hyperoctahedral quantum states, one is naturally led to consider larger families of symmetric states by reducing the size of the symmetry group. One choice is to consider the group cyclic permutations for H in Eq. (31). By replacing the diagonal orthogonal group with the larger group of all diagonal unitary matrices, we obtain the states that are invariant under the group $\mathfrak{CDU}(d)$, that can be defined as

$$\mathfrak{CDU}(d) := \mathrm{Cyc}(d) \ltimes \mathcal{DU}(d)$$

where $\mathcal{DU}(d)$ is the group of $d \times d$ diagonal unitaries.

We call these states as Local Cyclic Phase Invariant states (LCPI). These states have also been introduced and studied as a generalization of *axisymmetric states* [SES16] in the recent paper [SBSGS22]. They are special cases of LCSI states that we introduce in the next section. Importantly, this class of states contain PPT entangled states in all $d \geq 3$ (see Example 6.35 and Remark 6.36).

6.4 LOCAL CYCLIC SIGN PERMUTATION INVARIANCE

In this section, we will look at the basic definitions and properties of a new class of bipartite invariant quantum states, which we call *Local Cyclic Sign Invariant* (LCSI) states. The central group in this paper is the group of *cyclic sign permutations*, which we define below and denote by $\mathfrak{CDO}(d)$. We will denote the group of diagonal orthogonal matrices by $\mathcal{DO}_d$. This is just a matrix group that includes all orthogonal matrices O such that $O_{ii} = \pm 1$, and $O_{ij} = 0$ for all $i \neq j$. The group of $d \times d$ cyclic permutation matrices is denoted by Cyc_d. If we define $P = \mathsf{circ}(|1\rangle) \in \mathcal{M}_d(\mathbb{C})$, then Cyc_d is the (abelian) group generated by P.

Definition 6.20. The cyclic sign group is defined as

$$\mathfrak{CDO}(d) := \mathrm{Cyc}_d \ltimes \mathcal{DO}_d := \{P \cdot O : P \in \mathrm{Cyc}(d) \text{ and } O \in \mathcal{DO}_d\}$$

We can understand the group $\mathfrak{CDO}(d)$ as the group of cyclic permutation matrices, but with the 1 entries replaced by ± 1. For example, the permutation matrix P^{d-1} gives us

$$\begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & 0 & \cdots & 0 & \pm 1 \\ \pm 1 & 0 & \cdots & 0 & 0 \\ 0 & \pm 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \pm 1 & 0 \end{bmatrix}$$

More precisely, recall from the previous section that a general element of the group $\mathfrak{CDO}(d)$ corresponding to a cyclic permutation $\sigma = (1\,2\,\cdots\,d)^k \in \mathrm{Cyc}(d)$ and a sign vector $\varepsilon \in \{\pm 1\}^d$ is represented by a matrix $U_{\sigma,\varepsilon}$ having elements

$$[U_{\sigma,\varepsilon}]_{ij} = \mathbb{1}_{i=\sigma(j)}\varepsilon_i = 1_{i=j+k}\varepsilon_i.$$

Remark 6.21. The group $\mathfrak{CDO}(d)$ is *not* abelian even though both the groups of $\mathrm{Cyc}(d)$ and $D\mathcal{O}(d)$ are abelian:

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix} \neq \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

We come now to the main definition of this paper.

Definition 6.22. A bipartite matrix $X \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ is called *Local Cyclic Sign Invariant* (LCSI) if

$$\forall O \in \mathfrak{CDO}(d) : \qquad (O \otimes O)X(O \otimes O)^\top = X.$$

In the remainder of this section, we will investigate several properties of LCSI matrices.

6.4.1 *Linear Structure of LCSI matrices*

Since the condition in Definition 6.22 is linear, it is easy to see that the set of LCSI matrices (not necessarily quantum states) form a vector subspace of $\mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$. In this section, we explicitly characterize the structure of this space in terms of vector triples. Let us begin with a result from [SN21] to prove the following lemma.

Lemma 6.23. The linear space of LCSI_d matrices can be parametrized by $(A, B, C) \in \mathcal{M}_d(\mathbb{C})^{\times 3}_{\mathbb{C}^d}$ such that A, B, C are invariant under the action of $\mathrm{Cyc}(d)$: $PXP^{-1} = X$ for $X = A, B, C$.

Proof. The linear space of LDOI_d matrices can be parameterized using $(A, B, C) \in \mathcal{M}_d(\mathbb{C})^{\times 3}_{\mathbb{C}^d}$ such that any state can be written as

$$X_{(A,B,C)} = \sum_{ij} A_{ij} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{i \neq j} B_{ij} \left|ii\right\rangle\!\left\langle jj\right| + \sum_{i \neq j} C_{ij} \left|ij\right\rangle\!\left\langle ji\right|$$

such that $\mathrm{diag}(A) = \mathrm{diag}(B) = \mathrm{diag}(C)$

We begin the proof by noting that $\mathsf{LCSI}_d \subseteq \mathsf{LDOI}_d$. Therefore it is of the form $X_{(A,B,C)}$ and satisfies the invariance condition

$$(P \otimes P)X_{A,B,C}(P^{-1} \otimes P^{-1}) = X_{A,B,C}$$

Looking at both the sides of the equation,

$$\begin{aligned}
\mathrm{LHS} &= \sum_{ij} A_{ij} \left|\pi(i)\pi(j)\right\rangle\!\left\langle \pi(i)\pi(j)\right| + \sum_{ij} B_{ij} \left|\pi(i)\pi(i)\right\rangle\!\left\langle \pi(j)\pi(j)\right| + \sum_{ij} C_{ij} \left|\pi(i)\pi(j)\right\rangle\!\left\langle \pi(j)\pi(i)\right| \\
&= \sum_{ij} A_{\pi^{-1}(i)\pi^{-1}(j)} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{ij} B_{\pi^{-1}(i)\pi^{-1}(j)} \left|ii\right\rangle\!\left\langle jj\right| + \sum_{ij} C_{\pi^{-1}(i)\pi^{-1}(j)} \left|ij\right\rangle\!\left\langle ji\right| \\
\mathrm{RHS} &= \sum_{ij} A_{ij} \left|ij\right\rangle\!\left\langle ij\right| + B_{ij} \left|ii\right\rangle\!\left\langle jj\right| + C_{ij} \left|ij\right\rangle\!\left\langle ji\right|
\end{aligned}$$

This implies that $A_{ij} = A_{\pi^{-1}(i)\pi^{-1}(j)}$ for all π in $\mathrm{Cyc}(d)$. This condition can be written as $PAP^{-1} = A$ for all P in $\mathrm{Cyc}(d)$, and similarly for B and C. ■

Proposition 6.24. The set of matrices $X \in \mathcal{M}_d(\mathbb{C})$ satisfying $PXP^{-1} = X$ for all $P \in \mathrm{Cyc}(d)$ is precisely the set of circulant matrices, i.e. $X_{ij} = a_{i-j}$ for a vector $a \in \mathbb{C}^d$ having entries $(a_0, a_1, \ldots, a_{d-1})$.

Proposition 6.25. The linear space of LCSI_d is isomorphic to the vector space

$$(\mathbb{C}^d)^{\times 3}_{\mathbb{C}} := \{(a, b, c) \in (\mathbb{C}^d)^{\times 3} \text{ st } a_0 = b_0 = c_0\},$$

where the isomorphism can be written as

$$X_{(a,b,c)} = \sum_{j,k} a_k |j \oplus k, j\rangle\langle j \oplus k, j| + \sum_{j,k\geq 1} b_k |j \oplus k, j \oplus k\rangle\langle j, j| + \sum_{j,k\geq 1} c_k |j \oplus k, j\rangle\langle j, j \oplus k|$$

and $\oplus$ should be understood as sum $\mathrm{mod}(d)$

Proof. The proof follows directly from Lemma 6.23 and Proposition 6.24. ■

Remark 6.26. The dimension of the complex vector space of LCSI_d is $\dim_{\mathbb{C}}(\mathsf{LCSI}_d) = 3d - 2$. The stated isomorphism with vector triples shows that we have $3d$ parameters for 3 vectors, but since $a_0 = b_0 = c_0$, we get $\dim_{\mathbb{C}}(\mathsf{LCSI}_d) = 3d - 2$. This should be compared with the dimension of LDOI_d, which scales quadratically in d: $\dim_{\mathbb{C}}(\mathsf{LDOI}_d) = 3d^2 - 2$.

Symmetries of LCSI_d *subspace*

In [SN21, Proposition 4.3], the authors analyzed the symmetries of this space under permutations of wires. We write them here for the case of space of LSPI matrices. Recall that we denote by $a \to a^{\mathsf{R}}$ the transformation $a^{\mathsf{R}}_i = a_{d-i \bmod d}$.

Proposition 6.27. The vector subspace of LCSI_d matrices is invariant under the following tensor leg permutations:

$$\begin{aligned} FX_{(a,b,c)}F &= X_{(a^{\mathsf{R}},b,c^{\mathsf{R}})} & \left(X_{(a,b,c)}\right)^{\top} &= X_{(a,b^{\mathsf{R}},c^{\mathsf{R}})} \\ \left(X_{(a,b,c)}\right)^{\times} &= X_{(a^{\mathsf{R}},b^{\mathsf{R}},c)} & \left(X_{(a,b,c)}\right)^{\mathrm{Re}} &= X_{(b,a,c)} \end{aligned}$$

where F is the flip (or swap) operator, Re is the Realignment operator, and $\times$ permutes the indices diagonally. The space LCSI_d also has the following symmetries:

$$\begin{aligned} \left(X_{a,b,c}\right)^{\Gamma} &= X_{a,c,b} & FX_{a,b,c} &= X_{c^{\mathsf{R}},b,a^{\mathsf{R}}} \\ \left(X_{a,b,c}\right)^{\intercal} &= X_{a,c^{\mathsf{R}},b^{\mathsf{R}}} & X_{a,b,c}F &= X_{c,b,a} \end{aligned}$$

where Γ and $\intercal$ are the partial transposition of the tensor factor 1 and 2 respectively.

6.4.2 *Convex structure of LCSI matrices*

In this subsection, we will look at the cones of positive semi-definite LCSI matrices (by which we will also mean states), the PPT cone and finally the cone of separable matrices. Here, we prove some structure theorems on the vector triple (a, b, c) such that $X_{a,b,c}$ belongs to each of these cones. We look at these cones as they are the most important from the perspective of quantum information theory, particularly in entanglement theory. In the next few sections, we will be interested in exploring PPT entangled states and the separability problem in this class of quantum states. The next proposition characterizes membership in the positive semidefinite cone for a matrix and positivity under partial transpose.

Theorem 6.28. We define, for $k \in [d]$,

$$\lambda_k^{\pm} := \frac{(a_k + a_{d-k}) \pm \sqrt{(a_k - a_{d-k})^2 + 4c_{d-k}c_k}}{2}.$$

Then, the spectrum of $X_{a,b,c}$ is given by:

$$\mathrm{spec}[X_{a,b,c}] = \left(\sqrt{d}\mathcal{F}b\right) \cup \bigcup_{k=1}^{d-1} \{\lambda_k^{\pm}\}^{\times(d-k)}.$$

Moreover, for any $X_{a,b,c}$ it holds that:

- $X_{a,b,c} \in \mathsf{PSD}_{d^2} \iff a \in \mathbb{R}^d_+, \mathcal{F}b \in \mathbb{R}^d_+, c = \bar{c}^{\mathsf{R}}$ and, $\forall i \in [d]$, $a_i a_{d-i} \geq |c_i|^2$;
- $X^{\Gamma}_{a,b,c} \in \mathsf{PSD}_{d^2} \iff a \in \mathbb{R}^d_+, \mathcal{F}c \in \mathbb{R}^d_+, b = \bar{b}^{\mathsf{R}}$ and, $\forall i \in [d]$, $a_i a_{d-i} \geq |b_i|^2$;
- $X_{a,b,c} \in \mathsf{PPT}_{d^2} \iff a \in \mathbb{R}^d_+, \mathcal{F}b, \mathcal{F}c \in \mathbb{R}^d_+$ and, $\forall i \in [d]$, $a_i a_{d-i} \geq \max(|b_i|^2, |c_i|^2)$.

Proof. We can use the following block decomposition of the matrix $X_{a,b,c}$ to prove these results, see [SN21, Proposition 4.1]:

$$X_{a,b,c} = \mathsf{circ}(b) \oplus \bigoplus_{k=1}^{d-1} \begin{pmatrix} a_k & c_k \\ c_{d-k} & a_{d-k} \end{pmatrix}^{\oplus(d-k)}.$$

For any circulant matrix $\mathsf{circ}(b) \in \mathcal{M}_d(\mathbb{C})$, we have $\mathrm{spec}[\mathsf{circ}(b)] = \sqrt{d}\mathcal{F}(b)$. Finally, from Proposition 6.27, we know that $X^{\Gamma}_{a,b,c} = X_{a,c,b}$. ∎

Next, we look at the separable cone (SEP). Recall that $(a * b)_k = \sum_i a_i b_{k-i}$. For $a \in \mathbb{C}^d$, we define the reflected vector $a^{\mathsf{R}} \in \mathbb{C}^d$ as $a^{\mathsf{R}}_i = a_{d-i}$. The map $a \to \bar{a} * a^{\mathsf{R}}$ is called the autocorrelation map. We now derive the necessary and sufficient conditions for the separability of the LCSI matrix $X_{a,b,c}$. For this we introduce another notion of positivity for vectors a, b, c which will be called *Circulant* Triplewise Completely Positive, inspired by the cone of Triplewise Completely Positive matrices introduced in [NS21, Definition 7.4], which, in turn, generalizes [JM19, Definition 3.1].

Definition 6.29. A vector triple $(a, b, c) \in (\mathbb{C}^d)^{\times 3}_{\mathbb{C}}$ is called *Circulant Triplewise Completely Positive* if there exist a finite set of vectors $\{v_k, w_k\}_{k \in I}$ such that

$$a = \sum_{k \in I} (v_k \odot \overline{v_k}) * (\overline{w_k} \odot w_k)^{\mathsf{R}}, \qquad b = \sum_{k \in I} (v_k \odot w_k) * (\overline{v_k} \odot \overline{w_k})^{\mathsf{R}},$$
$$c = \sum_{k \in I} (v_k \odot \overline{w_k}) * (\overline{v_k} \odot w_k)^{\mathsf{R}},$$

where we recall that $*$ denotes the circular convolution and $\odot$ denotes the Hadamard (entrywise) product of vectors. We denote the set of all such vector triples (a, b, c) by $\overrightarrow{\mathsf{TCP}}_d$.

Theorem 6.30. The following holds true for LCSI matrices:

$$X_{a,b,c} \text{ is separable} \iff (a,b,c) \in \overrightarrow{\mathsf{TCP}}_d.$$

Proof. Following Section 6.16, we know that for a separable LDOI matrix $X^{\mathsf{LDOI}}_{(A,B,C)}$, there exist finite set of vectors v_k and w_k such that

$$A = \sum_k |v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}| \quad B = \sum_k |v_k \odot w_k\rangle\langle v_k \odot w_k| \quad C = \sum_k |v_k \odot \overline{w_k}\rangle\langle v_k \odot \overline{w_k}|$$

From Section 6.4.1, we know that LCSI states with the triple a, b, c are LDOI states with $A = \mathsf{circ}(a), B = \mathsf{circ}(b)$ and $C = \mathsf{circ}(c)$. Recall that $\mathsf{circ}(a) = \sum_{i=0}^{d-1} a_i P^i$, where P is the shift permutation from Remark 6.4 satisfying $P^i P^j = P^{i \oplus j}$ and $\mathrm{Tr}(P^i) = d\mathbb{1}_{i=0 \bmod d}$. Hence, we obtain

$$\sum_{i=0}^{d-1} a_i P^i = \sum_k |\overline{v_k} \odot v_k\rangle\langle \overline{w_k} \odot w_k| \,.$$

Taking the trace of both sides after multiplying by P^{-j}, we have:

$$\begin{aligned} d \sum_{i=0}^{d-1} a_i \delta_{i-j} = \mathrm{Tr}\left(\sum_{i=0}^{d-1} a_i P^i P^{-j}\right) &= \sum_{i=0}^{d-1} a_i \mathrm{Tr}(P^i P^{-j}) \\ &= \sum_k \mathrm{Tr}\left(|\overline{v_k} \odot v_k\rangle\langle \overline{w_k} \odot w_k| \, P^{-j}\right) \\ &= \sum_k \langle \overline{w_k} \odot w_k| \, P^{-j} \, |\overline{v_k} \odot v_k\rangle \,. \end{aligned}$$

This simplifies to

$$a = \frac{1}{d} \sum_k (w_k \odot \overline{w_k}) * (\overline{v_k} \odot v_k)^{\mathsf{R}}.$$

We can do a similar calculation for $B = \mathrm{circ}(b)$ and $C = \mathrm{circ}(c)$ to show that the vectors (a, b, c) form a $\overrightarrow{\mathsf{TCP}}_d$ triple of the form in Definition 6.29.

To show the converse, we begin with $(a, b, c) \in \overrightarrow{\mathsf{TCP}}_d$ that is of the form given in Definition 6.29 and show that $(\mathsf{circ}(a), \mathsf{circ}(b), \mathsf{circ}(c)) \in \mathrm{TCP}_d$. Again, we will do an explicit calculation for a, and a similar calculation can be done for b and c to show that $(\mathsf{circ}(a), \mathsf{circ}(b), \mathsf{circ}(c))$ is of the form in Definition 6.16. We start with the given expression:

$$a = \sum_k (v_k \odot \overline{v_k}) * (\overline{w_k} \odot w_k)^{\mathsf{R}} \implies a_j = \sum_k \langle \overline{v_k} \odot v_k| \, P^{-j} \, |\overline{w_k} \odot w_k\rangle \,.$$

Now, consider the circulant matrix generated by a:

$$\begin{aligned}
\mathsf{circ}(a) &= \sum_{i=0}^{d-1} a_i P^i \\
&= \sum_{k} \sum_{i=0}^{d-1} \langle \overline{v_k} \odot v_k | \, P^{-i} \, | \overline{w_k} \odot w_k \rangle \, P^i \\
&= \sum_{k} \sum_{i=0}^{d-1} \mathrm{Tr}\left(| \overline{w_k} \odot w_k \rangle\langle \overline{v_k} \odot v_k | \, P^{-i} \right) P^i \\
&= \sum_{k} \sum_{i=0}^{d-1} \frac{1}{d} \mathrm{Tr}\left(\sum_j P^j \, | \overline{w_k} \odot w_k \rangle\langle \overline{v_k} \odot v_k | \, P^{-j} P^{-i} \right) P^i \\
&= \sum_{k} \sum_{j} P^j \, | \overline{w_k} \odot w_k \rangle\langle \overline{v_k} \odot v_k | \, P^{-j} \\
&= \sum_{k,j} \left| \overline{w_{kj}} \odot w_{kj} \right\rangle\!\left\langle \overline{v_{kj}} \odot w_{kj} \right| ,
\end{aligned}$$

where $v_{kj} = P^j |v_k\rangle$ and $w_{kj} = P^j |w_k\rangle$. ■

6.5 EXAMPLES OF LCSI STATES

We gather in this section several simple examples of LCSI states. This can be achieved by considering special a, b, c vectors having equal entries or extra zeros. For similar results in the LDOI case, see [SN21, Table 1].

6.5.1 *Diagonal states*

It is clear from the isomorphism in Proposition 6.25 that when $a, b, c \in \mathbb{C}^d$ are such that $b = c = a_0 |0\rangle$, the matrix $X_{a,b,c}$ is diagonal. Hence the following is true for such vector triples:

$$X_{a,b,c} \in \mathsf{PSD}_d \iff X_{a,b,c} \in \mathsf{PPT}_d \iff X_{a,b,c} \in \mathsf{SEP}_d \iff a_k \geq 0 \quad \forall k \in [d].$$

6.5.2 *States with a uniform diagonal*

By analogy with the set of correlation matrices, we define

$$\mathsf{corr}_d := \{x \in \mathbb{C}^d \ : x_0 = 1, \ \mathcal{F}x \in \mathbb{R}^d_+\}.$$

Theorem 6.31. Let $\mathbb{C}^d \ni e := (1, 1, \ldots, 1)^\top$ be the all-ones vector. Then,

$$X_{e,b,c} \in \mathsf{SEP} \iff X_{e,b,c} \in \mathsf{PPT} \iff b, c \in \mathsf{corr}_d.$$

Proof. The forward implications are trivial to prove. Hence, it suffices to show $b, c \in \mathsf{corr}_d \implies X_{e,b,c} \in \mathsf{SEP}$. Let $b, c \in \mathsf{corr}_d$. We expand $\mathcal{F}b = \sum_i (\mathcal{F}b)_i |i\rangle$, so that

$$b = \sum_i (\mathcal{F}b)_i \mathcal{F}^{-1} |i\rangle = \sum_i (\mathcal{F}b)_i |f_i\rangle = \frac{1}{\sqrt{d}} \sum_i (\mathcal{F}b)_i |f_i\rangle * |\overline{f_i}\rangle^{\mathsf{R}},$$

and similarly for c. Note that since $b, c \in \mathsf{corr}_d$, we have $(\mathcal{F}b)_i, (\mathcal{F}c)_i \geq 0$ for all i and $\sqrt{d}\sum_i (\mathcal{F}b)_i = \sqrt{d}\sum_i (\mathcal{F}c)_i = d = \mathrm{Tr}(\mathsf{circ}(b)) = \mathrm{Tr}(\mathsf{circ}(c))$. Now, for each $i, j \in [d]$, we can find phase vectors $v_{ij}, w_{ij} \in \mathbb{T}^d$ such that

$$|v_{ij} \odot w_{ij}\rangle = \sqrt{d} |f_i\rangle \quad \text{and} \quad |v_{ij} \odot \overline{w_{ij}}\rangle = \sqrt{d} |f_j\rangle .$$

Then, we can write

$$\begin{aligned}(e, b, c) &= \left(e, \sum_i \frac{1}{\sqrt{d}} (\mathcal{F}b)_i \ |f_i\rangle * |\overline{f_i}\rangle^{\mathsf{R}}, \sum_j \frac{1}{\sqrt{d}} (\mathcal{F}c)_j \ |f_j\rangle * |\overline{f_j}\rangle^{\mathsf{R}}\right) \\ &= \sum_{i,j} \frac{1}{d} \mathcal{F}(b)_i \mathcal{F}(c)_j \left(e, |f_i\rangle * |\overline{f_i}\rangle^{\mathsf{R}}, |f_j\rangle * |\overline{f_j}\rangle^{\mathsf{R}}\right),\end{aligned}$$

where $\left(e, |f_i\rangle * |\overline{f_i}\rangle^{\mathsf{R}}, |f_j\rangle * |\overline{f_j}\rangle^{\mathsf{R}}\right) \in \overrightarrow{\mathsf{TCP}}_d$ for all i, j with the decomposition given as

$$\frac{1}{d} \left(|v_{ij} \odot \overline{v_{ij}}\rangle * |w_{ij} \odot \overline{w_{ij}}\rangle^{\mathsf{R}}, |v_{ij} \odot w_{ij}\rangle * |\overline{v_{ij}} \odot \overline{w_{ij}}\rangle^{\mathsf{R}}, |v_{ij} \odot \overline{w_{ij}}\rangle * |\overline{v_{ij}} \odot w_{ij}\rangle^{\mathsf{R}}\right).$$

This shows that $X_{e,b,c} \in \mathsf{SEP}$, and the proof is complete. ∎

The above result shows that PPT entanglement does not exist in the subspace of LCSI_d formed by matrices with uniform diagonal. In the next theorem, we show that the corresponding result for LDOI states is false, solving in the negative the question at the end of [SN21, Example 3.6].

Theorem 6.32. In the case of LDOI matrices, we have:

- $X^{\mathsf{LDOI}}_{(\mathbb{J},\mathbb{J},C)} \in \mathsf{PPT}_d \iff C \in \mathsf{Corr}_d := \{Z \in \mathsf{PSD}_d : \operatorname{diag} Z = \mathbb{I}_d\}$.
- $X^{\mathsf{LDOI}}_{(\mathbb{J},\mathbb{J},C)} \in \mathsf{SEP}_d \iff C \in \operatorname{conv}\{|z\rangle\langle z| : |z\rangle \in \mathbb{T}^d\} \subseteq \mathsf{Corr}_d$.

In particular, for local dimension $d \geq 4$, there exist PPT entangled LDOI matrices with triples of the form $(\mathbb{J}, \mathbb{J}, C)$.

Proof. The first point was shown in [SN21, see Example 3.6] and the discussion following it. For the second point, assume that $(\mathbb{J}, \mathbb{J}, C)$ is TCP so that it admits a decomposition given in Definition 6.16 with vectors $|v_k\rangle, |w_k\rangle \in \mathbb{C}^d$. Since $B = \mathbb{J}$ is rank-1 and hence extremal in PSD_d, for all k, $|v_k \odot w_k\rangle\langle v_k \odot w_k| \propto |e\rangle\langle e| \implies |v_k \odot \overline{w_k}\rangle\langle v_k \odot \overline{w_k}| \propto |z_k\rangle\langle z_k|$, where $|z_k\rangle \in \mathbb{T}^d$ is a phase vector. Thus,

$$C \in \mathrm{conv}\{|z\rangle\langle z| : |z\rangle \in \mathbb{T}^d\}.$$

However, for $d \geq 4$, there exist extreme points of Corr_d that are not rank one [GPW90, Loe80, LT94]. Hence, there exist matrices $C \in \mathsf{Corr}_d$ that do not belong in $\mathrm{conv}\{|z\rangle\langle z| : |z\rangle \in \mathbb{T}^d\}$ and for any such C, the triple $(\mathbb{J}, \mathbb{J}, C)$ cannot be TCP. ■

6.5.3 LCSI *states with* b *or* c *extremal*

In a recent paper [SBSGS22], the authors completely characterize the SEP cone on the facet $\{(a, b, a_0 |0\rangle) : b = (a_0, a_0 \ldots a_0) = a_0 |e\rangle)\} \subset (\mathbb{C}^d)^{\times 3}_{\mathbb{C}}$. In the theorem that follows, we will prove a more general result in our framework that also reproduces the results obtained in [SBSGS22]. Let us begin with a simple lemma.

Lemma 6.33. Let $x \in \mathbb{C}^d$ be such that for all $l \in [d]$, $|\sum_i \overline{x_i} x_{i-l}| = |\sum_i \overline{x_i} x_i|$. Then, $x \in \mu \mathbb{T}^d$ for some $\mu \in \mathbb{C}$, i.e., for all $i \in [d]$, $|x_i| = |\mu|$.

Proof. We can rewrite the assumption of the lemma as

$$\forall l \in [d] : \qquad |\langle x|P^{-l}|x\rangle| = |\langle x|x\rangle|,$$

where P is the shift permutation from Remark 6.4. Then, the equality condition of Cauchy Schwarz shows that x is an eigenvector of P, i.e. x is a scalar multiple of a phase vector. ■

Theorem 6.34. Let $X_{a,b,c}$ be such that $a \in \mathbb{R}^d_+$ and $b, c \in \overrightarrow{\mathsf{PSD}}_d$ (such that $b_0 = c_0 = a_0$) with either b or c being extremal, and $a_0 = b_0 = c_0$. Then, the following equivalences hold:

$$\begin{aligned} a_l a_{d-l} \geq a_0^2 \quad \forall l \in [d] &\iff X_{a,b,c} \in \mathsf{PPT} \\ a_l \geq a_0 \quad \forall l \in [d] &\iff X_{a,b,c} \in \mathsf{SEP}. \end{aligned}$$

Proof. The PPT equivalence follows easily from Theorem 6.28 (note that since b is extremal, Remark 6.15 shows that $|b_i| = b_0 = a_0$ for all i).

Here, we prove the SEP equivalence. Assume that $a_l \geq a_0 \geq 0$ for all l. We split

$$(a, b, c) = (a - a_0 |e\rangle, 0, 0) + (a_0 |e\rangle, b, c),$$

where the former triple is in $\overrightarrow{\mathsf{TCP}}_d$ because $a_l - a_0 \geq 0$ for all l and the latter triple is in $\overrightarrow{\mathsf{TCP}}_d$ as $a_0 |e\rangle$ is a uniform vector and $\mathcal{F}(b), \mathcal{F}(c) \in \mathbb{R}^d_+$, see Theorem 6.31. Hence, $X_{a,b,c} \in \mathsf{SEP}$ (note that in the forward implication, we did not actually make use of extremality of b or c).

To show the converse, assume (wlog) that b is extremal in $\overrightarrow{\mathsf{PSD}}_d$ and $X_{a,b,c} \in \mathsf{SEP}$, so that (a, b, c) admits a decomposition given in Definition 6.29 with vectors $|v_k\rangle, |w_k\rangle$. Let $|x_k\rangle = |v_k \odot w_k\rangle$, so that we can write

$$b = \sum_k |\overline{x_k}\rangle * |x_k\rangle^{\mathsf{R}} \implies |\overline{x_k}\rangle * |x_k\rangle^{\mathsf{R}} = \lambda_k |b\rangle$$

for some $\lambda_k \geq 0$, where the implication follows from the extremality of b. From Remark 6.15, we know that $|b_0| = |b_i|$ for all i. Hence, we can use Lemma 6.33 to deduce that $|x_k\rangle \in \mu_k \mathbb{T}^d$ is a scalar multiple of a phase vector for each k, i.e., $|v_k^i w_k^i| = |\mu_k|$ for all i, k. Now, the $\overrightarrow{\mathsf{TCP}}_d$ decomposition for a shows that

$$\begin{aligned} \forall l \in [d] : \quad a_l = \sum_k \sum_i |v_k^i|^2 |w_k^{l-i}|^2 &= \sum_k |\mu_k|^2 \sum_i |v_k^i|^2 \frac{1}{|v_k^{l-i}|^2} \\ &\geq d \sum_k |\mu_k|^2 \cdot \prod_i \left(|v_k^i|^2 \frac{1}{|v_k^{l-i}|^2} \right)^{1/d} \\ &= d \sum_k |\mu_k|^2 \\ &= a_0, \end{aligned}$$

where we used the AM-GM inequality. This completes the proof. ∎

Example 6.35. We borrow the example from [SN21, Example 9.1]: take $d = 3$, $a := (2\mu, 1, 4\mu^2)$ and $b := (2\mu, 2\mu, 2\mu)$ for $\mu \in \mathbb{R}$. The condition $b, c \in \overrightarrow{\mathsf{PSD}}_d$ reads $\mu \geq 0$. We have now that

$$X_{a,b,c} \in \mathsf{PPT} \iff \mu \geq 0$$
$$X_{a,b,c} \in \mathsf{SEP} \iff \mu = 1/2.$$

Hence, the matrix $X_{a,b,c}$ is PPT entangled for any $\mu \in (0, \infty) \setminus \{1/2\}$. Such an example can be easily generalized to any dimension $d \geq 3$.

Remark 6.36. Theorem 6.34 gives a very simple recipe to construct PPT entangled LCSI states in local dimension $d \geq 3$: take $b = c = e$, and a such that

$$a_1 = \alpha,\ a_{d-1} = 1/\alpha \quad \text{and} \quad a_i = 1 \text{ for } i \neq 1, d-1$$

for some $\alpha > 1$.

If b or c in the above theorem is of the form $\beta |e\rangle + (a_0 - \beta) |0\rangle$, the above argument doesn't hold, as it was essential to use the fact that the vectors b, c are extremal. However, the proof of Theorem 6.34.

Conjecture 6.37. Given $a \in \mathbb{R}^d_+$ and $\beta \in \mathbb{R}$, we have $X_{a,\beta|e\rangle+(a_0-\beta)|0\rangle,a_0|0\rangle} \in \mathsf{SEP}$ iff $a_i \geq a_0 \geq \beta$ for all $i \in [d]$.

6.6 CYCLIC MIXTURES OF DICKE STATES

In this section we focus on a special subset of bipartite quantum states with circular symmetry, those corresponding to *mixtures of Dicke states*. Such states have received a lot of attention in the general (no circulant symmetry) case [TAQ+18, Yu16, SN21], in particular due to the connection to the theory of *completely positive matrices* [BSM03].

Definition 6.38. A state $X \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ is said to be a *mixture of Dicke states* if it can be written as

$$X = \sum_{i,j=1}^{d} p_{ij} \, |D_{ij}\rangle\langle D_{ij}| \tag{32}$$

where $D_{ij} = \frac{1}{\sqrt{2}}(|ij\rangle + |ji\rangle)$ for $i \neq j$, $D_{ii} = |ii\rangle$, $p_{ij} = p_{ji} \geq 0$, and $\sum_{i,j=1}^{d} p_{ij} = 1$.

It has been well understood that characterizing PPT and separability for Dicke states reduce to checking membership in the cones of doubly non-negative and completely positive matrices, respectively [TAQ+18, Yu16]. Recall that a matrix $A \in \mathcal{M}_d(\mathbb{C})$ is called *completely positive* if it admits a decomposition $A = \sum_i |v_i\rangle\langle v_i|$ such that for each i, $v_i \in \mathbb{R}^d_+$ [BSM03]. The cone of all completely positive $d \times d$ matrices is denoted CP_d. The cone of $d \times d$ *doubly non-negative* matrices is defined as $\mathsf{DNN}_d := \mathsf{EWP}_d \cap \mathsf{PSD}_d$. Clearly, $\mathsf{CP}_d \subseteq \mathsf{DNN}_d$, where equality holds if and only if $d \leq 4$ [BSM03]. Note that Dicke states form a subclass of LDOI states with the corresponding matrix triples (A, B, C) satisfying $A_{ij} = C_{ij} = p_{ij}$ and $B = \mathrm{diag}(A)$ [SN21], which can be used to prove the following result.

Theorem 6.39. [TAQ+18] The following equivalences hold true for Dicke states:

- $X_{(A,\mathrm{diag}\,A,A)}$ is separable $\iff$ $(A, \mathrm{diag}\,A, A) \in \mathsf{TCP}_d$ $\iff$ $A \in \mathsf{CP}_d$.
- $X_{(A,\mathrm{diag}\,A,A)}$ is PPT $\iff$ $A \in \mathsf{DNN}_d$.

Similarly, mixtures of Dicke states with the following additional symmetry,

$$(P \otimes P)X(P \otimes P)^* = (P \otimes P)X(P \otimes P)^\top = X$$

for all cyclic permutation matrices $P \in \mathrm{Cyc}(d)$ can be understood as the subclass of LCSI_d states (see Section 6.4) with

$$a_k = c_k = p_{i,i+k}, \qquad \forall i, k \in [d].$$

In particular, this means that the symmetric matrix p defining the Dicke state mixture in Eq. (32) is circulant, and the vectors a, c in the LCSI writing are given by the first row of p, while the b vector is trivial (only its 0-th coordinate being non-zero).

Below is the general form of a circulant mixture of Dicke states, in the cases $d = 2, 3$ (dots represent 0 entries):

$$X_{(a_0,a_1),(a_0,0),(a_0,a_1)} = \left[\begin{array}{cc|cc} a_0 & \cdot & \cdot & \cdot \\ \cdot & a_1 & a_1 & \cdot \\ \hline \cdot & a_1 & a_1 & \cdot \\ \cdot & \cdot & \cdot & a_0 \end{array}\right]$$

$$X_{(a_0,a_1,a_2),(a_0,0,0),(a_0,a_1,a_2)} = \left[\begin{array}{ccc|ccc|ccc} a_0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & a_1 & \cdot & a_1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & a_2 & \cdot & \cdot & \cdot & a_2 & \cdot & \cdot \\ \hline \cdot & a_2 & \cdot & a_2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & a_0 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_1 & \cdot & a_1 & \cdot \\ \hline \cdot & \cdot & a_1 & \cdot & \cdot & \cdot & a_1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_2 & \cdot & a_2 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_0 \end{array}\right].$$

We define the cones $\overrightarrow{\mathsf{CP}}_d$ and $\overrightarrow{\mathsf{DNN}}_d$ as the intersection of the cones CP_d and DNN_d with the circulant subspace:

$$\overrightarrow{\mathsf{CP}}_d := \operatorname{cone}\{v * v^{\mathsf{R}} : v \in \mathbb{R}^d_+\} \quad \text{and} \quad \overrightarrow{\mathsf{DNN}}_d := \operatorname{cone}\{a \in \mathbb{R}^d_+ \,:\, \mathcal{F}a \in \mathbb{R}^d_+\} = \mathbb{R}^d_+ \cap \mathcal{F}\mathbb{R}^d_+.$$

Proposition 6.40. For all $d \geq 2$, we have $\overrightarrow{\mathsf{CP}}_d \subseteq \overrightarrow{\mathsf{DNN}}_d \subseteq \mathbb{R}^d_+$.

Proof. Consider an arbitrary element of the cone $\overrightarrow{\mathsf{CP}}_d$

$$a = \sum_k \lambda_k v_k * v_k^{\mathsf{R}}$$

for non-negative vectors $v_k \in \mathbb{R}^d_+$ and non-negative scalars $\lambda_k \geq 0$. Clearly, a is entrywise non-negative. Taking the Fourier transform of a we have

$$\sqrt{d}\mathcal{F}a = \sqrt{d}\sum_k \lambda_k \mathcal{F}(v_k * v_k^{\mathsf{R}}) = d\sum_k \lambda_k \mathcal{F}v_k \odot \mathcal{F}(v_k^R) = d\sum_k \lambda_k \mathcal{F}v_k \odot \overline{\mathcal{F}v_k} \in \mathbb{R}^d_+,$$

proving that $\mathcal{F}a$ is also entrywise non-negative and finishing the proof. ∎

The connection to separability and the PPT property of the corresponding LCSI states are given in the following result.

Proposition 6.41. The following equivalences are true for vector triples of the form $(a, a_0 |0\rangle, a)$

- $X_{a,a_0|0\rangle,a} \in \mathsf{SEP} \iff (a, a_0 |0\rangle, a) \in \overrightarrow{\mathsf{TCP}}_d \iff a \in \overrightarrow{\mathsf{CP}}_d$
- $X_{a,a_0|0\rangle,a} \in \mathsf{PPT} \iff a \in \overrightarrow{\mathsf{DNN}}_d$

The remainder of this section is devoted to characterizing the geometry of these cones. Importantly, for every $d \geq 5$, there exist $\overrightarrow{\mathsf{CP}}_d$ vectors that are not in $\overrightarrow{\mathsf{DNN}}_d$, signaling the presence of PPT entanglement in the class of symmetric states we consider.

6.6.1 *Euclidean formulation of the cones*

In this section we are considering cones $X \subseteq \mathbb{R}^d$ such that the $\mathcal{F} \cdot X \subseteq \mathbb{R}^d$ or equivalently we are looking at vectors $X \ni a = a^{\mathsf{R}}$. These conditions impose linear constraints on the cones, hence they have, in general, empty interior in $\mathbb{R}^d$. To remedy the situation, we shall consider their linear closure, hence reducing the total dimension of the underlying vector space.

Let us introduce the new parameter $n := 1 + \lfloor d/2 \rfloor$, which counts the number of free parameters of reflection-invariant real vectors. We can construct an orthonormal basis $\{f_j\}_{j\in[n]}$for the space

$$E_d := \{a \in \mathbb{R}^d \,:\, a = a^{\mathsf{R}}\}$$

as follows:

$$\{e_0\} \cup \left\{\frac{e_i + e_{-i}}{\sqrt{2}}\right\}_{i=1}^{n-2} \cup \{e_{n-1}\} \quad \text{if } d \text{ is even;} \qquad \{e_0\} \cup \left\{\frac{e_i + e_{-i}}{\sqrt{2}}\right\}_{i=1}^{n-1} \quad \text{if } d \text{ is odd.} \tag{33}$$

The space E is left invariant by the Fourier matrix $\mathcal{F}_{ij} = \omega^{ij}/\sqrt{d}$. We denote by G the restriction of $\mathcal{F}$ to the space E. One can compute the matrix elements of G from those of $\mathcal{F}$. For example, in the case where $f_j = (e_j + e_{-j})/\sqrt{2}$:

$$\langle f_0 | \mathcal{F} | f_j \rangle = \frac{\langle e_0 | \mathcal{F} | e_j \rangle + \langle e_0 | \mathcal{F} | e_{-j} \rangle}{\sqrt{2}} = \sqrt{2}\,\mathrm{Re}\,\langle e_0 | \mathcal{F} | e_j \rangle\,.$$

Clearly, G is a symmetric matrix ($G = G^\top$) and we have

$$G_{ij} = \begin{cases} \frac{1}{\sqrt{d}} & \text{if } i = j = 0, \\ \sqrt{\frac{2}{d}} & \text{if } i = 0 \text{ and } 1 \leq j < \frac{d}{2}, \\ \frac{1}{\sqrt{d}} & \text{if } i = 0 \text{ and } j = \frac{d}{2} \text{ (for even } d), \\ \frac{2}{\sqrt{d}} \cos\left(\frac{2\pi ij}{d}\right) & \text{if } 1 \leq i, j < \frac{d}{2}, \\ \sqrt{\frac{2}{d}}(-1)^i & \text{if } 1 \leq i < \frac{d}{2} \text{ and } j = \frac{d}{2} \text{ (for even } d), \\ \frac{(-1)^{d/2}}{\sqrt{d}} & \text{if } i = j = \frac{d}{2} \text{ (for even } d). \end{cases}$$

For d even, we have

$$G = \frac{1}{\sqrt{d}} \begin{pmatrix} 1 & \sqrt{2} & \sqrt{2} & \cdots & \sqrt{2} & 1 \\ \sqrt{2} & 2\cos\left(\frac{2\pi\cdot 1\cdot 1}{d}\right) & 2\cos\left(\frac{2\pi\cdot 1\cdot 2}{d}\right) & \cdots & 2\cos\left(\frac{2\pi\cdot 1\cdot \frac{d}{2}-1}{d}\right) & \sqrt{2}(-1)^1 \\ \sqrt{2} & 2\cos\left(\frac{2\pi\cdot 2\cdot 1}{d}\right) & 2\cos\left(\frac{2\pi\cdot 2\cdot 2}{d}\right) & \cdots & 2\cos\left(\frac{2\pi\cdot 2\cdot \frac{d}{2}-1}{d}\right) & \sqrt{2}(-1)^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \sqrt{2} & 2\cos\left(\frac{2\pi\cdot(\frac{d}{2}-1)\cdot 1}{d}\right) & 2\cos\left(\frac{2\pi\cdot(\frac{d}{2}-1)\cdot 2}{d}\right) & \cdots & 2\cos\left(\frac{2\pi\cdot(\frac{d}{2}-1)\cdot\frac{d}{2}-1}{d}\right) & \sqrt{2}(-1)^{\frac{d}{2}-1} \\ 1 & \sqrt{2}(-1)^1 & \sqrt{2}(-1)^2 & \cdots & \sqrt{2}(-1)^{\frac{d}{2}-1} & (-1)^{\frac{d}{2}} \end{pmatrix}.$$

For d odd, we have

$$G = \frac{1}{\sqrt{d}} \begin{pmatrix} 1 & \sqrt{2} & \sqrt{2} & \cdots & \sqrt{2} \\ \sqrt{2} & 2\cos\left(\frac{2\pi\cdot 1\cdot 1}{d}\right) & 2\cos\left(\frac{2\pi\cdot 1\cdot 2}{d}\right) & \cdots & 2\cos\left(\frac{2\pi\cdot 1\cdot \frac{d-1}{2}}{d}\right) \\ \sqrt{2} & 2\cos\left(\frac{2\pi\cdot 2\cdot 1}{d}\right) & 2\cos\left(\frac{2\pi\cdot 2\cdot 2}{d}\right) & \cdots & 2\cos\left(\frac{2\pi\cdot 2\cdot \frac{d-1}{2}}{d}\right) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{2} & 2\cos\left(\frac{2\pi\cdot\frac{d-1}{2}\cdot 1}{d}\right) & 2\cos\left(\frac{2\pi\cdot\frac{d-1}{2}\cdot 2}{d}\right) & \cdots & 2\cos\left(\frac{2\pi\cdot\frac{d-1}{2}\cdot\frac{d-1}{2}}{d}\right) \end{pmatrix}.$$

Below are the matrices G, for $d = 2, 3, 4, 5$ (and, respectively, $n = 2, 2, 3, 3$):

$$G^{(d=2)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad G^{(d=3)} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{bmatrix}$$

$$G^{(d=4)} = \frac{1}{2} \begin{bmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{bmatrix} \qquad G^{(d=5)} = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & \frac{\sqrt{5}-1}{2} & \frac{-\sqrt{5}-1}{2} \\ \sqrt{2} & \frac{-\sqrt{5}-1}{2} & \frac{\sqrt{5}-1}{2} \end{bmatrix}.$$

We shall identify in what follows the vector space E_d with $\mathbb{R}^n$ (recall that $n = 1 + \lfloor d/2 \rfloor$). Therefore, to every $a \in \overrightarrow{\mathsf{DNN}}_d$, we have assign $b \in \mathbb{R}^n$:

$$a \leftrightarrow b \iff \mathcal{F}a \leftrightarrow Gb$$

In this section, we prove some results to understand the geometry of the convex cones $\overrightarrow{\mathsf{DNN}}_d$ and $\overrightarrow{\mathsf{CP}}_d$ that characterize completely the cones of SEP and PPT in the class of states that we introduced in the preceding section. We will look at the convex geometry of these cones as subsets of $\mathbb{R}^n$.

6.6.2 *Extremal rays of polyhedral PPT cone*

Since $\overrightarrow{\mathsf{DNN}}_d$ is a polyhedral cone, it is generated by a finite number of extreme rays. As we shall see, the analytical enumeration of all extreme rays of $\overrightarrow{\mathsf{DNN}}_d$ is still difficult problem. Here we prove certain results about this cone, and provide a simple algorithm to calculate its extreme rays. In this section, we shall continue using the correspondence between $\overrightarrow{\mathsf{DNN}}_d \subseteq \mathbb{R}^d$ and the real vector space $E_d \approx \mathbb{R}^n$. We have

$$\overrightarrow{\mathsf{DNN}}_d \leftrightarrow \{b \in \mathbb{R}^n_+ \,:\, Gb \in \mathbb{R}^n_+\}.$$

We are thus considering the so-called *semi-positive cone* of the matrix G. We recall below the definition in the general case, see e.g. [ST18, HS20] and references therein, as well as Fig. 11.

Definition 6.42. Let A be a real $n \times n$ square matrix. The *semi-positive* cone with respect to A is the set

$$\mathsf{SPC}_A := \{x \in \mathbb{R}^n_+ \,:\, Ax \in \mathbb{R}^n_+\}.$$

Hence, finding the extremal rays of the cone $\overrightarrow{\mathsf{DNN}}_d$ (in $\mathbb{R}^d$) is equivalent to finding the extremal rays of the semi-positive cone of the matrix G (in $\mathbb{R}^n$). We shall focus on the latter problem in this section. For example, in the case $d = 2$ (resp. $d = 3$) the matrix G corresponds to a $\pi/4$ (resp. $\pi/6$) clock-wise rotation in $\mathbb{R}^2$. The extremal rays of the semi-positive cone of G are the first basis element f_0 and its image through G. We have the following result, showing that the extremal rays of SPC_G come in (possibly degenerate) pairs.

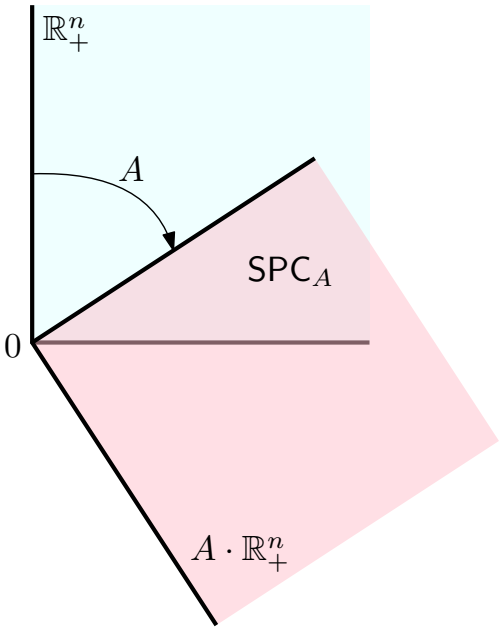


Figure 11: The semi-positive cone of a linear transformation $A : \mathbb{R}^n \to \mathbb{R}^n$ is the intersection of the non-negative orthant $\mathbb{R}^n_+$ with its image through A.

Proposition 6.43. If $x \in \mathbb{R}^n_+$ is an extreme ray of SPC_G if and only if $Gx \in \mathbb{R}^n_+$ is an extreme ray of SPC_G.

Proof. Since $G^2 = I$, G leaves invariant its semi-positive cone $G \cdot \mathsf{SPC}_G = \mathsf{SPC}_G$. Hence the set of extreme rays of SPC_G must have the same G-symmetry. Indeed, assume that x is an extreme ray of SPC_G. Assume there exist vectors $g_1, g_2 \in \mathsf{SPC}_G$ such that $G(x) = g_1 + g_2$. Then $x = G(g_1) + G(g_2)$. Since x is an extreme ray and $G(g_1), G(g_2) \in \mathsf{SPC}_G$, it $\implies$ $G(g_1), G(g_2) \propto x \implies g_1, g_2 \propto G(x)$. Hence $G(x)$ is an extreme ray. ■

The above proof shows that the extremal rays of SPC_G either satisfy $Ga = a$ (i.e. they are eigenvectors of the matrix G with eigenvalue 1) or they come in pairs (a, Ga).

Let us now make some general observation about the semi-positive cones of real matrices. We shall specialize these results in the following subsection to the matrices G corresponding to the $\overrightarrow{\mathsf{DNN}}_d$ cones. The next observation is that the supports of the vectors defining the extreme rays are severely constrained. Recall that the support of a vector $v \in \mathbb{C}^n$ is the set of indices of the non-zero elements of v:

$$\mathrm{supp}(v) := \{i \in [n] \,:\, v_i \neq 0\}.$$

We start with a slightly technical lemma.

Lemma 6.44. Let X be a real $n \times n$ matrix and $a \in \mathsf{SPC}_X$. Assume that there exists a vector $b \in \mathbb{R}^d$ such that the following conditions hold:

- the vectors a and b are not colinear, i.e. $\mathbb{R}a \neq \mathbb{R}b$
- $\mathrm{supp}(b) \subseteq \mathrm{supp}(a)$
- $\mathrm{supp}(Xb) \subseteq \mathrm{supp}(Xa)$

Then $\mathbb{R}_+ a$ is *not* an extremal ray of SPC_X.

Proof. Put

$$\varepsilon := \min\left[\min_{i\in\mathrm{supp}(a)}\left(\frac{|a_i|}{|b_i|}\right), \min_{i\in\mathrm{supp}(Xa)}\left(\frac{|(Xa)_i|}{|(Xb)_i|}\right)\right] > 0,$$

where we use the convention $|x|/0 = +\infty$. Using the condition on the supports, we have $a \pm \varepsilon b \in \mathsf{SPC}_X$, which provides a non-trivial decomposition of the ray $\mathbb{R}_+ a$ inside the cone SPC_X, proving the claim. ∎

For the main result of this section, we shall denote by $X[J, I]$ the submatrix of X consisting of rows indexed by J and columns indexed by I (here, $\emptyset \neq I, J \subseteq [n]$). We have

$$X[J, I] : \mathbb{R}^I \to \mathbb{R}^J.$$

Theorem 6.45. Let I and J be subsets of $\{0, 1, \ldots, n-1\}$. Define the integer function

$$\beta_X(I, J) := \dim \ker X[J^c, I].$$

We have then:

1. If $\beta_X(I, J) \geq 2$ for some index sets I and J, then any vector $a \in \mathsf{SPC}_X$ with $\mathrm{supp}(a) = I$ and $\mathrm{supp}(Xa) = J$ is not extremal in SPC_X.
2. If $\beta_X(I, J) = 1$ and $\ker X[J^c, I]$ is spanned by a vector v such that $v > 0$ entrywise and $X[J, I]v > 0$ entrywise, then the vector $a := v_I \oplus O_{I^c}$ is extremal in SPC_X with $\mathrm{supp}(a) = I$, and $\mathrm{supp}(Xa) = J$.
3. Conversely, let a be a vector lying on an extremal ray of SPC_X with $\mathrm{supp}(a) = I$ and $\mathrm{supp}(Xa) = J$. Then $\beta_X(I, J) = 1$ and $\ker X[J^c, I]$ is spanned by $a_I > 0$ entrywise which also satisfies $(Xa)_J > 0$ entrywise.

Proof. We will make repeated use of Lemma 6.44 to show this theorem.

1. Assume $\beta_X(I,J) \geq 2$ and let $a \in \mathsf{SPC}_X$ be a vector with $\operatorname{supp}(a) = I$ and $\operatorname{supp}(Xa) = J$. Since $\dim(\ker X[J^c, I])) \geq 2$, there exists at least one vector $b \in \ker X[J^c, I])$ not colinear to a. Hence, setting $b' := b_I \oplus 0_{I^c}$, we have

$$Xb' = X[J,I]b \oplus X[J^c,I]b = X[J,I]b \oplus 0_{J^c},$$

   thus $\operatorname{supp}(Xb') \subseteq J$. We can now apply Lemma 6.44, proving the first claim.

2. We only need to show extremality, all the other claims being clear. Assume, $a = b + c$ where $b, c \in \mathsf{SPC}_X$. We know that $\operatorname{supp}(b), \operatorname{supp}(c) \subseteq \operatorname{supp}(a) = I$ and similarly $\operatorname{supp}(Xb), \operatorname{supp}(Xc) \subseteq \operatorname{supp}(Xa) = J$, hence $b_I, c_I \in \ker X[J^c, I]$. Since the kernel has dimension 1, b_I and c_I must be colinear with v and thus b, c must be colinear with a, proving the claim.

3. For an extremal vector a with $\operatorname{supp}(a) = I$ and $\operatorname{supp}(Xa) = J$, we have $X[J^c, I]a_I = 0$, hence $\beta_X(I,J) \geq 1$. Moreover, since a is extremal, it follows from the first item in the result that $\beta_X(I,J) < 2 \implies \beta_X(I,J) = 1$. The strict positivity follows from the fact that $a \in \mathsf{SPC}_X$ and the support conditions.

■

The result above essentially tells us that, for every pair of subsets $\emptyset \neq I, J \subseteq [n]$, there is at most one extremal ray a of SPC_X such that $\operatorname{supp}(a) = I$ and $\operatorname{supp}(Xa) = J$. Moreover, the pairs (I,J) of supports of extremal rays have to satisfy $\beta_X(I,J) = 1$. Therefore the function $\beta_X(I,J)$ contains very useful information about the possible supports of the extremal rays of the cone SPC_X.

Lemma 6.46. The function β_X has the following monotonicity properties with respect to the inclusion partial order on index sets:

$$I \subseteq I' \implies \beta_X(I,J) \leq \beta_X(I',J)$$
$$J \subseteq J' \implies \beta_X(I,J) \leq \beta_X(I,J').$$

Proof. For the first point, assuming $I \subseteq I'$, if $v \in \ker X[J^c, I]$ then $v \oplus 0_{I'-I} \in \ker X[J^c, I']$, hence $\beta_X(I,J) \leq \beta_X(I',J)$.

For the second claim, let $v \in \ker X[J^c, I]$. Since $J'^c \subseteq J^c$, we have that $v \in \ker X[J'^c, I]$, proving the claim. ■

We have implemented a `Mathematica` routine to compute the extremal rays of SPC_X for an arbitrary matrix X by enumerating the possible support sets, see [Gul25]. For example, in the case of the matrix

$$X = \begin{bmatrix} 0 & 0 & 1 \\ \frac{1}{2} & \frac{1}{5} & -1 \\ 0 & 1 & 0 \end{bmatrix},$$

which was also considered in [HS20, Example 3.3], our code correctly identifies the extremal rays and their support:

$\mathrm{supp}(a)$	$\mathrm{supp}(Xa)$	a
$\{1\}$	$\{2\}$	$(1,0,0)$
$\{2\}$	$\{2,3\}$	$(0,1,0)$
$\{1,3\}$	$\{1\}$	$\left(1,0,\frac{1}{2}\right)$
$\{2,3\}$	$\{1,3\}$	$\left(0,1,\frac{1}{5}\right)$

6.6.3 *Enumeration of extremal rays*

Facets of $\overrightarrow{\mathsf{DNN}}_d$ *for small* d

Using the `Mathematica` routine [Gul25] we implemented for generating the extremal rays of semi-positive cones, we can generate the extremal rays of the doubly non-negative circulant cone $\overrightarrow{\mathsf{DNN}}_d$ for small values of d, by first computing the extremal rays of SPC_G for the matrix G and then embedding these vectors of $\mathbb{R}^n$ into the larger space $\mathbb{R}^d$ using the reverse basis change from Eq. (33); note the factor $\sqrt{2}$ that has to be taken into account. Note how the two vectors

$$|0\rangle = (1, \underbrace{0, \ldots, 0}_{d-1 \text{ times}}) \quad \text{and} \quad |e\rangle = (1, 1, 1, \ldots, 1)$$

are extremal for all $d \geq 2$. We present our results below, for $d = 2, 3, 4, 5, 6$.

For $d = 2$

$\mathrm{supp}(a)$	$\mathrm{supp}(\mathcal{F}a)$	a
$\{1\}$	$\{1,2\}$	$(1,0)$
$\{1,2\}$	$\{1\}$	$(1,1)$

For $d = 3$

$\mathrm{supp}(a)$	$\mathrm{supp}(\mathcal{F}a)$	a
$\{1\}$	$\{1,2,3\}$	$(1,0,0)$
$\{1,2,3\}$	$\{1\}$	$(1,1,1)$

For $d = 4$

$\mathrm{supp}(a)$	$\mathrm{supp}(\mathcal{F}a)$	a
$\{1\}$	$\{1,2,3,4\}$	$(1,0,0,0)$
$\{1,2,4\}$	$\{1,2,4\}$	$\left(1,\frac{1}{2},0,\frac{1}{2}\right)$
$\{1,3\}$	$\{1,3\}$	$(1,0,1,0)$
$\{1,2,3,4\}$	$\{1\}$	$(1,1,1,1)$

For $d = 5$

$\mathrm{supp}(a)$	$\mathrm{supp}(\mathcal{F}a)$	a
$\{1\}$	$\{1,2,3,4,5\}$	$(1,0,0,0,0)$
$\{1,2,5\}$	$\{1,2,5\}$	$\left(1,\frac{\sqrt{5}-1}{2},0,0,\frac{\sqrt{5}-1}{2}\right)$
$\{1,3,4\}$	$\{1,3,4\}$	$\left(1,0,\frac{\sqrt{5}-1}{2},\frac{\sqrt{5}-1}{2},0\right)$
$\{1,2,3,4,5\}$	$\{1\}$	$(1,1,1,1,1)$

For $d = 6$

$\mathrm{supp}(a)$	$\mathrm{supp}(\mathcal{F}a)$	a
$\{1\}$	$\{1,2,3,4,5,6\}$	$(1,0,0,0,0,0)$
$\{1,2,6\}$	$\{1,2,3,5,6\}$	$\left(1,\frac{1}{2},0,0,0,\frac{1}{2}\right)$
$\{1,3,5\}$	$\{1,4\}$	$(1,0,1,0,1,0)$
$\{1,4\}$	$\{1,3,5\}$	$(1,0,0,1,0,0)$
$\{1,2,3,5,6\}$	$\{1,2,6\}$	$\left(1,\frac{3}{4},\frac{1}{4},0,\frac{1}{4},\frac{3}{4}\right)$
$\{1,2,3,4,5,6\}$	$\{1\}$	$(1,1,1,1,1,1)$

Analytical enumeration of facets of $\overrightarrow{\mathsf{DNN}}_d$ *with small supports*

Although the cone $\overrightarrow{\mathsf{DNN}}_d$ has a polyhedral structure, the analytical enumeration of the extreme rays of this cone is still a significant challenge for general dimension d. In this section, we make some progress to understand the extreme rays of the $\overrightarrow{\mathsf{DNN}}_d$ cone which have support of size 3 or its Fourier transform (equal to the rank of the corresponding circulant matrix) has support of size 3.

Definition 6.47. For every $I \subseteq [0:d-1]$, we define a facet of the cone

$$\overrightarrow{\mathsf{DNN}}_d^I = \mathrm{conv}\{a \in \mathrm{ext}(\overrightarrow{\mathsf{DNN}}_d) \,:\, \mathrm{supp}(a) \subseteq I\}.$$

Since extremal rays of facets are extremal in the cone, we have the following result.

Proposition 6.48. The extreme rays of the cone $\overrightarrow{\mathsf{DNN}}_d^I$ are also extreme rays of the $\overrightarrow{\mathsf{DNN}}_d$ cone.

Lemma 6.49. For every subset $I = -I \subseteq [d]$ and any positive integer k, we have $\overrightarrow{\mathsf{DNN}}_{md}^{mI} \cong \overrightarrow{\mathsf{DNN}}_d^I$.

Proof. The matrix G satisfies the scaling property, $G_{mn}[mJ, I] = G_n[I, J]$. Since the extremal rays depend only on $\ker(G_n[J^c, I])$, we can show that the cones are isomorphic with

$$a \in \overrightarrow{\mathsf{DNN}}_d^I \longleftrightarrow b \in \overrightarrow{\mathsf{DNN}}_{md}^{mI} \text{ such that } b_{mi} = a_i \,\forall i \in [d] \text{ and } b_k = 0 \text{ otherwise.}$$

■

Proposition 6.50. In the case of trivial support $I = \{0\}$, we have $\overrightarrow{\mathsf{DNN}}_d^{\{0\}} = \mathrm{cone}\{|0\rangle\}$. Hence both $|0\rangle$ and e are extremal rays of the $\overrightarrow{\mathsf{DNN}}_n$ cone. Moreover these are the only extreme rays for $\overrightarrow{\mathsf{DNN}}_2$ and $\overrightarrow{\mathsf{DNN}}_3$.

Since the analytical enumeration of the extremal rays is a difficult problem, we provide some partial results when the supports of the rays are small. We look at the facet $\overrightarrow{\mathsf{DNN}}_d^{\{0,i,d-i\}}$ for each i and d.

Proposition 6.51. For $i \neq d/2$, the extreme rays of the $\overrightarrow{\mathsf{DNN}}_d^I$ for $I = \{0, i, d-i\}$ are:

- $\mathbb{R}_+ |0\rangle$
- $\begin{cases} \mathbb{R}_+ \left(2\cos\left(\frac{\gcd(i,d)\pi}{d}\right), 1, 1\right)_{\{0,i,d-i\}} & \text{if } \frac{d}{\gcd(i,d)} \text{ is odd,} \\ \mathbb{R}_+ \left(1, 1, 1\right)_{\{0,i,d-i\}} & \text{if } \frac{d}{\gcd(i,d)} \text{ is even.} \end{cases}$

where $\gcd(p, q)$ denotes the greatest common divisor of two positive integers p, q. For d even, and $i = d/2$ the extreme rays with the support $I = \{0, d/2\}$ are $\mathbb{R}_+(1, 1)$ and $\mathbb{R}_+(1, 0)$.

Proof. Let us start by considering the case $i \neq d/2$. The facet $\overrightarrow{\mathsf{DNN}}_d^{\{0,i,d-i\}}$ is described by the inequalities $a_0 \geq 0$, $a_i = a_{d-i} \geq 0$, and $a_0 + 2\cos\left(\frac{2\pi ij}{d}\right) a_i \geq 0$ for all j. Let $k = \gcd(i, d)$, and write $i = ka$ and $d = kb$. We have then

$$\min_{j\in[d]} \cos\left(\frac{2\pi ij}{d}\right) = \min_{j\in[d]} \cos\left(j \cdot \frac{2\pi a}{b}\right) = \min_{j\in[b]} \cos\left(\frac{2\pi j}{b}\right) = \begin{cases} -1 & \text{if } b \text{ is even} \\ -\cos\left(\frac{\pi}{b}\right) & \text{if } b \text{ is odd,} \end{cases}$$

where in the second equality above we have used the fact that $\exp\left(2\pi \mathrm{i} \frac{a}{b}\right)$ is a *primitive* root of unity. We conclude by plugging this minimum value in the inequality

$$a_0/a_i \geq -2 \min_{j\in[d]} \cos\left(\frac{2\pi ij}{d}\right).$$

In the case of d even, $i = d/2$, we can use the fact that $\overrightarrow{\mathsf{DNN}}_d^{\{0,d/2\}} \cong \overrightarrow{\mathsf{DNN}}_2^{\{0,1\}} = \overrightarrow{\mathsf{DNN}}_2$ by Lemma 6.49.

■

Corollary 6.52. The extremal rays of the $\overrightarrow{\mathsf{DNN}}_5$ cone are exactly $\{|0\rangle, e, a^{(1)}, a^{(2)}\}$, where

$$a^{(1)} = (2\cos(\pi/5), 1, 0, 0, 1), \qquad a^{(2)} = (2\cos(\pi/5), 0, 1, 1, 0).$$

Proof. These extremal rays have already been computed using computer assisted routine based on supports in Section 6.6.3. We provide below a full analytical proof of this result.

By Theorem 6.45 we know that the unique extremal ray having full support is e; we get for free its dual $|0\rangle$, see Proposition 6.43. The only other possible supports are $\{0,1,4\}$ and $\{0,2,3\}$. These fall under Proposition 6.51, and we recover the vectors $a^{(1,2)}$ which can be rewritten as

$$a^{(1)} = \left(1, \frac{\sqrt{5}-1}{2}, 0, 0, \frac{\sqrt{5}-1}{2}\right), \qquad a^{(2)} = \left(1, 0, \frac{\sqrt{5}-1}{2}, \frac{\sqrt{5}-1}{2}, 0\right),$$

obtaining expressions that match the results from the previous subsection. ■

6.6.4 *Geometry of separable states and entanglement witnesses*

This section contains the exact description of the cones $\overrightarrow{\mathsf{CP}}_d$ for $d \leq 5$ and some partial results for $d = 6, 7$. The main result is the complete characterization of the cone $\overrightarrow{\mathsf{CP}}_5$ (and also of its dual), that is not equal to the larger cone $\overrightarrow{\mathsf{DNN}}_5$, see Fig. 14, which allows us to construct examples of PPT entangled states.

Dimensions $d \leq 4$

In this case, the following proposition for the equality of the two sets (separable and PPT) can be shown

Proposition 6.53. For $d \leq 4$, $\overrightarrow{\mathsf{CP}}_d = \overrightarrow{\mathsf{DNN}}_d$: a circulant mixture of Dicke states is separable if and only if it is PPT.

Proof. This follows from the more general statement in [TAQ+18, Yu16] that (general) mixtures of Dicke states in local dimension 4 or less are separable if and only if they are PPT. In turn, this is a consequence of the well-know fact that a matrix of size 4 or less is completely positive if and only if it is positive semidefinite and entrywise positive [SMB21, Theorem 3.35]. ■

We display in Fig. 12 a slice through these cones, showing how randomly generated elements from the $\overrightarrow{\mathsf{CP}}_4$ cone slice fill the polyhedron spanned by the 4 extremal elements of the $\overrightarrow{\mathsf{DNN}}_4$ cone from Section 6.6.3.

Dimension $d = 5$

In this section, we discuss the geometry of the set $\overrightarrow{\mathsf{CP}}_d$ in the simplest non-trivial case $d = 5$. Indeed, for $d \leq 4$, since $\overrightarrow{\mathsf{CP}}_d = \overrightarrow{\mathsf{DNN}}_d$, the $\overrightarrow{\mathsf{CP}}_d$ cone is a polyhedron that was

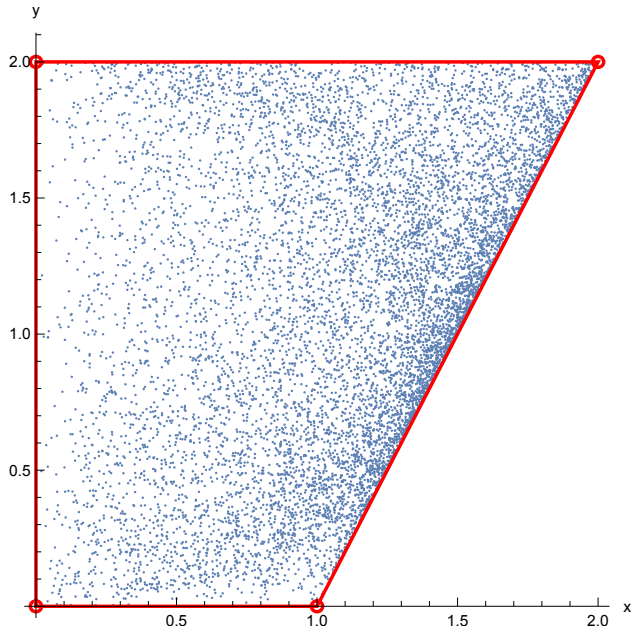


Figure 12: The slice $(2, x, y, x)$ through the cones $\overrightarrow{\mathsf{DNN}}_4 = \overrightarrow{\mathsf{CP}}_4$. In blue, 10^4 randomly generated points inside $\overrightarrow{\mathsf{CP}}_4$; in red, the 4 extreme points of $\overrightarrow{\mathsf{DNN}}_4$ from Section 6.6.3 and the polyhedral slice they generate

completely described via its (finitely many) extremal rays in the previous two sections. For $d \geq 5$, the $\overrightarrow{\mathsf{CP}}_d$ cone has more complex structure inside the $\overrightarrow{\mathsf{DNN}}_d$ which is still a polyhedral cone. We shall completely characterize the geometry of the $\overrightarrow{\mathsf{CP}}_5$ cone and its dual, providing a list of its (infinitely many) extremal rays. The main results of this section are Theorem 6.58 and Theorem 6.60, which are summarized in Fig. 13 and Fig. 14 respectively. To discuss the more interesting cases of $d \geq 5$, let us first introduce in the general case the dual objects needed in our analysis.

Definition 6.54. We can define the dual cone of $\overrightarrow{\mathsf{CP}}_d$ as follows:

$$(\overrightarrow{\mathsf{CP}}_d)^* = \{a \in \mathbb{R}^d \ : \ \langle a, (v * v^{\mathsf{R}})\rangle \geq 0 \quad \forall\, v \in \mathbb{R}^d_+\}.$$

Recall that *copositive matrices* [SMB21] are the dual of completely positive matrices:

$$\mathsf{COP}_d := \{A \in \mathcal{M}_d^{\mathrm{sa}}(\mathbb{R}) \ : \ \langle v, Av\rangle \geq 0 \quad \forall v \in \mathbb{R}^d_+\}.$$

The following proposition simply states that vectors in the dual of $\overrightarrow{\mathsf{CP}}_d$ correspond to circulant copositive matrices; we leave the proof to the reader.

Proposition 6.55. We have

$$(\overrightarrow{\mathsf{CP}}_d)^* = \mathsf{circ}^{-1}(\mathsf{Circ}_d \cap \mathsf{COP}_d) =: \overrightarrow{\mathsf{COP}}_d.$$

Therefore, elements of $\overrightarrow{\mathsf{COP}}_d$ behave like entanglement witnesses for circulant mixtures of Dicke states. An important example of a circulant copositive matrix is the *Horn matrix* [HJN63]:

$$H = \mathsf{circ}(1,-1,1,1,-1) = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix} \in \mathsf{COP}_5. \tag{34}$$

Note that elements in $\overrightarrow{\mathsf{COP}}_d$ can have negative elements; there are however some simple necessary conditions for membership in $\overrightarrow{\mathsf{COP}}_d$ that we gather in the following lemma.

Lemma 6.56. Let $a \in \overrightarrow{\mathsf{COP}}_d$. Then

- $a_0 \geq 0$;
- for all $k \in [d]$, $2a_0 + a_{2k} + a_{-2k} \geq 0$.

Proof. The result follows from the definition of the set $\overrightarrow{\mathsf{COP}}_d$ using vectors v of the respective forms:

- $v = |k\rangle$
- $v = |k\rangle + |-k\rangle$.

■

One can define similarly the dual cone of $\overrightarrow{\mathsf{DNN}}_d$:

$$(\overrightarrow{\mathsf{DNN}}_d)^* = \mathsf{circ}^{-1}(\mathsf{Circ}_d \cap (\mathsf{PSD}_d^{\mathbb{R}} + \mathsf{EWP}_d))) =: \overrightarrow{\mathsf{SPN}}_d.$$

We call such matrices *circulant* SPN matrices, where

$$\mathsf{SPN}_d = \mathsf{PSD}_d^{\mathbb{R}} + \mathsf{EWP}_d$$

is the cone of SPN matrices, see [SMB21, Theorem 1.167].

Proposition 6.57. The cone $\overrightarrow{\mathsf{SPN}}_5$ has 4 extremal rays, generated by the following vectors:

$$(0,1,0,0,1),(0,0,1,1,0),$$
$$(1,-\cos(\pi/5),\cos(2\pi/5),\cos(2\pi/5),-\cos(\pi/5)),$$
$$(1,\cos(2\pi/5),-\cos(\pi/5),-\cos(\pi/5),\cos(2\pi/5)).$$

Proof. Recall from the previous sections that the $\overrightarrow{\mathsf{DNN}}_d$ cone was defined via the conditions $a \in \mathbb{R}^d_+$ and $\mathcal{F}a \in \mathbb{R}^d_+$. Hence, there are at most $2(1+\lfloor d/2 \rfloor) = 6$ extremal rays of $\overrightarrow{\mathsf{SPN}}_5$:

$$(1,0,0,0,0),(0,1,0,0,1),(0,0,1,1,0),(1,1,1,1,1),$$
$$(1,-\cos(\pi/5),\cos(2\pi/5),\cos(2\pi/5),-\cos(\pi/5)),$$
$$(1,\cos(2\pi/5),-\cos(\pi/5),-\cos(\pi/5),\cos(2\pi/5)).$$

One can easily see that the first and the fourth elements in the list above can be obtained by positive linear combinations of the four others and that the remaining four rays are extreme. ■

We characterize *extremal* circulant copositive matrices (or circulant entanglement witnesses) in local dimension $d = 5$ in the result below, see also Fig. 13.

Theorem 6.58. Define, for $\theta \in \mathbb{R}$, the vectors

$$h_\theta := (1,-\cos\theta,\cos(2\theta),\cos(2\theta),-\cos\theta) \tag{35}$$
$$h'_\theta := (1,\cos(2\theta),-\cos\theta,-\cos\theta,\cos(2\theta)). \tag{36}$$

The extremal rays of the $\overrightarrow{\mathsf{COP}}_5$ cone are given by:

$$\operatorname{ext}\overrightarrow{\mathsf{COP}}_5 = \mathbb{R}_+ \cdot \left[\{(0,1,0,0,1),(0,0,1,1,0)\} \sqcup \{h_\theta : \theta \in [0,\pi/5]\} \sqcup \{h'_\theta : \theta \in [0,\pi/5]\}\right].$$

Proof. Let us first show that the proposed rays are extremal. We start with the ray generated by the vector $(0,1,0,0,1)$, leaving the proof for the ray generated by $(0,0,1,1,0)$ to the reader. First, note that $(0,1,0,0,1) \in \overrightarrow{\mathsf{SPN}}_5 \subseteq \overrightarrow{\mathsf{COP}}_5$ since it is entrywise positive. Consider a decomposition

$$(0,1,0,0,1) = a + b, \qquad \text{with } a,b \in \overrightarrow{\mathsf{COP}}_5.$$

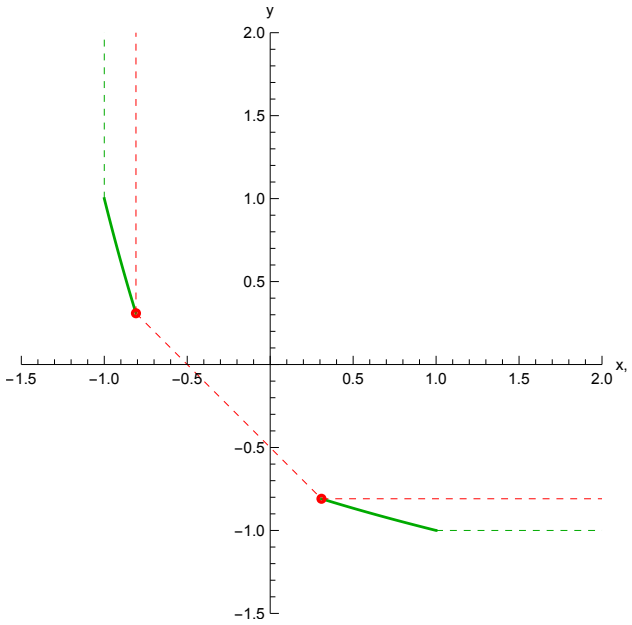


Figure 13: The slice $(1, x, y, y, x)$ through the cones $\overrightarrow{\mathsf{SPN}}_5 \subsetneq \overrightarrow{\mathsf{COP}}_5$. The red dots are the 2 extreme points $(1, -\cos(\pi/5), \cos(2\pi/5), \cos(2\pi/5), -\cos(\pi/5))$, $(1, \cos(2\pi/5), -\cos(\pi/5), -\cos(\pi/5), \cos(2\pi/5))$ of $\overrightarrow{\mathsf{SPN}}_5$ belonging to this slice. The red dashed lines correspond to the boundary of the (unbounded) slice. Solid green curves correspond to the extremal rays of $\overrightarrow{\mathsf{COP}}_5$ belonging to this slice: h_θ and h'_θ for $\theta \in [0, \pi/5]$. Dashed green lines depict the boundary of $\overrightarrow{\mathsf{COP}}_5$.

Using Lemma 6.56, we have $a_0, b_0 \geq 0$ hence $a_0 = b_0 = 0$. Moreover, taking $k = 1$, we obtain $a_2, b_2 \geq 0$ and thus also $a_2 = b_2 = 0$. We conclude that the vectors a is of the form $(0, a_1, 0, 0, a_1)$ and similarly for b, thus they are proportional to $(0, 1, 0, 0, 1)$, proving the extremality of the ray.

Let us now move on to the infinite families generated by the vectors h_θ and h'_θ. Consider the characterization of the extremal rays of the copositive cone from [Hil12, Theorem 3.1]. Note that the first infinite family we propose correspond to the choice $T(\psi)$ from [Hil12] with $\psi_i = \theta \in (0, \pi/5)$ for $i = 1, 2, 3, 4, 5$. The value $\theta = 0$ corresponds to the Horn matrix (which is extremal [HJN63]), while the value $\theta = \pi/5$ will be addressed later in the proof. The second family and the first family are conjugated by the (non-circulant!) permutation matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

hence theses are again extremal rays by [Hil12, Theorem 3.1].

To finish the proof, we need to show that the proposed family are the only extremal rays. First, we claim that the only extremal rays a with $a_0 = 0$ are the ones in the statement. Indeed, we have already shown that the slice $a_0 = 0$ of the $\overrightarrow{\mathsf{COP}}_5$ cone contains the extremal rays $(1,0)$ and $(0,1)$, in the (x,y) parametrization of the $(0,x,y,y,x)$ slice. A cone in $\mathbb{R}^2$ cannot have more than two extremal rays, proving the claim. To discuss extremal rays with $a_0 \neq 0$ (hence $a_0 > 0$ by Lemma 6.56), we can restrict our attention on the slice $a_0 = 1$, see Fig. 13. Using Lemma 6.56, we obtain $x = a_1 = a_4 \geq -1$ and $y = a_2 = a_3 \geq -1$. Hence, there are no elements of $\overrightarrow{\mathsf{COP}}_5$ (and thus no extreme points) below the $y = -1$ and to the left of the $x = -1$ lines in Fig. 13. Let us now show that $(1,-1,1,1,-1)$ (i.e. the Horn point) is the only extremal point on the $x = -1$ line. This follows from the fact that any other point $(1,-1,y,y,-1)$, with $y > 1$ can be decomposed as

$$(1,-1,y,y,-1) = (1,-1,1,1,-1) + (y-1)\cdot \underbrace{(0,0,1,1,0)}_{\in \mathrm{ext}\, \overrightarrow{\mathsf{COP}}_5},$$

hence it cannot be extreme.

Consider now the fact that $(1,1,1,1,1) \in \overrightarrow{\mathsf{CP}}_5$, as it can easily be seen by considering the convolution $e * e^{\mathsf{R}}$. Hence

$$(1,x,y,y,x) \in \overrightarrow{\mathsf{COP}}_5 \implies \langle (1,1,1,1,1), (1,x,y,y,x)\rangle \geq 0 \iff x + y \geq -\frac{1}{2}.$$

Graphically, this means that there are no (extreme) points of $\overrightarrow{\mathsf{COP}}_5$ strictly below the slanted red dashed line $x + y = -1/2$ in Fig. 13. Let us now consider the (extremal) points of $\overrightarrow{\mathsf{COP}}_5$ lying on this line. Clearly the two points

$$h_{\pi/5} = (1, -\cos(\pi/5), \cos(2\pi/5), \cos(2\pi/5), -\cos(\pi/5))$$

and $h'_{\pi/5} = (1, \cos(2\pi/5), -\cos(\pi/5), -\cos(\pi/5), \cos(2\pi/5))$ are elements of $\overrightarrow{\mathsf{COP}}_5$ since they are (extremal) elements of $\overrightarrow{\mathsf{SPN}}_5$. Note that they are the only elements of the families h_θ, h'_θ lying on this line, so they must be extremal (the contrary would contradict the extremality of the other elements in the family); this proves the only remaining case from the beginning of the proof. Since they are extremal, no other points on the line $x + y = -1/2$ can be extremal, finishing the proof. ■

For $d = 5$, as we only need three parameters to describe the cones of $\overrightarrow{\mathsf{CP}}_d$ and $\overrightarrow{\mathsf{DNN}}_d$, it is possible to visualize the complete cone after normalization. This visualization helps us gain more intuition about the set of separable as well as PPT entangled states in $d = 5$.

To do this, we look at the convex set of SEP states as the section obtained by setting $a_0 = 2$ in the $\overrightarrow{\mathsf{CP}}_5$ cone. Essentially, the convex set we obtain provides us all the information as the any ray of the cone is λx where x is the extreme point of this set. From the last

section, we know that the $\overrightarrow{\mathsf{CP}}_5$ cone can be described as the intersection of all the half-planes parametrized by the parameter $\theta \in [0, \pi/5]$. In the next step, we explicitly calculate the extreme rays of the cone generated by these half planes.

We shall need the following basic convexity lemma.

Lemma 6.59. Let $K \subseteq \mathbb{R}^2$ be a convex set. Consider a C^1 family $(h_t)_{t\in(-1,1)}$ of extremal points of the dual, $h_t \in \operatorname{ext} K^\circ$, parametrized in a regular way such that

$$\delta_0 := \lim_{t\to 0} \frac{h_t - h_0}{t} \neq 0.$$

Let $x_0 \in K$ be an element of K lying on the supporting hyperplane defined by h_0: $\langle h_0, x_0\rangle = 1$. Then x_0 is extremal in K: $x_0 \in \operatorname{ext} K$.

Proof. Assume that x_0 is not extremal in K, that is there exists $\Delta \in \mathbb{R}^2$, $\Delta \neq 0$, such that $x_0 \pm \Delta \in K$. First, note that Δ cannot be colinear to x_0:

$$1 \geq \langle h_0, x_0 \pm \Delta\rangle = 1 \pm \langle h_0, \Delta\rangle \implies \langle h_0, \Delta\rangle = 0,$$

while $\langle h_0, x_0\rangle = 1$. Define, for $t \neq 0$, $\delta_t := (h_t - h_0)/t$. We have, for $t \neq 0$:

$$1 \geq \langle h_t, x_0 \pm \Delta\rangle = 1 + t\langle \delta_t, x_0 \pm \Delta\rangle.$$

Hence, we have

$$\begin{aligned} \forall t \in (-1, 0) \qquad & \langle \delta_t, x_0 \pm \Delta\rangle \geq 0 \\ \forall t \in (0, 1) \qquad & \langle \delta_t, x_0 \pm \Delta\rangle \leq 0. \end{aligned}$$

Taking directional limits $t \to 0^+$, respectively $t \to 0^-$, we obtain:

$$\langle \delta_0, x_0 \pm \Delta\rangle = 0 \implies \langle \delta_0, x_0\rangle = 0 \quad \text{and} \quad \langle \delta_0, \Delta\rangle = 0.$$

This, together with the fact that x_0 and Δ span $\mathbb{R}^2$, contradicts the assumption $\delta_0 \neq 0$, finishing the proof. ∎

Theorem 6.60. Define, for $\theta \in \mathbb{R}$, the vectors

$$\begin{aligned} x_\theta &:= (2\cos(2\theta) + 4, 4\cos\theta, 1, 1, 4\cos\theta) \\ x'_\theta &:= (2\cos(2\theta) + 4, 1, 4\cos\theta, 4\cos\theta, 1). \end{aligned}$$

The extreme rays of the $\overrightarrow{\mathsf{CP}}_5$ cone are given by:

$$\operatorname{ext}\overrightarrow{\mathsf{CP}}_5 = \mathbb{R}_+ \cdot \Big[\{(1,0,0,0,0),(1,1,1,1,1),(2,1,0,0,1),(2,0,1,1,0)\} \sqcup \{x_\theta \,:\, \theta \in [0,\pi/5]\} \sqcup \{x'_\theta \,:\, \theta \in [0,\pi/5]\}\Big].$$

Proof. Nonzero elements a of the $\overrightarrow{\mathsf{CP}}_5$ cone must have $a_0 > 0$, so it is enough to study the slice $a_0 = 2$ of this cone, see Fig. 14.

Let us first show that the points in the statement are actually elements of $\overrightarrow{\mathsf{CP}}_5$. We have

$$\begin{aligned}
(1,0,0,0,0) &= (1,0,0,0,0) * (1,0,0,0,0)^{\mathsf{R}} \\
(1,1,1,1,1) &= \frac{1}{5} \cdot (1,1,1,1,1) * (1,1,1,1,1)^{\mathsf{R}} \\
(2,1,0,0,1) &= (0,0,1,1,0) * (0,0,1,1,0)^{\mathsf{R}} \\
(2,0,1,1,0) &= (0,1,0,0,1) * (0,1,0,0,1)^{\mathsf{R}}.
\end{aligned}$$

For the infinite families, write, for all $\theta \in [0,\pi/2]$,

$$x_\theta = v_\theta * v_\theta^{\mathsf{R}}, \qquad \text{with } v_\theta := (2\cos\theta, 1, 0, 0, 1) \in \mathbb{R}^5_+.$$

Hence $x_\theta \in \overrightarrow{\mathsf{CP}}_5$ for all $\theta \in [0,\pi/2] \supset [0,\pi/5]$; a similar result holds for x'_θ. See the solid and dashed green curves in Fig. 14.

Let us now prove that the points in the statement are extremal. Since the coordinates of elements of $\overrightarrow{\mathsf{CP}}_5$ are non-negative, e_0 is clearly extremal. Consider now the face

$$\{a \in \overrightarrow{\mathsf{CP}}_5 \,:\, \langle (0,1,0,0,1), a\rangle = 0\}$$

defined by the extremal point $(0,1,0,0,1)$ of the dual cone $\overrightarrow{\mathsf{COP}}_5$. Extremal points on this face must satisfy

$$v_0v_4 + v_1v_0 + v_2v_1 + v_3v_2 + v_4v_3 = 0, \qquad \text{where } v_i \geq 0.$$

Since we can shift cyclically the entries of the v vector, assume $v_0 \neq 0 \implies v_1 = v_4 = 0$. Moreover, one of $v_{2,3}$ must be zero. Again, by cyclic permutation, we can assume $v_3 = 0$. Hence, this face consists of vectors

$$(v_0,0,v_2,0,0) * (v_0,0,v_2,0,0)^{\mathsf{R}} = (v_0^2 + v_2^2, 0, v_0v_2, v_0v_2, 0)$$

Thus it is equal to the set

$$\{(x,0,y,y,0) \,:\, 0 \leq 2y \leq x\}.$$

The slice $x = 2$ of this face is the segment $y \in [0, 1]$ so it corresponds to the extremal rays e_0 and $(2, 0, 1, 1, 0)$. In a similar manner, considering the extremal hyperplane $(0, 0, 1, 1, 0) \in \operatorname{ext} \overrightarrow{\mathsf{COP}}_5$, one shows that $(2, 1, 0, 0, 1)$ is also an extremal ray of $\overrightarrow{\mathsf{CP}}_5$. The ray supported on $(1, 1, 1, 1, 1)$ is an extremal element of $\overrightarrow{\mathsf{DNN}}_5$ and an element of $\overrightarrow{\mathsf{CP}}_5$ so it must be extremal in $\overrightarrow{\mathsf{CP}}_5$. For the continuous families of points, observe that

$$\langle h_\alpha, x_\beta \rangle = 4(\cos\alpha - \cos\beta)^2.$$

Hence, for all $\theta \in (0, \pi/5)$, we have

$$\forall t \in (0, \pi/5) \quad \langle h_t, x_\theta \rangle \geq 0 \qquad \text{with equality iff} \qquad t = \theta.$$

Note that the slice corresponding to setting the first coordinate of the vector to 1 is a convex set of $\mathbb{R}^2$, see Figs. 13 and 14. Thus, we can apply Lemma 6.59 to conclude that the point x_θ is extremal (in that slice), using the fact that the family of extremal hyperplanes $(h_t)_{t\in(0,\pi/5)}$ is C^1. The non-vanishing gradient condition is satisfied for the chosen parametrization:

$$\nabla_t(-\cos t, \cos(2t)) = (\sin t, -2\sin(2t)) \neq 0 \qquad \forall t \in (0, \pi/5).$$

Finally, let us prove that the points in the statement exhaust the set of extremal points of $\overrightarrow{\mathsf{CP}}_5$. This follows, on the level of the slice $a_0 = 2$, from the analysis of the faces defined by the extremal rays of the dual cone $\overrightarrow{\mathsf{COP}}_5$, studied in Theorem 6.58:

$$\begin{aligned}
(0, 1, 0, 0, 1) &\to \text{1-dim. face } [x_0, (2, 0, 1, 1, 0)] \\
(0, 0, 1, 1, 0) &\to \text{1-dim. face } [x_0, (2, 1, 0, 0, 1)] \\
h_0 &\to \text{1-dim. face } [x_0, (2, 0, 1, 1, 0)] \\
h'_0 &\to \text{1-dim. face } [x'_0, (2, 0, 1, 1, 0)] \\
h_{\pi/5} &\to \text{1-dim. face } [x_{\pi/5}, (2, 2, 2, 2, 2)] \\
h'_{\pi/5} &\to \text{1-dim. face } [x'_{\pi/5}, (2, 2, 2, 2, 2)] \\
h_\theta &\to \text{0-dim. face } \{x_\theta\} \\
h'_\theta &\to \text{0-dim. face } \{x'_\theta\}.
\end{aligned}$$

■

Note that in Fig. 14, the region between the $\overrightarrow{\mathsf{DNN}}_5$ and $\overrightarrow{\mathsf{CP}}_5$ corresponds to quantum states that are PPT entangled. The two extremal $\overrightarrow{\mathsf{DNN}}_5$ rays that are not elements of $\overrightarrow{\mathsf{CP}}_5$ play an important role as *extremal PPT entangled states*.

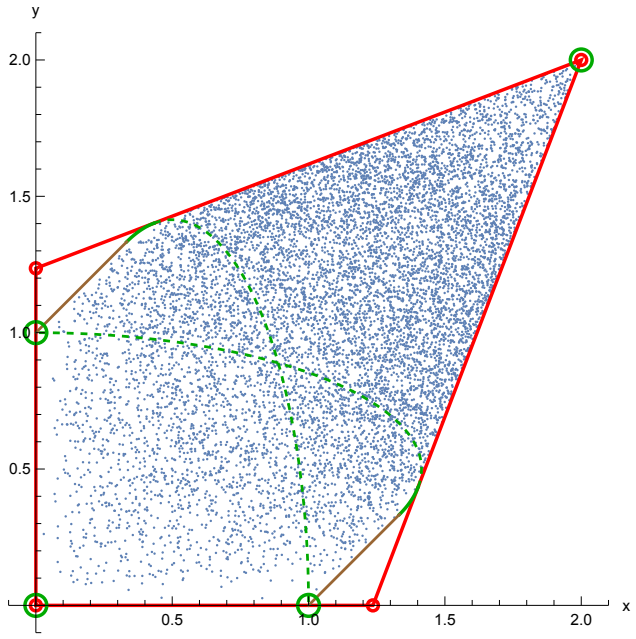


Figure 14: The slice $(2, x, y, y, x)$ through the cones $\overrightarrow{\mathsf{CP}}_5 \subsetneq \overrightarrow{\mathsf{DNN}}_5$. In blue, 10^4 randomly generated points inside $\overrightarrow{\mathsf{CP}}_5$. In red, the 4 extreme points of $\overrightarrow{\mathsf{DNN}}_5$ from Section 6.6.3 and the polyhedral slice they generate. Solid green curves correspond to the extremal rays x_θ and x'_θ for $\theta \in [0, \pi/5]$, while the three green points are the extremal rays in the directions $(1,0,0,0,0)$, $(1,1,1,1,1)$, $(2,1,0,0,1)$, $(2,0,1,1,0)$. Dashed green lines are non-extremal elements of $\overrightarrow{\mathsf{CP}}_5$ corresponding to x_θ and x'_θ in the parameter range $\theta \in (\pi/5, \pi/2]$. The two brown lines fill in the missing (non-extremal) part of the boundary of $\overrightarrow{\mathsf{CP}}_5$.

Dimensions $d = 6$ and $d = 7$

In these cases, the cones (due to symmetry) can be described by 4 independent parameters. When we normalize the first parameter ($a_0 = 1$), we have a convex set to describe in 3 dimensions. Although we do not have the complete geometry of the $\overrightarrow{\mathsf{CP}}_d$ cone, we characterize in this section the geometry on the three faces of this convex set with $a_i = 0$ for $i \in \{0, 1, 2\}$. To do this, let's define the face of the $\overrightarrow{\mathsf{CP}}_d$ cone,

$$\overrightarrow{\mathsf{CP}}_d^I = \{x \in \overrightarrow{\mathsf{CP}}_d \mid \operatorname{supp} x \subseteq I\}$$

Looking at the slice of the $\overrightarrow{\mathsf{CP}}_6$, and $\overrightarrow{\mathsf{CP}}_7$ cones with $a_0 = 1$, there are 3 free parameters that form a convex set. The next theorem completely characterizes these convex sets on each such face. The proofs can be found in Section 6.8; we use that the fact that the 0 in the vector restricts the possible supports of the terms $x * x^{\mathsf{R}}$ in the decomposition, making it possible to characterize the duals completely.

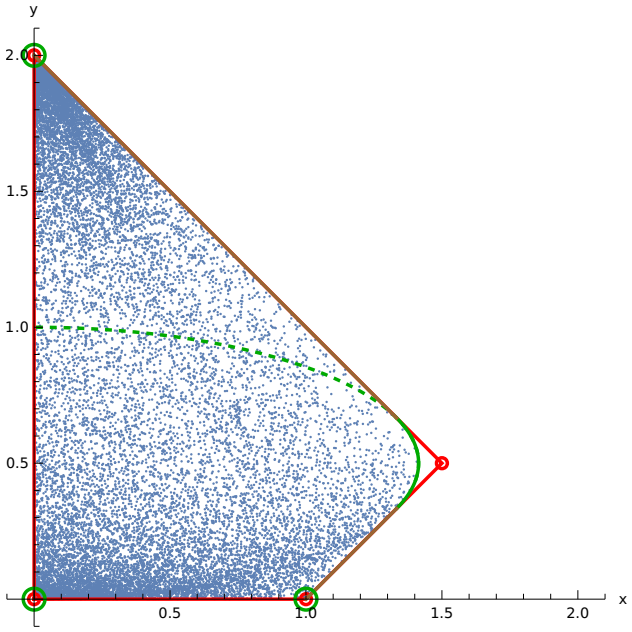


Figure 15: The slice $(2, x, y, 0, y, x)$ through the cones $\overrightarrow{\mathsf{CP}}_6$ and $\overrightarrow{\mathsf{DNN}}_6$. In blue, randomly generated points inside the $\overrightarrow{\mathsf{CP}}_6$ cone. In red, the four extreme points of $\overrightarrow{\mathsf{DNN}}_6$ on this face, and the polytope they generate. The solid green curve is the continuous family of extremal points, while the four other green points are also extremal. The PPT entangled states are present in the small "corner" formed by the continuous family extremal rays of $\overrightarrow{\mathsf{CP}}_6$ and the point $(2, 3/2, 1/2, 0, 1/2, 3/2)$ (which is the only extremal $\overrightarrow{\mathsf{DNN}}_6$ point that is not in $\overrightarrow{\mathsf{CP}}_6$).

Theorem 6.61. Let $x_\theta := (2\cos\theta, 1, 0, 0, 0, 1)$. The extreme rays of the faces corresponding to a zero entry of $\overrightarrow{\mathsf{CP}}_6$ are of the following form:

$$\begin{aligned}
\operatorname{ext} \overrightarrow{\mathsf{CP}}_6^{\{0,1,2,4,5\}} &= \mathbb{R}_+ \cdot \left[\{x_\theta * x_\theta^{\mathsf{R}} : \theta \in [0, \pi/3]\} \sqcup \{(2,1,0,0,0,1), (1,0,1,0,1,0), |0\rangle\}\right] \\
\operatorname{ext} \overrightarrow{\mathsf{CP}}_6^{\{0,1,3,5\}} &= \mathbb{R}_+ \cdot \{(2,1,0,0,0,1), (1,0,0,1,0,0), |0\rangle\} \\
\operatorname{ext} \overrightarrow{\mathsf{CP}}_6^{\{0,2,3,4\}} &= \mathbb{R}_+ \cdot \{(1,0,1,0,1,0), (1,0,0,1,0,0), |0\rangle\}\,.
\end{aligned}$$

From Proposition 6.51, we can conclude that the latter two the faces of the $\overrightarrow{\mathsf{CP}}_6$ are equivalent to the faces of $\overrightarrow{\mathsf{DNN}}_6$ as they have the same extremal rays. Hence, PPT entangled states are present only on the face $\overrightarrow{\mathsf{CP}}_6^{\{0,1,2,4,5\}}$. In particular, $X_{a,a_0|e_0\rangle,a}$ with $a = (4,3,1,0,1,3)$ is PPT entangled (and the only vector in $\operatorname{ext} \overrightarrow{\mathsf{DNN}}_6 \setminus \operatorname{ext} \overrightarrow{\mathsf{CP}}_6$). In Fig. 15, we show this face of the cone with $a_0 = 2$.

We now study the $\overrightarrow{\mathsf{CP}}_7$ cone. We postpone the proof of the following theorem that characterises completely the facets of $\overrightarrow{\mathsf{CP}}_7$ to the Section 6.8.

Theorem 6.62. Consider the following continuous families of vectors parametrized by a real parameter θ:

$$x_\theta^{(3)} := (2\cos(2\theta)+4, 4\cos\theta, 1, 0, 0, 1, 4\cos\theta),$$
$$x_\theta^{(1)} := (2\cos(2\theta)+4, 0, 4\cos\theta, 1, 1, 4\cos\theta, 0),$$
$$x_\theta^{(2)} := (2\cos(2\theta)+4, 1, 0, 4\cos\theta, 4\cos\theta, 0, 1).$$

Then the faces of the $\overrightarrow{\mathsf{CP}}_7$ cone can be completely characterized as:

$$\operatorname{ext}\overrightarrow{\mathsf{CP}}_7^{\{0,1,2,5,6\}} = \mathbb{R}_+ \cdot \left[\left\{x_\theta^{(3)} : \theta \in [0,\pi/2]\right\} \sqcup \{(2,1,0,0,0,0,1), |0\rangle\}\right],$$
$$\operatorname{ext}\overrightarrow{\mathsf{CP}}_7^{\{0,2,3,4,5\}} = \mathbb{R}_+ \cdot \left[\left\{x_\theta^{(1)} : \theta \in [0,\pi/2]\right\} \sqcup \{(2,0,1,0,0,1,0), |0\rangle\}\right],$$
$$\operatorname{ext}\overrightarrow{\mathsf{CP}}_7^{\{0,1,3,4,6\}} = \mathbb{R}_+ \cdot \left[\left\{x_\theta^{(2)} : \theta \in [0,\pi/2]\right\} \sqcup \{(2,0,0,1,1,0,0), |0\rangle\}\right].$$

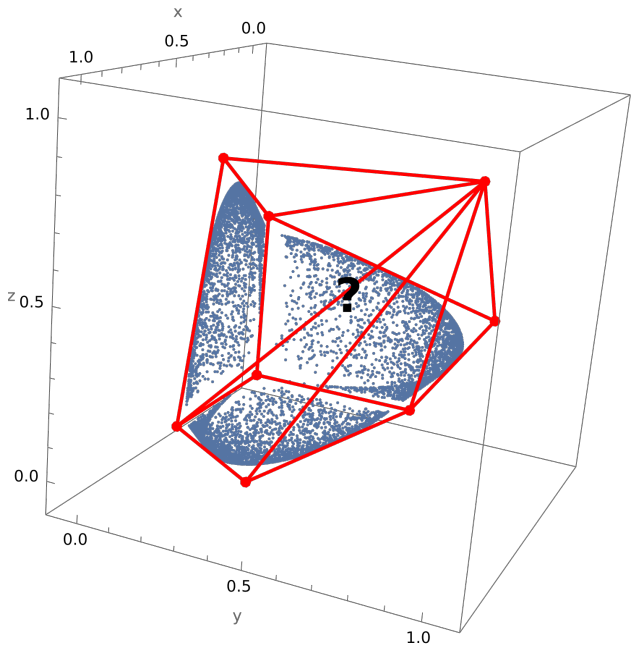


Figure 16: The slice $(2, x, y, 0, 0, y, x)$ through the cones $\overrightarrow{\mathsf{CP}}_7$ (corresponding to separable matrices) and $\overrightarrow{\mathsf{DNN}}_7$ (corresponding to PPT matrices). In blue, randomly generated points inside the face of the $\overrightarrow{\mathsf{CP}}_7$ cone. In red, the four extreme points of $\overrightarrow{\mathsf{DNN}}_7$ on this face, and the polytope they generate. The solid green curve is the continuous family of extremal points $x_\theta^{(3)}, \theta \in [0, \pi/2]$, while the three other green points (big green circles) are also extremal. All the extremal $\overrightarrow{\mathsf{DNN}}_d$ states (red dots) except $|0\rangle$ are not in $\overrightarrow{\mathsf{CP}}_d$. For $\overrightarrow{\mathsf{DNN}}_7$ and $\overrightarrow{\mathsf{CP}}_7$, all the other slices $(2, 0, x, y, y, x, 0)$ and $(2, y, 0, x, x, 0, y)$ are identical to the one above, up to permutation of the coordinates.

We display the slice of $\overrightarrow{\mathsf{CP}}_7$ and $\overrightarrow{\mathsf{DNN}}_7$ by setting $a_0 = 2$ (as $a_0 > 0$ for all non-zero elements of this cone) in Fig. 16. We leave the question of describing completely $\overrightarrow{\mathsf{CP}}_7$ cone for future work. Analyzing the geometry of the $\overrightarrow{\mathsf{CP}}$ cones discussed in this section, we arrive at the following simple result (see also Fig. 17).

Theorem 6.63. For every dimension d, and for the slice $a_0 = 1$ there exists a ball of radius $\varepsilon > 0$ around the point $|e\rangle = (1, 1, \ldots, 1)^\top \in \overrightarrow{\mathsf{CP}}_d$ such that all $\overrightarrow{\mathsf{DNN}}_d$ vectors in this ball are also in $\overrightarrow{\mathsf{CP}}_d$.

Proof. Define the vector $|x\rangle_\varepsilon = |e\rangle + (0, \varepsilon, \varepsilon, \ldots)^\top$. Then, we can do the following computation

$$\begin{aligned} |x\rangle_\varepsilon * |x\rangle_\varepsilon^{\mathsf{R}} &= \Big(|e\rangle + (0, \varepsilon, \varepsilon, \ldots)^\top\Big) * \Big(|e\rangle + (0, \varepsilon, \varepsilon, \ldots)^\top\Big)^{\mathsf{R}} \\ &= |e\rangle + \varepsilon(d-1)\,|e\rangle + \varepsilon^2\Big(d, (d-2), (d-2), \ldots, (d-2)\Big)^\top, \end{aligned}$$

Rewriting this, we have:

$$|x\rangle_\varepsilon * |x\rangle_\varepsilon^{\mathsf{R}} = \Big((d + (d-1)\varepsilon) + d\varepsilon^2\Big)\,|e\rangle - \varepsilon^2\Big(0, 2, 2, \ldots, 2\Big)^\top.$$

By definition, this vector belongs to $\overrightarrow{\mathsf{CP}}_d$ for all $\varepsilon \geq -1$. Let us define:

$$\tilde{\varepsilon} := \frac{2\varepsilon^2}{d + (d-1)\varepsilon + d\varepsilon^2} > 0, \quad \forall \varepsilon > 0.$$

Then, for any $x \in \overrightarrow{\mathsf{DNN}}_d$ such that the Euclidean norm $\|x - |e\rangle\|_2 = \sqrt{\sum_{i=1}^{d-1} |x_i - 1|^2} \leq \tilde{\varepsilon}$, we can ensure that x admits a $\overrightarrow{\mathsf{CP}}_d$ decomposition. ∎

Remark 6.64. This result is analogous to the existence of a ball of separable matrices around the maximally mixed state $\rho = \mathbb{I}/d$ [GB02]. Determining the maximum radius of such a ball for the $\overrightarrow{\mathsf{CP}}_d$, as a function of the local dimension d, remains an open question. Notice that the previous result cannot be obtained from the result in [GB02] because $X_{e/d,e_0,e/d} \neq \mathbb{I}/d$.

We finally present in Fig. 17, a partial geometry of the $\overrightarrow{\mathsf{CP}}_7$ cone using the previous results, leaving the full case to be addressed in future work.

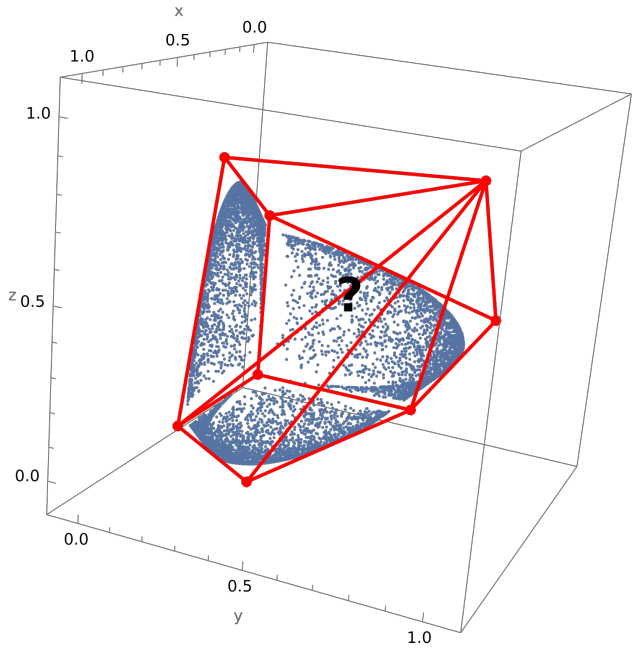


Figure 17: The figure shows the $(2, x, y, z, z, y, x)$ slice of the the $\overrightarrow{\mathsf{CP}}_7$ and $\overrightarrow{\mathsf{DNN}}_7$ cone. The polytope with the red edges/red vertices is the slice of $\overrightarrow{\mathsf{DNN}}_7$. In blue, the faces with zeros of the $\overrightarrow{\mathsf{CP}}_7$ cone and randomly generated points on the faces of $\overrightarrow{\mathsf{CP}}_7$. The geometry of the bulk is an open question.

6.6.5 *Detecting* PPT *entangled mixtures of Dicke states*

In this section, we address the question of detecting PPT entangled mixtures of Dicke states, which is equivalent to detecting if a matrix does not belong to the CP cone. Note that we address here the general (i.e. not circulant) case, using techniques for the circulant case developed in this paper. This question has been addressed in the some of the previous papers relating entanglement and completely positive matrices, see e.g. [TAQ+18]. We propose a new strategy to do this, by first projecting the matrices into the *circulant* subspace, and then testing if they are in not in $\overrightarrow{\mathsf{CP}}_d$.

Definition 6.65. We define the projection to the circulant subspace as $\mathcal{P}_d : \mathcal{M}_d(\mathbb{C}) \to \mathsf{Circ}_d(\mathbb{C})$ as $X \mapsto \sum_k P^{-k} X P^k$.

It is easy to check that this operation preserves all the cones $\mathcal{P}_d(\mathsf{CP}_d) \subseteq \mathsf{CP}_d$, $\mathcal{P}_d(\mathsf{DNN}_d) \subseteq \mathsf{DNN}_d$ and also their duals $\mathcal{P}_d(\mathsf{SPN}_d) \subseteq \mathsf{SPN}_d$ and $\mathcal{P}_d(\mathsf{COP}_d) \subseteq \mathsf{COP}_d$. This allows us to conclude the next proposition,

Proposition 6.66. Let $a \in \overrightarrow{\mathsf{DNN}}_d \backslash \overrightarrow{\mathsf{CP}}_d$. For any matrix $X \in \mathsf{DNN}_d$ such that $\mathrm{circ}^{-1}(\mathcal{P}_d(X)) = a$, we have that $X \notin \mathsf{CP}_d$. Similarly for $a \in \overrightarrow{\mathsf{COP}}_d \backslash \overrightarrow{\mathsf{SPN}}_d$, for any matrix $X \in \mathsf{COP}_d$ such that $\mathrm{circ}^{-1}(\mathcal{P}_d(X)) = a$, we have $X \notin \mathsf{SPN}_d$.

Example 6.67. In [TAQ+18], it is shown that the following 5×5 matrix is not in CP_5:

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 3 \end{bmatrix}.$$

We can recover this result using Proposition 6.66 as follows. First, project the matrix A to the circulant subspace and extract the vector $a = (9, 5, 0, 0, 5)$. We claim that $a \notin \overrightarrow{\mathsf{CP}}_5$. Indeed, since a has a zero coordinate, it lies on the x axis in Fig. 14, with $x = 10/9$. We note that $1 < 10/9 < \sqrt{5} - 1$, proving the claim. Since $a \notin \overrightarrow{\mathsf{CP}}_5$, we conclude by Proposition 6.66 that $A \notin \mathsf{CP}_5$.

6.7 CONCLUSION AND FUTURE DIRECTIONS

We introduce and investigate bipartite mixed quantum states with local cyclic sign invariance. By leveraging the associated symmetry conditions, we show that these matrices can be parametrized in terms of triples of vectors. Exact conditions are derived for these vector triples to ensure that the corresponding matrices lie within the cones of positive semidefinite matrices and the PPT matrices. For vector triples, we define the concept of *Circulant* Triplewise Complete Positivity ($\overrightarrow{\mathsf{TCP}}$), which provides a comprehensive characterization of separability. This framework enables the construction of simple examples of PPT-entangled states in all dimensions $d \geq 3$. In the context of *mixtures of Dicke states*, the PPT is shown to correspond to the semi-positive polyhedral cone of the Fourier matrix. We further establish new results regarding semi-positive cones and their supports, which may have independent significance for developing algorithms to enumerate extreme rays of these cones. One of the principal contributions of our work is the complete analytical characterization of the PPT and the set of separable states for $d \leq 5$ in mixtures of Dicke states with cyclic symmetry. Substantial progress is also achieved for the cases $d = 6$ and

$d = 7$. Several examples of entangled mixtures of Dicke states available in the literature can be detected using the methods outlined in Section 6.6.5.

This work opens numerous avenues for future research. A key open problem is to understand the cone of circulant TCP vectors and to derive some better conditions for membership in this cone. This might be essential to provide new techniques to resolve the PPT^2 conjecture for channels with cyclic sign covariance. The concept of factor width of PCP/TCP cones, introduced in [SN22a], has already been instrumental in proving the conjecture for DUC maps and is likely to play a significant role in addressing this problem.

Since Choi's discovery of the first example of a positive non-decomposable map in the 1970s, there has been sustained interest in understanding its generalizations, particularly in light of their connections to Entanglement Theory. In this work, we observe that all Choi-type maps are special cases of a broader class of maps defined by cyclic sign covariance property. A comprehensive characterization of positive maps within the class of cyclic sign-covariant maps could enable further generalizations of these results.

Furthermore, it would be valuable to explore the entanglement properties of states invariant under other semi-direct product constructions with the diagonal orthogonal group. These additional symmetry constraints impose further structure on the matrix triples (A, B, C) defining the LDOI states [SN21]. A particularly intriguing research avenue is to investigate the relationship between symmetry and PPT entanglement, particularly how much symmetry can be imposed on quantum states while ensuring the presence of PPT entanglement. As far as we are aware, the hyperoctahedral states [PJPY24] are the most general class of invariant states for which the PPT condition implies separability, see Table 13 for reference. Is there even a larger class of states where this is true?

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6.8 GEOMETRY OF SEPARABLE CYCLIC MIXTURES OF DICKE STATES FOR $d = 6, 7$

Recall that a circulant graph is a graph such that its adjacency matrix is circulant. A circulant graph with a connection set $I = -I$ on d vertices has edges $i \leftrightarrow i \oplus s$ where $s \in I$. We denote this graph by C_d^I. We do not consider graphs with loops so $0 \notin I$. We display in Fig. 18 the example of the circulant graph $C_5^{1,4}$.

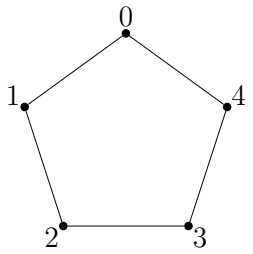


Figure 18: A cycle on 5 vertices is the circulant graph $C_5^{1,4}$. The connection set $I = \{1, 4\}$ signifies that the vertex 0 is connected to vertices 1 and $4 = -1$.

A *vertex cover* of a graph is a subset of vertices such that every edge is incident to at least one vertex of this set. A *clique* of a graph is a subgraph that is complete. A maximal clique is a clique that is not contained in any strictly larger clique. Vertex covers correspond to cliques of the complimentary graph. For more details on graph properties, see [BM08, Die24]. Using this, we prove an important lemma that uses the fact that when the support is not full, any element $x * x^R \in \overrightarrow{\mathsf{CP}}_d$ will have only some allowed possible supports for $\mathrm{supp}(x)$. This approach is inspired by the results in [BSM03] about completely positive matrices, and $\triangle$-free graphs.

Lemma 6.68. For all terms $x * x^R \in \overrightarrow{\mathsf{CP}}_d^I$, the $\mathrm{supp}(x)$ is a *clique* in the circulant graph with the connection set $C_d^{I\setminus\{0\}}$. Therefore,

$$\overrightarrow{\mathsf{CP}}_d^I = \mathrm{cone}\{x * x^R : x \geq 0, \mathrm{supp}\, x \text{ is contained in a maximal clique of } C_d^{I\setminus\{0\}}\}$$

Moreover, $x * x^R = P^l x * (P^l x)^{\mathsf{R}}$ where $P^l = \mathsf{circ}(|l\rangle)$.

Proof. We denote $I^c = [d-1]\setminus I$. Let us denote $a := x * x^{\mathsf{R}} \in \overrightarrow{\mathsf{CP}}_d^I$. Since the support of a is I, this means that means that $a_l = 0$ for all $l \in I^c$. Using the fact that these terms are non-negative, this means that $x_i x_{i+l} = 0$, so either $x_i = 0$ or $x_{i+l} = 0$ for all $l \in I^c$. Consider now $\mathsf{C}_d^{I^c}$, the circulant graph on d vertices labeled as $[d]$ with the connection set I^c. Recall that the edges of this graph connect the points $i \leftrightarrow i + l$. Let there be some assignment of 0 to x_i such that $a_l = 0$ for $l \in I^c$. It will imply that there exists a vertex cover of the circulant graph where $x_i = 0$. Recall that the complement of the vertex cover of graph is clique of the complementary graph. Moreover, we can show that if $\mathrm{supp}(x)$ is a clique of the graph $C_d^{I\setminus\{0\}}$, then $\mathrm{supp}(x * x^{\mathsf{R}}) \in I$. In case of circulant graphs, $(C_d^{I^c})^c = C_d^{I\setminus\{0\}}$. Therefore, the support (non-zero entries) of x is *any clique* of the circulant graph C_d^I. Since all cliques are contained in maximal cliques, we are done.

The second statement follows from the fact that $P^l x * (P^l x)^{\mathsf{R}} = \sum_i x_{i+l} x_{i+l-k} = \sum_i x_i x_{i-k} = x * x^{\mathsf{R}}$ for all x. ■

Notice that since the cone $\overrightarrow{\mathsf{CP}}_d^I$ does not have full support, the relint in the real vector space of symmetric vectors, $Q_d^{\mathsf{sym}} := \{a \in \mathbb{R}^d \ : \ a = a^{\mathsf{R}}\}$ is empty. Since we will be computing the polar dual of this cone, we start by defining the the vector space that accurately captures the dimensions of these faces of the $\overrightarrow{\mathsf{CP}}_d$ cone:

$$Q_I := \{x \in \mathbb{R}^d : x = x^{\mathsf{R}} \text{ such that } \operatorname{supp}(x) = I\}.$$

For any index set I, the dual of the cone $\overrightarrow{\mathsf{CP}}_d^\circ$ will be computed in the space Q_I and *not* with respect to the vector space Q_d^{sym}. We will use the following important result called the *Fejér-Riesz theorem*, with important contributions by Szegő [Fej16, RN12].

Theorem 6.69. Let $a = (a_0, a_1, a_2, \ldots, a_d)$ satisfy the following inequality for all θ:

$$\sum_{k=0}^{d} a_k \cos(k\theta) \geq 0.$$

Then there exist coefficients $c_0, c_1, \ldots, c_d \in \mathbb{R}$ such that

$$a_k = \sum_{j=0}^{d-k} c_j c_{j+k}.$$

Define the following continuous families of vectors:

$$h_\theta^{(3)} := (1, -\cos\theta, \cos(2\theta), 0, \cos(2\theta), -\cos\theta)$$
$$x_\theta := (2\cos\theta, 1, 0, 0, 0, 1).$$

We can state now the main result of this appendix, regarding the dual of the face of the $\overrightarrow{\mathsf{CP}}_6$ cone given by setting to zero the fourth coordinate.

Theorem 6.70. The extremal rays the cone $(\overrightarrow{\mathsf{CP}}_6^I)^\circ$, corresponding to the face given by $I = \{0, 1, 2, 4, 5\}$, are:

- $\{\mathbb{R}_+ h_\theta^{(3)}\}_{\theta \in [0, \pi/3]}$
- $\mathbb{R}_+(0, 0, 1, 0, 1, 0)$
- $\mathbb{R}_+(0, 1, 0, 0, 0, 1)$

Proof. We first begin by analyzing the graph C_6^I for $I = \{1, 2, 4, 5\}$. We observe that all the maximal cliques of this graph are of the form $\{0, 1, 2\} \oplus p_1$ and $\{0, 2, 4\} \oplus p_2$ for $p_1, p_2 \in \{0, 1, \ldots, 5\}$.

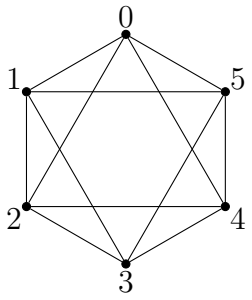


Figure 19: The graph $C_6^{1,2}$

By defining

$$K_1 := \text{cone}\{x * x^{\mathsf{R}} \,:\, x \geq 0,\, \text{supp}(x) \subseteq \{0, 1, 2\}\}$$
$$K_2 := \text{cone}\{x * x^{\mathsf{R}} \,:\, x \geq 0,\, \text{supp}(x) \subseteq \{0, 2, 4\}\}$$

we can use Lemma 6.68 to show that, $\overrightarrow{\mathsf{CP}}_6^I = K_1 + K_2$. Using the results about convex cones in Theorem 6.11, it follows that $(\overrightarrow{\mathsf{CP}}_6^I)^\circ = K_1^\circ \cap K_2^\circ$. We claim that the following is true

$$K_1 = \text{cone}\{a \in Q_I \,:\, a \geq 0,\, \langle h_\theta^{(3)}, a\rangle \geq 0 \quad \forall \theta \in [0, \pi)\}. \tag{37}$$

This is easy to see. The elements of K_1 are of the form $x * x^{\mathsf{R}}$ for $x = (c_0, c_1, c_2, 0, 0, 0)$ (which has the support {0,1,2}) for $c_0, c_1, c_2 \geq 0$.

$$a := x * x^{\mathsf{R}} = (c_0^2 + c_1^2 + c_2^2, c_0c_1 + c_1c_2, c_0c_2, 0, c_0c_2, c_0c_1 + c_1c_2).$$

Each such vector satisfies the inequality,

$$\begin{aligned}\langle h_\theta^{(3)}, a\rangle &= c_0^2 + c_1^2 + c_2^2 - 2(c_0c_1 + c_1c_2)\cos\theta + 2c_0c_2\cos(2\theta) \\ &= \text{Re}\left|c_0 - c_1e^{\mathrm{i}\theta} + c_2e^{\mathrm{i}2\theta}\right|^2 \geq 0\end{aligned}$$

and elements $x * x^{\mathsf{R}}$ are non-negative for $x \geq 0$. This is also true for any element K_1, which is just a sum of elements of this form. Now assume that some vector $a \in Q_I$ that satisfies $a \geq 0$ and also the continuous family of inequalities

$$\forall \theta \in [0, \pi), \qquad \langle (1, -\cos\theta, \cos(2\theta), 0, \cos(2\theta), -\cos\theta), a\rangle \geq 0.$$

By the Fejér-Riesz Theorem 6.69, we can write $a = (c_0, c_1, c_2, 0, 0, 0) * (c_0, c_1, c_2, 0, 0, 0)^{\mathsf{R}}$ for $c_i \in \mathbb{R}$. Since $a \geq 0$, we have that all the parameters $c_i \geq 0$ or $c_i \leq 0$. In the first

case, it shows that $a \in K_1$. In the latter case, we can flip all the signs to show that $a = c * c^{\mathsf{R}} = (-c) * (-c)^{\mathsf{R}} \in K_1$, proving the claim in Eq. (37).

Eq. (37) implies that the dual cone (remember that the duals are taken in Q_I) of K_1 is given by the inequalities defining K_1 itself:

$$K_1^\circ = \operatorname{cone}\left\{\{h_\theta^{(3)}\}_{\theta\in[0,\pi)} \sqcup \{(0,1,0,0,0,1),(0,0,1,0,1,0)\}\right\}.$$

For $\theta \in (0,\pi/2)$, note that

$$h^{(3)}_{\pi-\theta} = h^{(3)}_\theta + 2\cos\theta\cdot(0,1,0,0,0,1).$$

We now claim that (see Fig. 20, left panel, black curve)

$$\operatorname{ext} K_1^\circ = \operatorname{cone}\left\{\{h_\theta^{(3)}\}_{\theta\in[0,\pi/2]} \sqcup \{(0,1,0,0,0,1),(0,0,1,0,1,0)\}\right\}.$$

The "$\subseteq$" inclusion is clear. Fix $\theta \in [0,\pi/2)$. To show that $h_\theta^{(3)}$ is extremal, assume $h_\theta^{(3)} = \sum \lambda_i h^{(3)}_{\theta_i} + \mu_1(0,1,0,0,0,1) + \mu_2(0,0,1,0,1,0)$ with $\lambda_i, \mu_j > 0$ and $\theta_i \in [0,\pi/2]$. Considering the scalar product with

$$x_\theta * x_\theta^{\mathsf{R}} = (2+4\cos^2\theta, 4\cos\theta, 1, 0, 1, 4\cos\theta),$$

we get:

$$\begin{aligned} 0 &= \langle h_\theta^{(3)}, x_\theta * x_\theta^{\mathsf{R}}\rangle \\ &= \sum_i \lambda_i \langle h^{(3)}_{\theta_i}, x_\theta * x_\theta^{\mathsf{R}}\rangle + \mu_1\langle(0,1,0,0,0,1), x_\theta * x_\theta^{\mathsf{R}}\rangle + \mu_2\langle(0,0,1,0,1,0), x_\theta * x_\theta^{\mathsf{R}}\rangle \\ &= \sum_i \lambda_i \cdot 4(\cos\theta_i - \cos\theta)^2 + \mu_1\cdot 8\cos\theta + \mu_2\cdot 2. \end{aligned}$$

This implies $\theta_i = \theta$ for all i and $\mu_2 = 0$; the case $\theta = \pi/2$ can be easily dealt with separately. Thus, $h_\theta^{(3)}$ is extremal. The extremality of the rays generated by the vectors $(0,1,0,0,0,1)$ and $(0,0,1,0,1,0)$ follows easily from their zero-pattern.

Let us analyze now the cone K_2 and its dual. The elements of K_2 are of the form $x * x^{\mathsf{R}}$ for $x = (c_0,0,c_1,0,c_2,0)$ with $c_{0,1,2} \geq 0$. Expanding this, we have

$$a := x * x^{\mathsf{R}} = (c_0^2 + c_1^2 + c_2^2, 0, c_0c_1 + c_1c_2 + c_2c_0, 0, c_0c_1 + c_1c_2 + c_2c_0, 0).$$

Such vectors a are of the form $a = (a_0,0,a_2,0,a_2,0)$ and satisfy $a_{0,2} \geq 0$ and $a_0 \geq a_2$. Conversely, it is easy to see that any such vector a satisfying these inequalities can be factorized as $a := x * x^{\mathsf{R}}$ with $x \in Q_I$, $x \geq 0$. Therefore, $K_2 = \operatorname{cone}\{a \in Q_I \,:\, a \geq$

0 and $a_0 \geq a_2\}$ hence its dual (in Q_I, which is the vector space of $b \in \mathbb{R}^6$ with $b_3 = 0$) is easily computed:

$$K_2^\circ = \operatorname{cone}\{\{(1, x, -1/2, 0, -1/2, x) : x \in \mathbb{R}\} \cup \{(0,1,0,0,0,1), (0,0,1,0,1,0\}\}$$

Note that support of K_2 is a strict subset of the support of K_1, and the dual of K_2 is *not* pointed. Putting everything together, we arrive at the following result,

$$\operatorname{ext}(\overrightarrow{\mathsf{CP}}_6^I)^\circ = \operatorname{ext}(K_1^\circ \cap K_2^\circ) = \left\{\mathbb{R}_+ h_\theta^{(3)}\right\}_{\theta\in[0,\pi/3]} \sqcup \{\mathbb{R}_+(0,1,0,0,0,1), \mathbb{R}_+(0,0,1,0,1,0)\},$$

hence completing the proof. We plot in Fig. 20 the illustration of the geometry of the slice $(1, x, y, 0, y, x)$ of this cone. ■

Theorem 6.71. The extremal rays the cone $\overrightarrow{\mathsf{CP}}_6^I$, corresponding to the face given by $I = \{0, 1, 2, 4, 5\}$, are:

- $(1, 0, 1, 0, 1, 0)$
- $(1, 0, 0, 0, 0, 0)$
- $(2, 1, 0, 0, 0, 1)$.
- $x_\theta * x_\theta^{\mathsf{R}}$ for $\theta \in [0, \pi/3]$

Proof. The first three vectors are extremal as they belong to $\operatorname{ext} \overrightarrow{\mathsf{DNN}}_6$ and have the following $\overrightarrow{\mathsf{CP}}_6$ decompositions

$$(1,0,1,0,1,0) = 1/3 \cdot (1,0,1,0,1,0) * (1,0,1,0,1,0)^{\mathsf{R}}$$

$$(1,0,0,0,0,0) = (1,0,0,0,0,0) * (1,0,0,0,0,0)^{\mathsf{R}}$$

$$(2,1,0,0,0,1) = (1,1,0,0,0,0) * (1,1,0,0,0,0)^{\mathsf{R}}$$

For the continuous families of points, observe that

$$\langle h_\alpha^{(3)}, x_\beta \rangle = 4(\cos\alpha - \cos\beta)^2$$

Hence, for all $\theta \in (0, \pi/3)$, we have

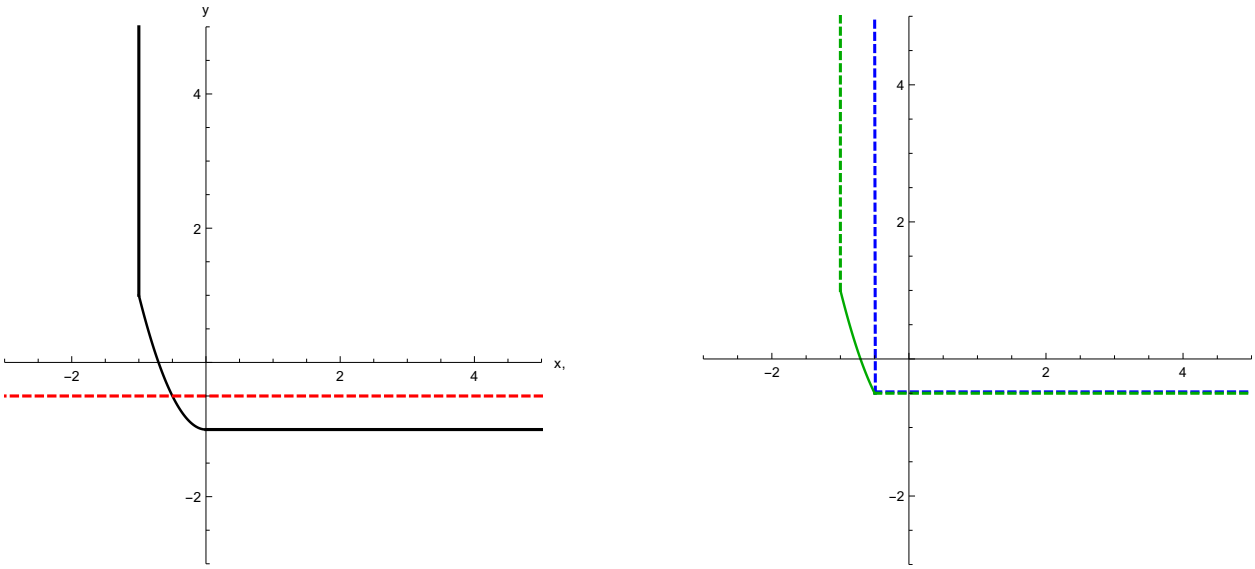
$$\forall t \in (0, \pi/3) \quad \langle h_t^{(3)}, x_\theta \rangle \geq 0 \qquad \text{with equality iff} \qquad t = \theta.$$

Note that the slice corresponding to setting the first coordinate of the vector to 1 is a convex set of $\mathbb{R}^2$, see Fig. 15. Thus, we can apply Lemma 6.59 to conclude that the

point x_θ is extremal (in that slice), using the fact that the family of extremal hyperplanes $(h_t^{(3)})_{t\in(0,\pi/3)}$ is C^1. The non-vanishing gradient condition is satisfied for the chosen parametrization:

$$\nabla_t(-\cos t, \cos(2t)) = (\sin t, -2\sin(2t)) \neq 0 \qquad \forall t \in (0, \pi/3).$$

■



(a) (b)

Figure 20: Visualization of the geometry of the slice $(1, x, y, 0, y, x)$ of $\overrightarrow{\mathsf{CP}}_6^\circ$ cone. The left panel shows the individual boundaries of the slices of K_1° (black) and K_2° (red, dashed), while the right panel highlights their intersection (green boundary) and its relation to $\overrightarrow{\mathsf{SPN}}_6$ (blue boundary)

Similar computations can be done for the faces of the cone $d = 7$. We provide the basic steps needed for characterizing the geometry of the face $\overrightarrow{\mathsf{CP}}_7^I$ for $I = \{0, 1, 2, 5, 6\}$. Again, we proceed by looking at the maximal cliques of the graph $C_7^{\{1,2\}}$ and using Lemma 6.68.

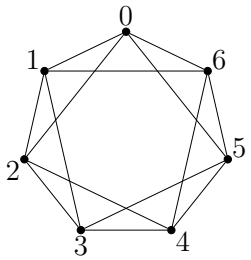


Figure 21: The graph $C_7^{\{1,2\}}$

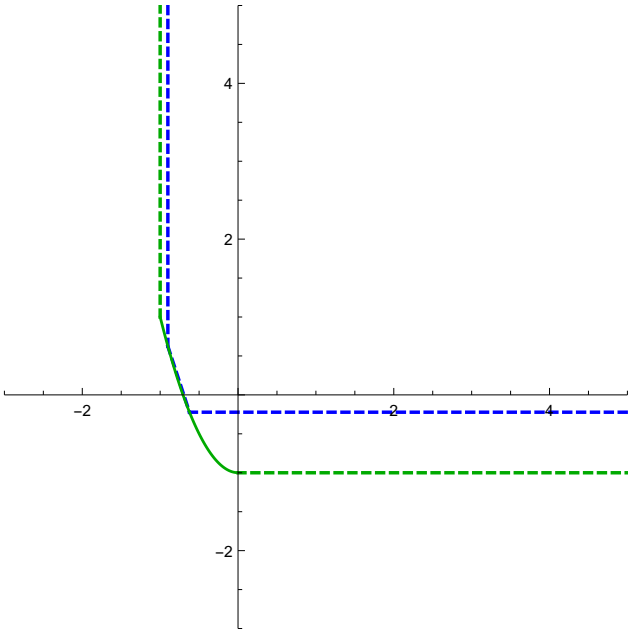


Figure 22: The following figure describes the slice $(1, x, y, 0, 0, y, x)$ of the $\overrightarrow{\mathsf{CP}}_7^{\circ}$ cone. In green, we have the boundary of the cone $\overrightarrow{\mathsf{CP}}_7^{\circ}$. In blue, we have the cone $\overrightarrow{\mathsf{SPN}}_7$ which is the dual of the cone $\overrightarrow{\mathsf{DNN}}_7$.

The maximal cliques of the graph are $\{0, 1, 2\} \oplus p$ for all $p \in \{0, 1, 2, 3, 4, 5\}$. Using the same arguments as for the $\overrightarrow{\mathsf{CP}}_6$ con, one can show that the dual cone (w.r.t. the space Q_I) is completely characterized as

$$\mathrm{ext}(\overrightarrow{\mathsf{CP}}_7^I)^{\circ} = \left\{\mathbb{R}_+ h_\theta^{(3,4)}\right\}_{\theta\in[0,\pi/2]} \sqcup \{\mathbb{R}_+(0,1,0,0,0,0,1), \mathbb{R}_+(0,0,1,0,0,1,0)\}$$

where $h_\theta^{(3,4)} := (1, \cos\theta, \cos(2\theta), 0, 0, \cos(2\theta), \cos\theta)$. This allows to completely determine the face of the cone $\overrightarrow{\mathsf{CP}}_7$. By defining $v_\theta := (2\cos\theta, 1, 0, 0, 0, 0, 1)$ it can be shown that for $I = \{0, 1, 2, 5, 6\}$

$$\mathrm{ext}\,\overrightarrow{\mathsf{CP}}_7^I = \left\{\mathbb{R}_+(v_\theta * v_\theta^{\mathsf{R}})\right\}_{\theta\in[0,\pi/2]} \sqcup \{\mathbb{R}_+ |0\rangle, \mathbb{R}_+(2,1,0,0,0,0,1)\}$$

which is shown in the Fig. 16. Moreover, the following graphs are isomorphic $C_7^{\{1,2\}} \cong C_7^{\{2,3\}} \cong C_7^{\{3,1\}}$, allowing for the same computations to be done for all faces.

7

Rank-based entanglement detection for bound entangled states

This is the reproduction of the article **Rank-based entanglement detection for bound entangled states** by Aabhas Gulati. Phys. Rev. A 113, 022415 (2025). [Gul26]

7.1 INTRODUCTION

With the advent of quantum information, entanglement is now recognized as an essential resource, enabling tasks such as quantum cryptography [Eke91], quantum teleportation [BBC+93], and measurement-based quantum computation [RB01]. Despite significant progress in this field, the theoretical understanding of entanglement in mixed quantum states remains challenging. Even the fundamental question of deciding if any given mixed quantum state is entangled or separable is NP-hard [Gur03, Gha10]. This fact alone points to a fundamental hardness in detecting entanglement in arbitrary states, implying that a complete characterization in terms of necessary and sufficient conditions that can be checked efficiently is unattainable (of course, unless P=NP). Still, several algorithms whose complexities scale quasi-polynomially in the system size have been developed [BCY11]. The complexity of this problem led to the strategy of necessary separability criteria, such that any state that violates any of these criteria is certainly entangled. Many such criteria to detect entanglement in mixed quantum states have been identified; for a comprehensive review, see [GT09].

The PPT (Positive under partial transposition) criterion, [Per96], sometimes also referred to as the Peres-Horodecki criterion, is arguably the most popular criterion to detect entanglement. This test can be applied to quantum states by checking if the matrix obtained by partial transposition on one subsystem is positive semidefinite. If not, the state is entangled. Surprisingly, this test is also sufficient in two-qubit and qutrit-qubit systems [Stø63, HHH96]. In quantum systems of other dimensions, there exist states

that are PPT but are still entangled. The first few examples of two qutrit and a qubit-ququart were constructed in [Hor97]. The PPT criterion is also sufficient for the class of quantum systems with complete unitary symmetries, the Werner states, the isotropic states [VW01], and their generalizations with weaker symmetries [PJPY24]. Although the PPT criterion originally had purely mathematical motivations, the states that are PPT entangled were found to satisfy quite interesting physical properties. Particularly, these states cannot be converted into pure entangled states under LOCC operations [HHH98], a fact that is intimately connected to the fundamental irreversibility of entanglement [VC01]. For this reason, they are sometimes called bound entangled states. Although for high enough dimensions, random-matrix arguments imply that these states have significant volume for some chosen noise thresholds [ASY14, LDB25, NP25], the systemic construction of examples of PPT entangled states remains open, and highly researched [Bre06, SHB$^+$12, PM07, Sin21, GWKB23]. Recently, some bound entangled states with high Schmidt numbers were also constructed in [PV19, HLLMH18, KG24].

In this article, we present a new technique in entanglement detection, which we use to find novel examples of PPT entangled quantum states. We do this by making useful connections between PPT entanglement and the so-called “rank-1 generated property" for conic subsets of positive-semidefinite (PSD) cones. This area of research has been prominent in matrix analysis and optimization theory, see, for example, [AKKW23, Hil16]. It is well-known that the convex cone of PSD matrices has extremal elements of rank-1, and any element in the PSD cone is a finite sum of such rank-1 elements. In general, this is not true for conic subsets of PSD, i.e, by imposing appropriate constraints on the matrices, the ranks of some of the extremal elements of the corresponding conic subset can be strictly greater than 1. Many examples of such conic subsets can be found in [AKKW23, Hil16]. In general, this problem is usually understood on a case-by-case basis [AKKW23], and only a few general conditions for a cone to satisfy this property are known, only when the number of constraints is small.

Let us briefly summarise our approach here: We map the bipartite PPT states to a constrained PSD convex cone that is not rank-1 generated. The main observation is that whenever a state is separable, this mapping results in a rank-1 generated matrix, i.e, a sum of *only* rank-1 elements of a constrained PSD cone. As we show, this provides a non-trivial necessary condition for separability, since any matrix that is mapped to any element that is not rank-1 generated can only arise from a PPT entangled state. To test the validity of the considered approach, we provide constructions of such a mapping to convex cones where the rank-1 generated property has already been studied in the literature, and for different faces of the PSD cone, we can detect PPT entangled states. Although the core idea of the method is quite simple to state, we achieve a wide variety of constructions

within this approach, with a high number of free parameters. In effect, this approach is analogous to the range criterion for entanglement, which detects PPT entangled states in various cases, but is not as easy to compute for arbitrary states.

We now provide the outline of this article. In Section 7.2, we discuss the preliminary topics to understand this article. In particular, we focus on separability of quantum states, local diagonal orthogonally invariant (LDOI) states, the rank-1-generated property of convex cones, and some graph-theoretic notions. In Section 7.3, we discuss the core ideas, along with the main result in Theorem 7.15, that provides a method to detect entanglement by checking whether an element in a convex conic subset of PSD is rank-1 generated. In Section 7.3.1, we show that the method can be applied to successfully detect entanglement in various families of states, and construct PPT entangled states in high dimensions and with a large number of parameters. These families of states we construct are connected to conic subsets of PSD for which the rank-1-generated property is well-studied.

7.2 PRELIMINARIES

7.2.1 *Notation*

The sets of complex, real, and non-negative real numbers will be denoted as $\mathbb{C}, \mathbb{R}$ and $\mathbb{R}_+$ respectively. Let $[d]$ denote the finite set $\{1, 2 \dots d\}$. We adopt Dirac's *bra-ket* notation to denote vectors, elements of $\mathbb{F}^d$ where $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and, the notation $\mathbb{R}^d_+$ will denote the set of d dimesional non-negative vectors. We denote the standard basis vector $e_i \in \mathbb{C}^d$ with the ket $|i\rangle$, and its dual vector, e_i^* as $\langle i|$. For vectors $v, w \in \mathbb{C}^d$, the linear map $vw^* : \mathbb{C}^d \to \mathbb{C}^d$ is written as $|v\rangle\langle w|$, and it represents a rank-1 matrix. To denote complex, and real matrices of size $d \times d'$, we use the notation $\mathcal{M}_{d,d'}$ and, $\mathcal{M}_{d,d'}(\mathbb{R})$, respectively. If the dimensions $d = d'$, we shorten it to $\mathcal{M}_d := \mathcal{M}_{d,d}$ and to $\mathcal{M}_d(\mathbb{R}) := \mathcal{M}_{d,d}(\mathbb{R})$. The rank and range of a matrix will be denoted by $\mathrm{rk}(A)$ and $\mathrm{ran}(A)$, respectively. The set of self-adjoint matrices is denoted by $\mathcal{M}_d^{\mathrm{sa}}$. The set of complex (resp. real) positive semidefinite matrices is denoted as $\mathcal{M}_d^+$ (resp. $\mathcal{M}_d^+(\mathbb{R})$) and the set of matrices with non-negative entries as $\mathcal{M}_d(\mathbb{R}_+)$. For bipartite positive semidefinite matrices, we use the notation, $(\mathcal{M}_d \otimes \mathcal{M}_d)^+$. We use $\mathrm{supp}(v)$ to denote the support of the vector $v \in \mathbb{C}^d$, i.e, $\mathrm{supp}(v) := \{i \in [d] \mid v_i \neq 0\}$. We use $\odot$ to denote the entrywise product of vectors $(v \odot w)_i := v_i \cdot w_i$ and matrices $(A \odot B)_{ij} := A_{ij} \cdot B_{ij}$. We use $\mathbb{I}_n$, and $\mathbb{J}_n$ to denote $n \times n$ identity matrix, and all ones matrix, respectively.

7.2.2 *Convex analysis*

In this section, we provide a brief introduction to convex analysis. As is usual in mathematical literature on entanglement theory, we work with convex cones rather than convex sets. Consider the following definition.

Definition 7.1 (Convex cones)**.** Let V be a real vector space. A *convex cone* $\mathcal{C}$ is a non-empty subset of V having the following two properties:

- If $x \in \mathcal{C}$ and $\lambda \in \mathbb{R}_+ = [0, \infty)$, then $\lambda x \in \mathcal{C}$.
- If $x, y \in \mathcal{C}$, then $x + y \in \mathcal{C}$.

In particular, $0 \in \mathcal{C}$.

The cone $\mathcal{C}$ is said to be *pointed* if $\mathcal{C} \cap (-\mathcal{C}) = \{0\}$; in other words, $\mathcal{C}$ is pointed if it does not contain any line. The important elements of a convex cone are those that cannot be decomposed into other ones, called *extremal* rays. For a vector $v \neq 0$, the half-line $\mathbb{R}_+ v := \{\lambda v : \lambda \in \mathbb{R}_+\} \subseteq \mathcal{C}$ is called an *extremal ray* of $\mathcal{C}$ (we write $\mathbb{R}_+ v \in \operatorname{ext} \mathcal{C}$) if

$$v = x + y \quad \text{with } x, y \in \mathcal{C} \implies x, y \in \mathbb{R}_+ v.$$

The set of non-negative matrices, $\mathcal{M}_d(\mathbb{R}_+)$, and the set of positive semidefinite matrices, $\mathcal{M}_d^+$, are two well-studied convex cones in the literature. The extreme rays of both these cones can be completely characterized, as $\operatorname{ext} \mathcal{M}_d^+ = \{\mathbb{R}_+ |v\rangle\langle v| \,|\, v \in \mathbb{C}^d\}$ and $\operatorname{ext} \mathcal{M}_d(\mathbb{R}_+) = \{\mathbb{R}_+ |i\rangle\langle j|\}_{i,j}$ respectively. Moreover, the extremal rays of both these cones consist only of matrices that are rank-1.

In this article, $\operatorname{cone}(X)$ denotes the *smallest* convex cone containing X. We call this the cone generated by the set X. In finite-dimensional vector spaces, a closed convex and pointed cone is generated by its extremal rays [Roc70], but the same result is not necessarily true for infinite dimensions.

Definition 7.2. Let $\mathcal{C}$ be a convex cone. Then, the convex sub-cone $\mathcal{F} \subseteq \mathcal{C}$ is called a *face* of $\mathcal{C}$, if for any element $\alpha \in \mathcal{C}$, and for all decompositions, $\alpha = \alpha_1 + \alpha_2$ such that both $\alpha_1, \alpha_2 \in \mathcal{C}$, it implies that $\alpha_1, \alpha_2 \in \mathcal{F}$.

This means that any element in the face of a convex cone has a possible conic decomposition only into the elements of the face itself. An extremal ray of the cone is a face of dimension 1.

For the PSD cone, it is well-known that the faces have a one-to-one correspondence with the subspaces of $\mathbb{C}^d$. This result can be found in [Bar25, Corollary 12.4].

Theorem 7.3. The following statements are true :

1. Let L be a linear subspace of $\mathbb{C}^d$, then,

$$\mathcal{F}_L := \{A \in \mathcal{M}_d^+ \mid \mathrm{ran}(A) \subseteq L\} \tag{38}$$

   is a face of the PSD cone.

2. Any face of the PSD cone is of the form $\mathcal{F}_L$ for some linear space L.

3. Let $X \in \mathcal{M}_d^+$. Then, $F_{\mathrm{ran}(X)}$ is the smallest face containing X.

Rank-1 generated cones: Let $\mathcal{L} := \{M_i \in \mathcal{M}_d^{\mathrm{sa}}\}_{i=1}^N$ be a finite set of complex self-adjoint matrices of size $d \times d$. Let us define the convex cone of PSD matrices with linear *half-space* constraints,

$$\mathcal{M}_d^+(\mathcal{L}) := \{X \in \mathcal{M}_d^+ \mid \forall\, M_i \in \mathcal{L},\, \langle M_i, X\rangle \geq 0\}.$$

To deal with the case of $\langle M, X\rangle = 0$, we can also impose the constraint $-M$ along with M, since,

$$\langle M, X\rangle \geq 0 \text{ and } \langle M, X\rangle \leq 0 \iff \langle M, X\rangle = 0.$$

If $\mathcal{L}$ is the empty set, $\mathcal{M}_d^+(\mathcal{L})$ corresponds to the full set of PSD matrices $\mathcal{M}_d^+$. Since $\mathcal{M}_d^+(\mathcal{L}) \subseteq \mathcal{M}_d^+$, any rank-1 element of the the $\mathcal{M}_d^+(\mathcal{L})$ is an extreme ray of $\mathcal{M}_d^+(\mathcal{L})$, as it is extremal in the larger cone $\mathcal{M}_d^+$. For $\mathcal{M}_d^+$ matrices, we know that *all* the extremal rays are only rank-1 elements. This result is not true generally for the cones $\mathcal{M}_d^+(\mathcal{L})$, which may have extremal rays of higher rank.

We now focus on the rank-1 generation property of convex conical subsets in PSD. Any such cone is said to satisfy the *rank-1 generated property* if all the elements in the cone have a conic decomposition into rank-1 elements. Formally, for every convex matrix cone $\mathcal{C} \subseteq \mathcal{M}_d^+$, let $\mathrm{R}_1[\mathcal{C}]$ denote the cone generated by its rank-1 elements.

$$\mathrm{R}_1[\mathcal{C}] := \mathrm{cone}\{|v\rangle\langle v| \in \mathcal{C}\}. \tag{39}$$

Definition 7.4 (Rank-1 generated cones)**.** A matrix cone $\mathcal{C}$ is said to be rank 1 generated if

$$\mathrm{R}_1[\mathcal{C}] = \mathcal{C}. \tag{40}$$

Clearly, the PSD cone satisfies Eq. (40), and is rank-1 generated.

We consider an example of a conic subset of 2×2 PSD matrices in which the rank-1 generated property does not hold. Recall that 2×2 PSD matrices with trace 1 can be mapped to the bloch sphere in $\mathbb{R}^3$ with the coordinates,

$$\begin{aligned} r_x &:= \langle X, \sigma_x \rangle , \\ r_y &:= \langle X, \sigma_y \rangle , \\ r_z &:= \langle X, \sigma_z \rangle . \end{aligned}$$

Let us consider the following set of self-adjoint matrices,

$$\mathcal{L} := \{\sigma_z, -\sigma_z, \sigma_x, \sigma_y\}.$$

For the set $\mathcal{M}_d^+(\mathcal{L})$, this corresponds to the half-space constraints,

$$\begin{aligned} r_x &\geq 0, \\ r_y &\geq 0, \\ r_z &= 0. \end{aligned}$$

In Section 7.2.2, we represent the set of matrices satisfying these constraints, $\mathcal{M}_d^+(\mathcal{L})$. Note that the rank-1 elements lie on the boundary of the sphere, and hence, $\mathrm{R}_1[\mathcal{M}_d^+(\mathcal{L})] \subsetneq \mathcal{M}_d^+(\mathcal{L})$.

Any closed, convex, and pointed matrix cone is rank-1 generated if and only if all the extremal rays of the cone are rank-1. We phrase it as the next lemma.

Lemma 7.5. A closed convex cone $\mathcal{C} \subseteq \mathcal{M}_d^+$ is rank-1 generated if and only if $\operatorname{ext}\mathcal{C}$ consists of only rank-1 elements.

Proof. ($\implies$) To prove the implication, we assume that $\mathrm{R}_1[\mathcal{C}] = \mathcal{C}$, i.e $\mathcal{C}$ is rank-1 generated. Let there be any element X in $\operatorname{ext}\mathcal{C}$. Since the cone is rank-1 generated, by

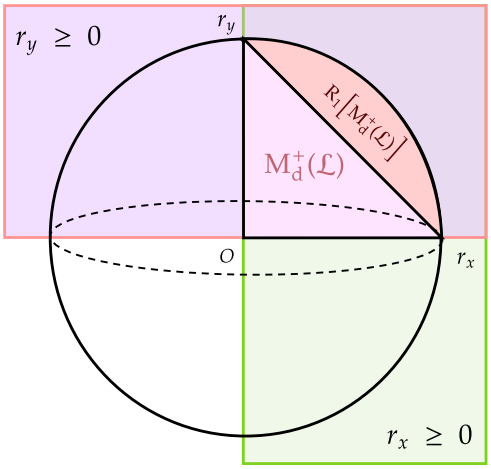


Figure 23: We plot the slice of the (normalised) Bloch sphere with $r_z = 0$ and represent the constraints $r_x \geq 0$ and $r_y \geq 0$ in (light purple and light green, respectively). The extremal points (points on the boundary of the sphere) are the rank-1 extremal elements. The region in pink is the set $\mathcal{M}_d^+(\mathcal{L})$ and in orange is the $\mathrm{R}_1[\mathcal{M}_d^+(\mathcal{L})]$.

definition, there exists a decomposition of $X = \sum_k X_k$ such that each X_k is rank 1. Also, since X is extremal, we have $X_k \propto X$ for all k which implies X is rank-1.

($\Longleftarrow$) We assume that the extremal rays of $\mathcal{C}$ are rank-1. Then the proof follows from the fact that a closed convex pointed cone is the convex hull of its extreme rays [Roc70]. ■

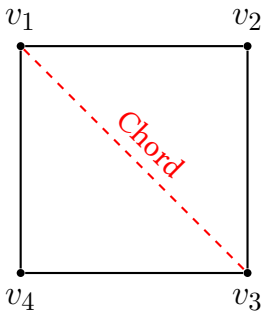
The rank-1 generated property of matrices is related to problems in optimisation theory, see [AKKW23] for more details.

7.2.3 *Graph theory*

A (simple and undirected) *graph* G consists of a finite vertex set V, and a finite set E of two-element (unordered) subsets of V, which is called the edge-set. For $k \geq 3$, a k*-cycle* in a graph is a sequence of edges $\{v_0, v_1\}, \{v_1, v_2\}, \ldots, \{v_{k-1}, v_k\}$ such that $v_1 \neq v_2 \neq \ldots \neq v_k$, and $v_0 = v_k$. 3-cycles in a graph are called *triangles*. A graph which does not contain any triangles is called triangle-free (or triangle-free). A graph is termed *cyclic* if it contains a cycle and *acyclic* otherwise. A graph is called *chordal* if all cycles of size ≥ 4 have a chord, i.e, an edge connecting two vertices not in the cycle. The *adjacency matrix* $A_G \in \mathcal{M}_d(\{0,1\})$ of a graph G on d vertices is defined as follows: $\operatorname{diag} A_G = 0$ and $(A_G)_{ij} = (A_G)_{ji} = 1$ if $\{i, j\}$ is an edge for $i \neq j$. (Implicitly, $(A_G)_{ij} = (A_G)_{ji} = 0$ otherwise for $i \neq j$). The adjacency matrix is hermitian, and for isomorphic graphs G

and H, the adjacency matrices are related as $P\left(A_G\right)P^* = A_H$. where P is a permutation matrix.

Figure 24: The figure represents a cycle of the graph $v_1 \to v_2 \to v_3 \to v_4 \to v_1$ and $v_1 \to v_3$ is the called the chord of the graph.



7.2.4 *Separability, PPT and PPT-edge states*

Definition 7.6 (Separability and Entanglement)**.** A bipartite positive matrix $\rho \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ is said to be separable if

$$\rho = \sum_{i=1}^{N} |v_i\rangle\langle v_i| \otimes |w_i\rangle\langle w_i|$$

for some finite set of vectors $|v_i\rangle, |w_i\rangle \in \mathbb{C}^d$, and it is said to be entangled otherwise.

We denote the convex cone of all separable matrices in $\mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ by SEP_d. By the Hahn-Banach hyperplane theorem, it is possible to separate this set from every entangled state using a hyperplane. For any *entangled state* ρ we can find a Hermitian operator W such that

- $\mathrm{Tr}(\sigma W) \geq 0$ for all σ in SEP_d,
- $\mathrm{Tr}(\rho W) < 0$.

This Hermitian operator is called an entanglement witness. Horodecki's criterion [HHH96] gives us an operational way to detect entanglement, by finding a positive map Φ such that $(\mathrm{id}_d \otimes \Phi)(\rho)$ is not positive semi-definite. One important positive map in this regard is the transposition map T. The quantum states that are not positive under

transposition are entangled, and are called NPT (Non-Positive-Transpose) states. The states satisfying the PPT condition are called PPT states, which also include the set of separable states. This criterion to verify entanglement is called the PPT (Positivity under Partial Transpose) criterion. In the case of $d = 2$, the reverse implication is also true, i.e., any state that is PPT is also separable [Stø63, HHH96]. This is not true for $d \geq 3$. The states that satisfy the PPT condition but are still entangled (for $d \geq 3$) are called PPT entangled states [Hor97].

Definition 7.7 (Separability Problem (Informal))**.** Given a bipartite density matrix $\rho \in \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$, decide whether $\rho \in \mathsf{SEP}_d$ or not.

It is well known that the membership problem (and the weak membership problem) for SEP is NP-hard [Gur03, Gha10]. Unless P = NP, there is no computationally efficient criterion to decide if a state is separable or entangled. We mention here one such important approach for detecting PPT entangled states using the range of the density matrix.

Definition 7.8 (Range criterion [Hor97])**.** A bipartite mixed state is said to satisfy the range criterion if there exist vectors $|a_i\rangle, |b_i\rangle \in \mathbb{C}^d$ such that $\mathrm{ran}(\rho) = \mathrm{span}(|a_i\rangle \otimes |b_i\rangle)$ and $\mathrm{ran}(\rho^\Gamma) = \mathrm{span}(|a_i\rangle \otimes |\bar{b_i}\rangle)$.

Let ρ be a separable state. Then,

$$\rho = \sum_k |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k| ,$$

and its partial transpose,

$$\rho^\Gamma = \sum_k |v_k\rangle\langle v_k| \otimes |\overline{w_k}\rangle\langle \overline{w_k}| .$$

Clearly $|v_k\rangle \otimes |w_k\rangle$ span the range of ρ and $|v_k\rangle \otimes |\overline{w_k}\rangle$ span the range of ρ^Γ, hence all separable states trivially satisfy this criterion. There has been considerable interest in studying the states that maximally violate this criterion.

Definition 7.9 ([LKCH00])**.** A PPT entangled state is called an edge-state if there is no product vector $|a\rangle \otimes |b\rangle \in \mathrm{ran}(\rho)$ such that $|a\rangle \otimes |\bar{b}\rangle \in \mathrm{ran}(\rho^\Gamma)$.

These edge states lie on the boundary of the PPT cone. There is another equivalent characterization of edge states that will be useful for constructing new examples of such states.

Proposition 7.10 ([LKCH00]). A PPT entangled state ρ is an edge-state if for all (un-normalized) $|ab\rangle := |a\rangle \otimes |b\rangle$, $|ab\rangle \neq 0$ that

$$\rho - |ab\rangle\langle ab| \notin \mathrm{PPT}\,.$$

Remark 7.11. There exist particular faces of quantum states well-suited to the application of the range-criterion, i.e, the set of states that have the range only in *entangled* subspaces. This face can be constructed using "Unextendible Product Basis", or UPBs. Any PPT state that is orthogonal to the UPBs is automatically PPT entangled as it violates the range criterion [DMS+03, Ter01, Bra04].

It is clear from the definition that all extremal PPT states are edge-states. But it is known that not all edge states are extremal [LKCH00]. There are only a few systematic constructions of PPT entangled edge states [CKK20] known in the literature. The ranks of PPT entangled edge states have been amply scrutinized, and a complete classification obtained in $3 \otimes 3$ [KO12]. Such states are also useful to construct entanglement witnesses [LKCH00], and any PPT state can be decomposed into a PPT edge state and a separable state [LKCH00], making them useful to analyse from the perspective of entanglement theory.

7.2.5 *Local Diagonal Orthogonal Invariant States*

In this section, we provide a small introduction to local diagonal orthogonal invariant states, or in short, LDOI states. These states are characterized by their local invariance,

$$(O \otimes O)X(O \otimes O) = X$$

for all O in the diagonal orthogonal matrices. This is the group of matrices,

$$\mathcal{DO}_d := \{\mathrm{diag}(x_1, x_2 \ldots x_n) \mid x_i \in \{-1, 1\}\}.$$

These are exactly the states parametrized by a matrix triple (X, Y, Z) with equal diagonals.

$$\rho_{X,Y,Z} := \sum_{i,j} X_{ij} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{i \neq j} Y_{ij} \left|ii\right\rangle\!\left\langle jj\right| + \sum_{i \neq j} Z_{ij} \left|ij\right\rangle\!\left\langle ji\right| .$$

In particular, their PSD and PPT properties can be readily inferred from the matrices (X, Y, Z). The matrix is PSD if and only if Y is self-adjoint, $\forall i, j \in [d],\ X_{ij}X_{ji} \geq |Z_{ij}|^2$ and $Y \in \mathsf{PSD}_d$. For the PPT property, we have the following result,

Theorem 7.12 ([SN21]). The family of quantum states $\rho_{X,Y,Z}$ is PPT if and only if,

- $\forall i, j \in [d] \quad X_{ij}X_{ji} \geq |Y_{ij}|^2, |Z_{ij}|^2$,
- $Y, Z \in \mathsf{PSD}_d$.

Theorem 7.13 ([SN21]). The family of quantum states $\rho_{X,Y,Z}$ is separable if and only if there exists a finite set of vectors $\{|v_k\rangle, |w_k\rangle\}_{k \in I} \subset \mathbb{C}^d$ such that

$$\begin{aligned} X &= \sum_{k \in I} \left|v_k \odot \overline{v_k}\right\rangle\!\left\langle w_k \odot \overline{w_k}\right| \\ Y &= \sum_{k \in I} \left|v_k \odot w_k\right\rangle\!\left\langle v_k \odot w_k\right| , \\ Z &= \sum_{k \in I} \left|v_k \odot \overline{w_k}\right\rangle\!\left\langle v_k \odot \overline{w_k}\right| . \end{aligned}$$

In particular, deciding if a LDOI state is separable or entangled is still NP-hard [SN21], and there exist PPT entangled states. For properties of LDOI states and the separability problem, we recommend [SN21, Sin21, GNS25]. Even in the smallest non-trivial $3 \otimes 3$ system, there is still no complete characterization of entanglement available for these states. Finally, we show that the popular CCNR (computable cross norm or realignment) criterion for LDOI states can be understood as a positivity condition on the triple of matrices.

Theorem 7.14 ([SN21]). Let $||X||_1 = \sum_{i,j=1}^{d} |X_{ij}|$ and $||X||_{\mathrm{tr}} = \mathrm{tr}(\sqrt{X^* X})$. Then the LDOI state $\rho_{X,Y,Z}$ satisfies the CCNR criterion if and only if

$$||X||_1 - ||X||_{\mathrm{tr}} \geq 2 \sum_{1 \leq i < j \leq d} \max |B_{ij}|, |C_{ij}|.$$

7.3 MAIN RESULTS

Let ρ be a mixed (but un-normalised) bipartite quantum state in $\mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$. Our goal is to provide the necessary conditions for separability using the rank-1 generated property. Note that a rank-1 PSD matrix $|v\rangle\langle v|$ is PPT if and only if $|v\rangle = |v_1\rangle \otimes |v_2\rangle$. Hence, the cone of separable states, or SEP, is exactly equal to $\mathrm{R}_1[\mathrm{PPT}]$, that is, the rank-1 generated matrices in PPT states.

The constraint of PPT is *not* a linear matrix constraint. We want to look at mappings of these cones to $n \times n$ matrices that allow us to reduce the PPT condition to *linear* constraints. Let us state our main idea as the next theorem.

Theorem 7.15. For all $K \in \mathcal{M}_{n,d^2}$, we define the following positive map $Z_K : \mathcal{M}_d \otimes \mathcal{M}_d \cong \mathcal{M}_{d^2} \to \mathcal{M}_n$

$$Z_K(\rho) := K\rho K^*.$$

Let $\mathcal{F}$ be a face of the bipartite psd matrices $(\mathcal{M}_d \otimes \mathcal{M}_d)^+$ and $\mathcal{F}_{PPT} := \mathcal{F} \cap \mathsf{PPT}$. Furthermore, assume that $Z_K(\mathcal{F}_{PPT}) \in \mathcal{M}_n^+(\mathcal{L})$. Then the following statements are true.

1. We have for all separable states on $\mathcal{F}$, the matrix $Z_K(\rho) \in \mathrm{R}_1[\mathcal{M}_n^+(\mathcal{L})]$. This is a *necessary criterion* for separability for states in $\mathcal{F}$.
2. If for a PPT state on $\mathcal{F}$ such that, $Z_K(\rho) \in \operatorname{ext} \mathcal{M}_n^+(\mathcal{L})$ and has rank ≥ 2, the state ρ is a PPT entangled edge state.

Proof. Firstly, note that Z_K maps positive matrices into positive matrices, and rank-1 matrices to rank-1 matrices as $Z_K(|v\rangle\langle v|) = (K|v\rangle)(K|v\rangle)^*$. If ρ is a separable state, it has a decomposition into rank-1 states that are PPT.

$$\rho = \sum_{k=1}^{N} |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k| . \tag{41}$$

Define $\rho_k := |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k|$, that is a rank-1 PPT state. Moreover, if we assume that ρ is separable and lies on the face $\mathcal{F}$, it implies that each $\rho_k \in \mathcal{F}$, hence by assumption in the theorem, each $Z_K(\rho_k) \in \mathcal{M}_d^+(\mathcal{L})$. Therefore, combined with the rank-1 preserving quality of the map, we conclude that $Z_K(\rho) = \sum_{k=1}^{N} Z_K(\rho_k) \in \mathrm{R}_1[\mathcal{M}_d^+(\mathcal{L})]$ as ρ_k and hence $Z_K(\rho_k)$ is rank-1. This concludes the proof of the first part of the theorem. For the second part, note that for any product state $|ab\rangle$, the matrix $Z_K(|ab\rangle\langle ab|) = |v\rangle\langle v| \in \mathcal{M}_d^+(\mathcal{L})$. Let ρ satisfy the condition in part 2. Assume the converse, that there is some product state $|ab\rangle$

such that $\rho - |ab\rangle\langle ab| = \delta \in \text{PPT}$. Then $\rho = |ab\rangle\langle ab| + \delta \implies Z_K(\rho) = |v\rangle\langle v| + Z_K(\delta)$. Since $Z_K(\rho)$ is extremal, $Z_K(\rho) \propto |v\rangle\langle v|$, that violates the fact that it is rank ≥ 2. ■

We also state the analogous theorem that maps the *partial transpose* of the state. The proof of this theorem is similar to that of the Theorem 7.15.

Theorem 7.16. For all $K \in \mathcal{M}_{n,d^2}$, we define the following positive map $Z_K^\Gamma : (\mathcal{M}_d \otimes \mathcal{M}_d) \cong \mathcal{M}_{d^2} \to \mathcal{M}_n$

$$Z_K^\Gamma(\rho) := (Z_K \circ \Gamma)(\rho) = K\rho^\Gamma K^*$$

Let $\mathcal{F}$ be a face of the bipartite psd matrices in $\mathcal{M}_d \otimes \mathcal{M}_d$ and $\mathcal{F}_{PPT} := \mathcal{F} \cap \text{PPT}$. Furthermore, assume that $Z_K^\Gamma(\mathcal{F}_{PPT}) \in \mathcal{M}_n^+(\mathcal{L})$. Then the following statements are true.

1. We have for all separable states on $\mathcal{F}$, the matrix $Z_K^\Gamma(\rho) \in \mathrm{R}_1[\mathcal{M}_n^+(\mathcal{L})]$. This is a *necessary criterion* for separability for states in $\mathcal{F}$.
2. If for a PPT state on $\mathcal{F}$, $Z_K^\Gamma(\rho) \in \operatorname{ext} \mathcal{M}_n^+(\mathcal{L})$ and has rank ≥ 2, the state ρ is a PPT entangled edge state.

7.3.1 *Detection of PPT entangled quantum states*

We use the following strategy based on the Theorem 7.15 to detect PPT entangled states.

1. Let $\mathcal{F}$ be a face of the bipartite $(\mathcal{M}_d \otimes \mathcal{M}_d)^+$ matrices.
2. We choose K such that $Z_K(\mathcal{F}_{PPT}) \in \mathcal{M}_n^+(\mathcal{L})$ or $Z_K^\Gamma(\mathcal{F}_{PPT}) \in \mathcal{M}_n^+(\mathcal{L})$.
3. By Theorem 7.15, when the state ρ is separable, $Z_K(\rho) \in \mathrm{R}_1[\mathcal{M}_n^+(\mathcal{L})]$ or $Z_K^\Gamma(\rho) \in \mathrm{R}_1[\mathcal{M}_n^+(\mathcal{L})]$ (resp.).
4. We use the gap in the inclusion $\mathrm{R}_1[\mathcal{M}_n^+(\mathcal{L})] \subsetneq \mathcal{M}_n^+(\mathcal{L})$ to detect PPT entangled states.

In some cases that we consider in this article, this problem of rank-1 generated cones has been well-studied in the literature, even though the connection to PPT entanglement has not been considered.

Sparse States

For a $n \times n$ matrix X, we define the (undirected) graph of a matrix $G(X)$ with vertices in $[n]$ and the edge set $\{\{i,j\} \mid X_{ij} \cdot X_{ji} > 0\}$, i.e the graph has an edge whenever X_{ij} and X_{ji} are both non-zero. This allows us to define the linear space of self-adjoint matrices with a sparsity pattern given by an undirected graph H,

$$\mathcal{M}_n(H) := \{X \in \mathcal{M}_n(\mathbb{C}) \mid X^* = X,\, G(X) \subseteq H\}$$

Note that for the complete graph on d vertices, which we denote by K_n, this space $\mathcal{M}_n(K_n)$ is the real vector space of $n \times n$ self adjoint matrices. In the other extreme case, when the graph is empty (denoted by E_n), $\mathcal{M}_n(E_n)$ is the vector space of diagonal matrices with real entries. We denote the set of sparse PSD matrices [AHMR88, PPS89] as

$$\mathcal{M}_n^+(H) := \mathcal{M}_n^+ \cap \mathcal{M}_n(H)$$

Let $\{|i_A\rangle\}_{i=1}^n$ and $\{|j_A\rangle\}_{j=1}^n$ be two orthogonal sets of vectors of size n each. We define the following $n \times n$ matrix $D(\rho)$ entrywise as

$$D(\rho)_{ij} := \langle i_A j_B|\, \rho\, |i_A j_B\rangle\,.$$

To understand the sparsity pattern of this matrix $D(\rho)$, we look at the graph $G(D(\rho))$. Note that elements of $D(\rho)$ are just the diagonal elements of the density matrix. Then, we define the face of the cone using the sparsity pattern of matrix A, and a graph H on n vertices.

$$\mathcal{F}[H] := \{\rho \in (\mathcal{M}_d \otimes \mathcal{M}_d)^+ \mid G\big(D(\rho)\big) \subseteq H\} \tag{42}$$

For the case of triangle-free graphs in [Sin21], this class of states was referred to as triangle-free quantum states. Let us quickly show that this is a face of the cone. Firstly, note that $D(\rho)$ is a non-negative matrix for all PSD matrices ρ. Let us pick an element $\rho \in \mathcal{F}_H$, and write a decomposition into PSD matrices,

$$\rho = \rho_1 + \rho_2 \implies D(\rho) = D(\rho_1) + D(\rho_2)$$

If $D(\rho)_{ij} = 0$, it implies that $k = \{1,2\}$, $D(\rho_i)_{ij} = 0$, and hence $G\big(D(\rho_k)\big) \subseteq G\big(D(\rho)\big) \subseteq H$, showing that $\rho_1, \rho_2 \in \mathcal{F}_H$. We show that for all PPT states on this face, the following constraints hold.

Theorem 7.17. Let $\rho \in \mathcal{F}_H$ be a bipartite quantum state satisfying the PPT condition, then, by choosing,

- $K := \sum_{i=1}^{n} |i\rangle\langle i_A i_B| \implies Z_K(\rho) \in \mathcal{M}_n^+(H)$
- $K := \sum_{i=1}^{n} \left|i\right\rangle\!\left\langle i_A \overline{i_B}\right| \implies Z_K^\Gamma(\rho) \in \mathcal{M}_n^+(H)$

Proof. Let $\rho \in \mathcal{F}_H$ be a bipartite quantum state satisfying the PPT condition. We have,

$$Z_K(\rho) = \sum_{i,j=1}^{n} \langle i_A i_B|\rho|j_A j_B\rangle \, |i\rangle\langle j| \, .$$

For any PPT state, ρ^Γ is PSD. Hence, any 2×2 block of ρ^Γ is PSD. This implies for all i, j,

$$\begin{aligned} \langle i_A \overline{j_B}|\rho^\Gamma|i_A \overline{j_B}\rangle \, \langle j_A \overline{i_B}|\rho^\Gamma|j_A \overline{i_B}\rangle &\geq \left|\langle i_A \overline{j_B}|\rho^\Gamma|j_A \overline{i_B}\rangle\right|^2 \\ \langle i_A j_B|\rho|i_A j_B\rangle \, \langle j_A i_B|\rho|j_A i_B\rangle &\geq |\langle i_A i_B|\rho|j_A j_B\rangle|^2 \\ \iff D(\rho)_{ij} D(\rho)_{ji} &\geq |Z_K(\rho)|_{ij}^2. \end{aligned}$$

Therefore, we have $G(Z_K(\rho)) \subseteq G(D(\rho)) \subseteq G(H)$. The proof of the second statement is similar. ■

Note that the intersection $\mathcal{M}_n^+(H)$ is a convex cone with constraints encoded in the sparsity pattern of this matrix using the graph H. Now, by using our main theorem, Theorem 7.15 and applying it to the previous result, Theorem 7.17, we can derive the following necessary criterion for separability.

Corollary 7.18. Let $K := \sum_{i=1}^{n} |i\rangle\langle i_A i_B|$. Let $\rho \in \mathcal{F}_H$ be a separable quantum state, then,

$$Z_K(\rho) \in \mathrm{R}_1[\mathcal{M}_n^+(H)] \tag{43}$$

Therefore, we find that the matrix $\sum_{i,j=1}^{n} \langle i_A i_B|\rho|j_A j_B\rangle \, |i\rangle\langle j|$ is rank-1 generated in $\mathcal{M}_n^+(H)$ for all separable states in the face of sparse states, $\mathcal{F}_H$. For the empty graph, E_n on n vertices, $\mathrm{R}_1[\mathcal{M}_n^+(E_n)]$ is the set of diagonal matrices with positive entries. On the other extreme, for the complete graph, which we denote as K_n, we have $\mathrm{R}_1[\mathcal{M}_n^+(K_n)] = \mathcal{M}_n^+ = \mathcal{M}_n^+(K_n)$ is the set of PSD matrices. In both of these cases, the cone is equal to its rank-1 generated sub-cone. There is actually a complete characterization of all such graphs.

Theorem 7.19 ([PPS89]). The cone $\mathcal{M}_n^+(G)$ is rank-1 generated, i.e $\mathrm{R}_1[\mathcal{M}_n^+(G)] = \mathcal{M}_n^+(G)$ if and only if the graph is chordal.

For all non-chordal graphs, these results allow us to detect entangled states by checking that the matrix $Z_K(\rho)$ is not rank-1 generated. Although in general a complex problem, a semi-definite characterisation of this rank-1 generated property can be shown for triangle-free graphs based on the so-called comparison matrices. This characterization has also recently been made in [Sin21]. For every matrix X, we can define the comparison matrix $M(X)$ entrywise such that $[M(X)]_{ii} = |X_{ii}|$ and $[M(X)]_{ij} = -|X_{ij}|$ for all $i \neq j$. Then, we have the following result.

Theorem 7.20 (Triangle-free graphs). Assume G is a triangle free graph, and $X \in \mathcal{M}_n^+(G)$. Then it is true that,

$$X \in \mathrm{R}_1[\mathcal{M}_n^+(G)] \iff M(X) \geq 0$$

Proof. The proof of the implication follows the strategy in [Sin21, Theorem III.2]. For any rank 1 element $|v\rangle\langle v| \in \mathcal{M}_n^+(G)$, the $\mathrm{supp}(v)$ has to be a clique of the graph G. Therefore, for triangle-free graphs, since we only have the largest cliques of size 2, we have $|\mathrm{supp}(v)| \leq 2$. Therefore, for all $X \in \mathrm{R}_1[\mathcal{M}_n^+(G)]$, i.e rank-1 generated elements, we have (denote $\mathrm{supp}(v) =: \sigma(v)$)

$$X = \sum_{\sigma(v_k)=i_k} |v_k\rangle\langle v_k| + \sum_{\sigma(z_k)=\{i_k,j_k\}} |z_k\rangle\langle z_k| \tag{44}$$

and hence the comparison matrix can be computed as,

$$M(X) = \sum_{\sigma(v_k)=i_k} |v_k\rangle\langle v_k| + \sum_{\sigma(z_k)=\{i_k,j_k\}} M\left(|z_k\rangle\langle z_k|\right) \tag{45}$$

For any matrix with a support on a 2×2 block, $B \geq 0 \iff M(B) \geq 0$. Hence, from this we conclude that $M(|z_k\rangle\langle z_k|) \geq 0$, and hence also $M(X) \geq 0$. This shows the implication. To show the other direction, we use the result from [SN22a, Theorem 3.9] which states that for any matrix $X \in \mathcal{M}_n^+$, $M(X) \geq 0 \iff X = DBD$ where $B \in \mathcal{M}_n^+$ is a diagonally dominant matrix such that $G(B) = G(X)$ and D is a strictly positive diagonal matrix. Then by expanding, $B = \sum_{\{i,j\}\in E(G)} B^{(i,j)} + C$ where

$$B^{(i,j)} = \begin{bmatrix} |B_{ij}| & B_{ij} \\ B_{ij}^* & |B_{ij}| \end{bmatrix}_{i,j} = |B_{ij}|\big(\,|i\rangle\langle i| + |j\rangle\langle j|\,\big) + B_{ij}\,|i\rangle\langle j| + B_{ij}^*\,|j\rangle\langle i|$$

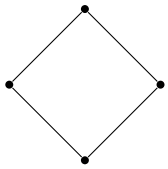


Figure 25: The graph $\mathcal{C}_4$ is the smallest non-chordal graph. It is also triangle-free, hence for any state with $G(A) \subseteq \mathcal{C}_4$, we can apply the theorem Theorem 7.20 to detect entanglement

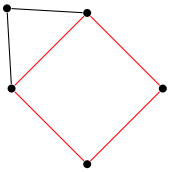


Figure 26: The graph in the figure is not triangle-free, but it has a triangle-free induced subgraph (the subgraph in red), allowing the application of Corollary 7.21

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and C is a diagonal matrix with $C_{ii} := B_{ii} - \sum_{i \neq j} |B_{ij}|$. Note that $C_{ii} \geq 0$ as B is diagonally dominant. Also for all $B^{(i,j)}$, we have $\det\left(B^{(i,j)}\right) = 0$, which implies it is rank-1 and hence $B^{(i,j)} = |z_{ij}\rangle\langle z_{ij}|$ for $z_{ij} \in \mathbb{C}^n$ with the support $\{i, j\} \in E$. Now for any positive-diagonal matrix D, $D\,|z_{ij}\rangle\langle z_{ij}|\,D \in \mathcal{M}_n^+(G)$ as $D\,|z_{ij}\rangle$ has support $\{i, j\} \in E$. Moreover, DCD is a diagonal matrix, and hence trivially belongs to $\mathcal{M}_n^+(G)$. ■

Corollary 7.21. Assume that graph H on vertex set I_H is a triangle-free induced subgraph of G. Then, for every $X \in \mathrm{R}_1[\mathcal{M}^+_{|I_H|}(G)]$, we have

$$M(X[I_H]) \geq 0$$

Proof. It is easy to see that $X[I_H] \in \mathrm{R}_1[\mathcal{M}^+_{|I_H|}(H)]$, and hence the result follows from Theorem 7.20. ■

Since every non-chordal graph contains a graph which is triangle-free (because it contains a cycle without chords), these tests provide an easy-to-implement family of tests for inclusion into the rank-1 generated cone (and also, novel necessary conditions on separability in the face of quantum states). We want to point out that these tests are not complete, in the sense that some matrices that are not included in $\mathrm{R}_1[\mathcal{M}_n^+(G)]$ possibly satisfy all the conditions in Corollary 7.21. The complete family of matrix maps that characterize the inclusion into the rank-1 generated cone of sparse PSD matrices has been completely characterized in [PPS89]. These tests are based on checking positivity of the

matrix after application of certain Schur maps, and this apparatus is intimately connected to the problem of positive-semidefinite completions [GJSW84]. For any matrix $Z \in \mathcal{M}_d$, we define the map $\mathcal{T}_Z(X) = Z \odot X$ where $\odot$ is the entrywise (or Schur) product of matrices $(Z \odot X)_{ij} = Z_{ij}X_{ij}$. It is well known that this Schur product map is a positive map if and only if $Z \in \mathcal{M}_n^+$. Recall that a matrix is PSD if and only if all its principal submatrices are PSD matrices. We extend this to define the convex cone of matrices that have *few* principal minors PSD. To do this, recall that a clique of a graph is a subgraph that is complete. For any graph G, let $\mathrm{cliq}[G]$ denote the set of cliques. For any matrix in $X \in \mathcal{M}_n$, and $I \subseteq [n]$, we define the principal submatrix $X[I] \in \mathcal{M}_{|I|}$ on the indices in I. Then, we define the following notion,

Definition 7.22. For a graph G,

$$\mathcal{M}_n^*(G) := \{Z \in \mathcal{M}_n \mid \forall I \in \mathrm{cliq}[G],\ Z[I] \geq 0\}.$$

Note that for a complete graph, i.e, $G = K_n$, this reduces to the PSD matrix cone, as *all* the principal submatrices are PSD. We show that this is the dual notion to the rank-1 generated cone $\mathrm{R}_1[\mathcal{M}_n^+(G)]$, in the next theorem.

Theorem 7.23. Let $X \in \mathcal{M}_n^+(G)$. Then the following is true,

$$X \in \mathrm{R}_1[\mathcal{M}_n^+(G)] \iff \mathcal{T}_Z(X) \geq 0$$

for all $Z \in \mathcal{M}_n^*(G)$.

Proof. For the forward implication, let $|x\rangle\langle x| \in \mathcal{M}_n^+(G)$. Then, $|x\rangle$ must have the support only on a clique of the graph G, say I, and therefore, $|x\rangle\langle x|$ must be supported in I. Moreover, we claim that $\mathcal{T}_Z(|x\rangle\langle x|) = |x\rangle\langle x| \odot Z \geq 0$ for all $Z \in \mathcal{M}_n^*(G)$. This holds because $Z[I] \geq 0$. This proves the implication. For the reverse implication, we refer the reader to [PPS89, Lemma 2.3]. ∎

Therefore, it directly follows that for $X \notin \mathrm{R}_1[\mathcal{M}_n^+(G)]$, there exists a $Z \in \mathcal{M}_n^*(G)$ such that $\mathcal{T}_Z(X) \ngeq 0$. By Corollary 7.18, this also detects entanglement in the class of sparse states we consider. This result also allows us to provide another proof of the forward implication in Theorem 7.20.

Corollary 7.24. For a triangle-free graph, G, $X \in \mathcal{M}_n^+(G) \implies M(X) \geq 0$.

Proof. Choose $Z_{ij} = e^{-i \arg(X_{ij})}$. We show that this matrix belongs to $\mathcal{M}_n^*(G)$. Since the graph is triangle-free, all its cliques are of size 2. Hence, the matrix $Z[i,j] \geq 0$ for every 2×2 principal minor of the matrix. Applying Theorem 7.23, we get $\mathcal{T}_Z(X) = M(X) \geq 0$. ■

Let us proceed with defining the notion of PSD-completable matrices. A matrix $X \in \mathcal{M}_n^*(G)$ is called to be PSD-*completable* if there exists a matrix $\tilde{X} \in \mathcal{M}_n^+$ such that $\tilde{X}[I] = X[I]$ for all $I \in \mathrm{cliq}[G]$.

Theorem 7.25. $\mathcal{T}_Z(X) \geq 0$ for all $X \in \mathcal{M}_n^+(G)$ if Z is PSD-completable. Therefore $X \notin \mathrm{R}_1[\mathcal{M}_n^+(G)]$ can be detected only by non-completable matrices.

Proof. Let Z' be the completion of the matrix Z. Then $\mathcal{T}_Z(X) = Z \odot X = Z' \odot X \geq 0$. ■

Note that these witnesses are analogous to decomposable ones, which do not detect PPT entangled states. It is important to note that in this dual picture, we have the analogous theorem for chordal graphs. (See also [PPS89, Theorem 2.4]).

Theorem 7.26. The following are equivalent for a graph G,

1. All $Z \in \mathcal{M}_n^*(G)$ are completable.
2. The graph is chordal.

Let us summarise our results in the following slogan. *If the graph of the matrix A is non-chordal, then the gap between the sparse PSD cone and its rank-1 generated version detects PPT entanglement.* This result provides a huge diversity for the construction of such states, each of which has $\approx O(d^2)$ free parameters. We show that this is very useful for constructing families of PPT entangled LDOI states. Select a *non-chordal* graph G on d vertices. Take $Y \notin \mathrm{R}_1[\mathcal{M}_n^+(G)]$, and select $Z \geq 0$ such that diag(Z) = diag(Y) and $G(Z) = G$. Then, select a non-negative X (ensuring diag(X) = diag(Y)) such that $G(X) = G$ and $X_{ij}X_{ji} \geq |Z_{ij}|^2$.

Then, the following state is PPT entangled.

$$\rho_{X,Y,Z} = \sum_{i,j} X_{ij} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{i\neq j} Y_{ij} \left|ii\right\rangle\!\left\langle jj\right| + \sum_{i\neq j} Z_{ij} \left|ij\right\rangle\!\left\langle ji\right| .$$

Proof of entanglement. The PPT property can be readily verified from Theorem 7.12. To check that the state is entangled, note that these states lie on the face $\mathcal{F}_G$, and for $K = \sum_{i=1}^{d} \left|i\right\rangle \left\langle ii\right|$, $Z_K(\rho) \notin \mathrm{R}_1[\mathcal{M}_d(G)]$. ■

Example 7.27. We select the smallest non-chordal graph, the cycle graph $\mathcal{C}_4$, and we use the extremal matrix of C that has rank 2 [AHMR88, Example 1]:

$$Y = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 1 & -1 \\ 1 & 0 & -1 & 2 \end{bmatrix}.$$

Then, by using the following free parameters,

$$X = \begin{bmatrix} 1 & X_{12} & 0 & X_{14} \\ X_{21} & 2 & X_{23} & 0 \\ 0 & X_{23} & 1 & X_{34} \\ X_{41} & 0 & X_{43} & 2 \end{bmatrix} \quad Z = \begin{bmatrix} 1 & Z_{12} & 0 & Z_{14} \\ Z_{12}^* & 2 & Z_{23} & 0 \\ 0 & Z_{23}^* & 1 & Z_{34} \\ Z_{14}^* & 0 & Z_{34}^* & 2 \end{bmatrix}$$

such that $Z \geq 0$ and $X_{ij}X_{ji} \geq |Z_{ij}|^2$, results in a PPT entangled state. Note that due to extremality, the constructed matrix forms a family of PPT entangled edge-states.

7.3.2 *Restricted Rank-1 States*

In this section, we provide another face of PSD bipartite matrices for which our result in Theorem 7.16 detects PPT entangled states. Let $V = \mathrm{span}_{i=1}^{n}\{\left|ii\right\rangle\}$. Then, we can define the following face of quantum states,

$$\mathcal{F}_{|\varphi\rangle} := \{\rho \in (\mathcal{M}_d \otimes \mathcal{M}_d)^+ \mid \rho|_V \propto \left|\varphi\right\rangle\!\left\langle\varphi\right|\}.$$

This is the face in which all the density matrices restricted to V are proportional to the rank-1 matrix, $\left|\varphi\right\rangle\!\left\langle\varphi\right|$. It is easy to see why these matrices form a face of the convex cone. Particularly, let's assume $\rho \in \mathcal{F}_{|\varphi\rangle}$ has a conic decomposition into sum of two PSD matrices, i.e $\rho = \rho_1 + \rho_2 \mid \rho_1, \rho_2 \in (\mathcal{M}_d \otimes \mathcal{M}_d)^+$. Then, it implies that,

$$\rho|_V = \rho_1|_V + \rho_2|_V.$$

Since $\rho|_V \propto |\varphi\rangle\langle\varphi|$ that is extremal, we have, $\rho_1|_V$ and $\rho_2|_V$ also are $\propto |\varphi\rangle\langle\varphi|$. This shows that this is a face of the bipartite states.

We now define the key convex cone for this section, that is, the cone of positive semidefinite matrices that have diagonal elements with some fixed proportions. Note that the cone of positive-semidefinite matrices with all diagonal elements equal has been well-studied in the literature, under the name of complex *correlation matrices* [CV79]. In the case of real matrices, this cone is sometimes referred to as the *elliptope*. Let us define the linear space of matrices for which the diagonal of the matrix is proportional to some fixed non-negative vector.

Definition 7.28. Let $x \in \mathbb{R}^n_+$ and,

$$\mathcal{M}_n[x] := \{X | \exists \lambda,\ \forall i,\ X_{ii} = \lambda x_i\}. \tag{46}$$

Let e be the vector with all elements 1.

Definition 7.29 (Correlation matrices)**.** $\mathcal{M}^+_n[e] = \mathcal{M}^+_n \cap \mathcal{M}_n[e]$ is the cone of PSD matrices with the diagonal elements equal.

For any vector $q \in \mathbb{C}^n$, we can embed the vector into a diagonal matrix, $D_q := \mathrm{diag}(q_1, q_2 \ldots q_n)$. We proceed with the following definition.

Definition 7.30 (Scaled correlation matrices)**.** For any vector $x \geq 0$, the scaled correlation matrices,

$$\mathcal{M}^+_n[x] := D_{\sqrt{x}}\, \mathcal{M}^+_n[e]\, D_{\sqrt{x}}$$

is the convex cone of positive semidefinite matrices with the diagonal $\propto x$.

Moreover, the ranks of the extremal matrices in the cone $\mathcal{M}^+_n$ have been completely characterized. It is known that any extremal matrix has a rank-r if and only if $r^2 \leq d$. [GPW90] [LT94]. Hence, we want to point out that the maximum ranks that are achieved by such extremal matrices are $\lfloor \sqrt{n} \rfloor$. Also, it follows that,

Theorem 7.31 ([LT94]). For all $n \geq 4$, we have

$$\mathrm{R}_1[\mathcal{M}_n^+[e]] \subsetneq \mathcal{M}_n^+[e].$$

This means that the cone of such matrices is not rank-1 generated for any $n \geq 4$. The same holds for the scaled correlation matrices $\mathcal{M}_n^+[x]$. We show that these sets can also be connected to detecting PPT entanglement in the face $\mathcal{F}_{|\varphi\rangle}$. Let us define $K := \sum_{i=1}^n |i\rangle \langle ii|$. Let ρ be a bipartite PPT state in the face $\mathcal{F}_{|\varphi\rangle}$. Then, we can see that,

$$Z_K^\Gamma(\rho)_{ii} = |\varphi_i|^2. \tag{47}$$

This implies that $Z_K^\Gamma(\rho) \in \mathcal{M}_n^+[\varphi \odot \varphi]$. Then, the following proposition follows from the application of Theorem 7.16.

Proposition 7.32. If the state ρ is separable in $\mathcal{F}_{|\varphi\rangle}$, then the matrix,

$$Z_K^\Gamma(\rho) \in \mathrm{R}_1[\mathcal{M}_n^+[\varphi \odot \varphi]]$$

Therefore, we find that if such a state in $\mathcal{F}_\varphi$ is separable, the necessary condition on the matrix $Z_K^\Gamma(\rho)$ is that it has to be a rank-1 generated element of the $\mathcal{M}_n^+[\varphi \odot \varphi]]$. This also allows us to construct new PPT entangled states. We first provide an example of a witness to detect the violation of the rank-1 generated property in the first non-trivial case of $n = 4$, which we borrow from the [JLLL20], which outlines a general strategy to witness the separation between correlation matrices and their rank-1 generated version. To this end, note that for complex correlation matrices, i.e, $\mathcal{M}_n^+[e]$, we also have the following characterization,

$$\mathrm{R}_1[\mathcal{M}_n^+[e]] = \mathrm{cone}\{|z\rangle\langle z| \mid z \in \mathbb{T}^n\}.$$

Consider the following 4×4 matrix,

$$W = \begin{bmatrix} 0 & -i & i & 1 \\ i & 0 & -i & 1 \\ -i & i & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}.$$

Then, it is shown [JLLL20] that $\langle z|W|z\rangle \leq 6$ for all $z \in \mathbb{T}^4$ and hence we have $\mathrm{Tr}(WZ) \leq 6\,\mathrm{Tr}(\mathrm{Z})$ for all $Z \in \mathrm{R}_1[\mathcal{M}_4^+[e]]$. Let us consider the following parametrized matrix,

$$H(x) = \begin{bmatrix} 1 & -ix & ix & x \\ ix & 1 & -ix & x \\ -ix & ix & 1 & x \\ x & x & x & 1 \end{bmatrix}.$$

It is easy to verify by direct computation of its eigenvalues that $H(x) \geq 0 \iff |x| \leq 1/\sqrt{3}$ and also $\mathrm{Tr}(H(x)W) = 12x \leq 6 \iff x \leq 1/2$. Hence, for the parameter range $1/2 < x \leq 1/\sqrt{3}$, the matrix $H(x)$ is not a rank-1 generated correlation matrix. Note that, for $1/2 < x < 1/\sqrt{3}$, the matrix also has full rank 4, and is not extremal.

Theorem 7.33. The matrix $H(x)$ is rank-2 and extremal in $\mathcal{M}_4^+[e]$ for $x = \frac{1}{\sqrt{3}}$.

Proof. The rank-2 property can be immediately verified by the computation of eigenvalues. For extremality, we use the results of [LT94, Theorem 1]. Consider the matrix X whose columns are the eigenvectors of the matrix. We need to show that the following holds.

$$\mathrm{span}\{x_i x_i^* \mid x_i \in X^*\} = \mathcal{M}_2^{\mathrm{sa}}. \tag{48}$$

Here the matrix, $X^* = \begin{bmatrix} 1 & 1 & 1 & -\sqrt{3} \\ 1 & \omega^2 & \omega & 0 \end{bmatrix}$ where $\omega := e^{i2\pi/3}$. Then it is easy to verify that the Eq. (48) is satisfied for $x_1 = (1,1), x_2 = (1,\omega^2), x_3 = (1,\omega), x_4 = (-\sqrt{3},0)$. ■

Finally, we provide examples of PPT entangled states using extremal matrices with rank ≥ 2. We consider the following parametric family of quantum states ($\forall i, A_{ii} = 1$),

$$|\omega\rangle\langle\omega| + \sum_{i\neq j}^{4} A_{ij} |ij\rangle\langle ij| + \sum_{i\neq j}^{4} H(x)_{ij} |ij\rangle\langle ji| \tag{49}$$

where $\omega = \sum_i |ii\rangle$ is the maximally entangled Bell state (un-normalized). These states belong to the face $\mathcal{F}_{|e\rangle}$. The PPT property can be verified readily from Theorem 7.12 by having $\forall i,j, A_{ij}A_{ji} \geq 1$. Moreover, it is easy to show that by choosing $K = \sum_{i=1}^4 |i\rangle\langle ii|$ we have $Z_K^\Gamma(\rho) = H(x)$. Since this matrix is not a rank-1 generated correlation matrix for $1/2 < x \leq 1/\sqrt{3}$, the state is PPT entangled by Proposition 7.32. Moreover, for $x = \frac{1}{\sqrt{3}}$ this is also a PPT entangled edge-state by Theorem 7.33.

Note that the states considered in the equation Eq. (49) are exactly the LDOI states with the triple $(A, \mathbb{J}_4, H(x))$. We have the following theorem from [SN21], which shows our necessary condition is also sufficient in the case of $A = \mathbb{J}$.

Theorem 7.34 ([SN21]). The LDOI state in $\mathcal{M}_d \otimes \mathcal{M}_d$ with the triple $(\mathbb{J}_d, \mathbb{J}_d, X)$ is separable if and only if $X \in \mathrm{R}_1[\mathcal{M}_d^+[e]]$.

We also show that two commonly used criteria for detecting entangled states fail to do so. CCNR criterion: From Theorem 7.14, it follows that the states we consider in Eq. (49) satisfy the CCNR criterion if and only if

$$||A||_1 - ||A||_{\mathrm{Tr}} \geq 12.$$

For the case $A = \mathbb{J}_4$ we have $||A||_1 = 16$, and $||A||_1 = 4$, so the state satisfies the CCNR criterion. Moreover, by choosing $A = \mathbb{I}_4 + t(\mathbb{J}_4 - \mathbb{I}_4)$, we have that the state satisfies the realignment criterion if $t \geq 1$, which is also ensured by the PPT criterion. This shows that the rank-based criterion is more powerful than CCNR (and also PPT) for some classes of states.

7.3.3 *Bose-symmetric states*

In this section, we analyze another class of quantum states for which our main result, Theorem 7.16, provides a method of detecting entanglement. We consider the states for which the range lies in the symmetric subspace, which we denote by $\mathbb{C}^d \vee \mathbb{C}^d$, $\vee$ being the symmetric product. Clearly, this forms a face of the bipartite PSD cone, due to the restriction of its range (see Theorem 7.3). Let F denote the flip operator,

$$F = \sum_{i,j=1}^{d} |ij\rangle\langle ji|$$

and $\Pi := \frac{\mathbb{I}+F}{2}$ denote the projection into the symmetric subspace. Then, for a bipartite PSD matrix, the following are equivalent,

- $\mathrm{ran}(\rho) \subseteq \mathbb{C}^d \vee \mathbb{C}^d$,
- $\Pi\rho\Pi = \rho$,
- $\rho F = F\rho = \rho$.

Interestingly, for all bosonic states, all the usual entanglement criteria, like PPT, realignment, and the covariance criterion, are equivalent [TG09], hence, any PPT entangled bosonic state cannot be detected by such criteria. Let us call the bosonic PSD matrices as $\mathcal{F}_\vee$. Let us consider the convex cone of doubly non-negative matrices,

$$\mathsf{DNN}_n := \mathcal{M}_n^+ \cap \mathcal{M}_n(\mathbb{R}_+).$$

Then, we have the following proposition.

Proposition 7.35. Assume $\rho \in \mathcal{F}_\vee$ is PPT. Let $\{|i\rangle\}_{i=1}^n$ denote the orthonormal set of vectors of size n. Let $K = \sum_{i=1}^n |i\rangle \langle i, \bar{i}|$. Then, the following is true,

$$Z_K^\Gamma(\rho) \in \mathsf{DNN}_n.$$

Proof. Let ρ be a PSD state in $\mathcal{F}_\vee$. Moreover, we have,

$$\begin{aligned} Z_K^\Gamma(\rho) &= \sum_{i=1}^n \sum_{j=1}^n \langle i, \bar{i}|\rho^\Gamma|j, \bar{j}\rangle \ |i\rangle \langle j| \\ &= \sum_{i=1}^n \sum_{j=1}^n \langle i, j|\rho|j, i\rangle \ |i\rangle \langle j| \\ &= \sum_{i=1}^n \sum_{j=1}^n \langle i, j|\rho F|i, j\rangle \ |i\rangle \langle j| \\ &= \sum_{i=1}^n \sum_{j=1}^n \langle i, j|\rho|i, j\rangle \ |i\rangle \langle j| \end{aligned}$$

Since ρ is PSD, we have $\langle i, j|\rho|i, j\rangle \geq 0 \implies Z_K^\Gamma(\rho) \in \mathcal{M}_d(\mathbb{R}_+)$. Moreover, this matrix is PSD by Theorem 7.16. ■

Using our result in Theorem 7.15, we can provide another necessary criterion for the separability of bosonic states.

Corollary 7.36. Assume ρ is a separable state in $\mathcal{F}_\vee$. Then, by choosing $K := \sum_{i=1}^n \left|i\middle\rangle\middle\langle i, \bar{i}\right|$, we have

$$Z_K^\Gamma(\rho) \in \mathrm{R}_1[\mathsf{DNN}_n].$$

The ranks of the extremal rays of the doubly non-negative cone have been scrutinized in [HJL96].

Theorem 7.37 (Ranks of extremal DNN matrices)**.** Let $A \neq 0 \in \operatorname{ext} \mathsf{DNN}_n$. Then, we have,

- If $n = 2$, $\operatorname{rk}(A) \leq 1$.
- If $n > 2$ is even, $\operatorname{rk}(A) \leq n - 3$.
- If $n > 2$ is odd, $\operatorname{rk}(A) \leq n - 2$.

Face of PSD	PPT $\Longrightarrow$	SEP $\Longrightarrow$
Sparse States (7.3.1)	Sparse PSD matrices (7.17)	Rank-1 generated G-sparse PSD matrices (7.18)
Restricted Rank-1 States (7.3.2)	Scaled correlation matrices (47)	Rank-1 generated scaled correlation matrices (7.32)
Bosonic states (7.3.3)	DNN matrices (7.35)	Rank-1 generated DNN matrices (7.36)

Table 14: Summary of the considered faces of the state space and the mappings of PPT states on these faces. The separable states are mapped to the corresponding rank-1 generated convex cones.

> Moreover, we have elements $A \in \operatorname{ext} \mathsf{DNN}_n$ for all ranks satisfying the conditions above.

Moreover, the rank-1 generated version of this cone is the well-known cone of completely positive matrices.

$$\mathrm{R}_1[\mathsf{DNN}_n] = \{|v\rangle\langle v| \mid v \in \mathbb{R}_+^d\} := \mathsf{CP}_n.$$

Theorem 7.37 implies that $\mathrm{R}_1[\mathsf{DNN}_n] = \mathsf{DNN}_n$ if and only if $n \leq 4$. For more details on these cones and examples of doubly non-negative matrices that are not rank-1 generated (i.e, not CP), we refer you to the book [SMB21]. The extremal DNN matrices also allow us to construct PPT entangled edge states (that are also bosonic). In general, it is computationally NP-hard to decide whether a DNN_n matrix belongs to CP_n. Lots of results are known about these matrices in special cases, like matrices having sparsity patterns corresponding to triangle-free graphs [SMB21].

Let us also briefly introduce the witnesses for detecting states that are not rank-1 generated. These are well-known under the name of copositive matrices, denoted as COP_n, that is, exactly the set of all matrices satisfying,

$$\forall v \in \mathbb{R}_+^n \quad \langle v|X|v\rangle \geq 0.$$

It is clear from the previous definition that if a matrix is the sum of a non-negative matrix and a PSD matrix, then it is copositive. Such matrices are called SPN_n matrices.

This convex cone is the conic-dual to DNN_n matrices [SMB21], and hence if $X \in \mathsf{SPN}_n$ then

$$\forall Y \in \mathsf{DNN}_n \quad \operatorname{Tr}(XY) \geq 0.$$

To detect non-rank-1 generated matrices, we can construct a witness that is copositive but not SPN. The paradigmatic example of such a matrix is the *Horn's matrix*.

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

To construct an example of a DNN_5 matrix that is not rank-1 generated, we borrow the example from [GNS25].

$$A = \begin{pmatrix} 2\cos\frac{\pi}{5} & 1 & 0 & 0 & 1 \\ 1 & 2\cos\frac{\pi}{5} & 1 & 0 & 0 \\ 0 & 1 & 2\cos\frac{\pi}{5} & 1 & 0 \\ 0 & 0 & 1 & 2\cos\frac{\pi}{5} & 1 \\ 1 & 0 & 0 & 1 & 2\cos\frac{\pi}{5} \end{pmatrix}.$$

By computing $\operatorname{Tr}(AH) = 10(\cos \pi/5 - 1) < 0$, we can verify that the matrix A is not rank-1 generated in the doubly non-negative matrix cone.

Example 7.38. Let us present an example of a family of PPT bosonic edge states that we can detect using the entanglement criterion in Corollary 7.36.

$$\sum_{i,j} A_{ij} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{i \neq j} Y_{ij} \left|ii\right\rangle\!\left\langle jj\right| + \sum_{i \neq j} A_{ij} \left|ij\right\rangle\!\left\langle ji\right|$$

for any $A \in \operatorname{ext} \mathsf{DNN}_d$ such that $\operatorname{rk}(A) \geq 2$, $Y \geq 0$ and $|A_{ij}| \geq Y_{ij}$. We can obtain these states as soon as $d \geq 5$, for constructions see [HJL96]. It can be verified to be PPT entangled, bosonic, and an edge state by choosing $K := \sum_{i=1}^{d} \left|i\right\rangle \left\langle i,i\right|$. and applying the previous results (Corollary 7.36, Theorem 7.16).

We want to point out that for $Y_{ij} = 0$, the states considered above are called *mixtures of Dicke states* [TAQ+18, SN21], which are separable if and only if $A \in \mathrm{R}_1[\mathsf{DNN}_n]$.

7.4 DISCUSSION AND OUTLOOK

In this article, we presented a rank-based criterion to detect PPT entanglement in mixed bipartite quantum states by mapping PPT states to cones that are not rank-1 generated. This allows us to use a variety of results and examples of matrix analysis, optimization, and graph theory to construct new methods and examples of PPT entangled states.

Our work definitely opens avenues for future research. The entanglement-theoretic properties of the states constructed by the above methods should be scrutinized (for example, Schmidt numbers and entanglement measures). It remains to be seen whether PPT entangled states can provide meaningful advantages over separable (unentangled) states in quantum protocols, some evidence for which has been recently obtained in [TTV+25, TV18, PTBV21] in the area of quantum metrology and non-local games. We hope that the methods used in this paper and examples of PPT entangled states are useful test states for such advantages. It will also be useful to analyse whether the witnesses that detect matrices that are not rank-1 generated in all cases considered in this paper can be used to construct positive indecomposable maps, an important topic of research in operator algebras. This was recently accomplished for copositive matrices [GNP25b], the witnesses discussed in Section 7.3.3.

Finally, the faces of the PSD cone we consider can be mapped to known convex cones that are not rank-1 generated. In general, it would be useful to understand how this machinery can be expanded to other faces of the PSD cone and appropriately chosen mappings, to construct new interesting examples of PPT entangled and PPT edge-states. It might be useful to first understand this question in low-dimensional quantum systems, i.e, in the case of two qutrits, or qubit-ququarts.

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8

Positive maps and extendibility hierarchies from copositive matrices

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8.1 INTRODUCTION

The study of positive linear maps between matrix algebras is a cornerstone of modern functional analysis and operator theory [Stø63, Cho75a, Wor76]. A linear map $\Phi : \mathcal{M}_n(\mathbb{C}) \to \mathcal{M}_n(\mathbb{C})$ is called *positive* if it maps positive semidefinite matrices to positive semidefinite matrices. A stronger condition is that of *complete positivity* [Pau02], where the amplification $\Phi \otimes \mathrm{I}_k$ remains positive for all ancilla dimensions k. While completely positive maps admit a simple structural characterization via the Choi-Kraus representation, the set of maps that are positive but not completely positive possesses a far more intricate structure.

Originating in operator algebra, the distinction between positivity and complete positivity turns out to have profound implications for *quantum entanglement theory* [HHHH09]. The celebrated *Horodecki criterion* [HHH96] established that a bipartite quantum state ρ is entangled if and only if there exists a positive but not completely positive map Φ such that $[\Phi \otimes \mathrm{I}_]\(\rho)$ is not positive semidefinite. Consequently, such maps Φ are synonymous with *entanglement witnesses* [Ter00], and the challenge of constructing and classifying them is one of the foremost problems in quantum information science [NC10, AS17, Wat18]. Within the set of positive maps lies the important convex cone of *decomposable maps*, that can be written as the sum of a completely positive map and a completely co-positive map (the composition of a completely positive map with the matrix transpose). Maps that are positive but not decomposable, known as *indecomposable maps*, are of particular interest as they can detect subtle forms of entanglement, such as that found in *PPT*

(positive partial transpose) entangled states [Hor97]. While it was shown by Størmer and Woronowicz that every positive map $\mathcal{M}_2(\mathbb{C}) \to \mathcal{M}_{2,3}(\mathbb{C})$ is known to be decomposable [Stø63, Wor76], Choi [Cho75c] provided the first example of a positive indecomposable map $\mathcal{M}_3(\mathbb{C}) \to \mathcal{M}_3(\mathbb{C})$, which was later generalized in various related forms (see, e.g., [CL77, TT88, Osa91, Kye92, CKL92, Ha03, SBSC24]). However, a general theory has remained largely out of reach. *Unextendible Product Bases* (UPBs) underpin a range of methods for constructing positive indecomposable maps in quantum information theory. DiVincenzo et al. [DMS$^+$03] define UPBs using orthogonality graphs, tiling patterns, and algebraic constructions; they show that the complement of a UPB yields a bound entangled state with a positive partial transpose that furnishes indecomposable maps. Terhal [Ter01] leverages these UPBs to generate positive maps that resist decomposition by standard methods. Bravyi [Bra04] classifies three-qubit UPBs and demonstrates that uncompletable product bases yield bound entangled states, while Alon and Lovász [AL01] employ graph-theoretic techniques to construct multipartite UPBs and derive bounds from orthogonality graphs. Several studies focus on explicit algebraic constructions of positive indecomposable maps: Chruściński and Kossakowski [CK06, CK07] introduce classes of maps based on cyclic bistochastic matrices and generalizations of the Choi map, as well as atomic maps characterized by their action on rank one projectors. Sarbicki and Chruściński [SC12] construct exposed indecomposable maps in $2n \times 2n$ matrices using reduction maps, generalizing the Robertson map. Ha and Kye [HK16] present parameterized families of exposed indecomposable maps, with explicit conditions for exposedness and the bi-spanning property. Collins, Hayden, and the second author [CHN16] employ random matrix and free probability techniques, constructing k-positive maps via free convolution and random matrix models. Marciniak and Rutkowski [MR17] introduce a geometric "merging" technique, systematically combining two positive maps with additional operators and functionals to produce new positive, often exposed, indecomposable maps. Müller-Hermes [**?**] uses symmetrization and tensor product techniques, particularly with Werner maps, to analyze decomposability under tensor powers and construct new non-decomposable maps. Siudzińska [Siu22] uses symmetric measurements (positive operator-valued measures) and operator bases to construct positive maps and indecomposable entanglement witnesses.

Other than or beyond the PPT criterion, the study of bipartite entanglement has also motivated the study of the notion of *extendibility* [DPS04, CKMR07, NOP09, Doh14, HNW17]. In particular, the notion of *bosonic (or Bose-symmetric) extendibility* plays a central role in the study of quantum entanglement, providing one of the most powerful and systematic separability criteria. Introduced in the seminal work of Doherty, Parrilo, and Spedalieri [DPS04], the hierarchy of r-extendible states forms an increasing sequence of convex sets that converges to the set of separable states. This completeness ensures that every

entangled state eventually fails some level of the hierarchy. Moreover, each level can be efficiently tested using semidefinite programming (SDP), making the DPS hierarchy not only theoretically elegant but also computationally tractable.

A stronger version of this idea arises when one focuses on bipartite *bosonic* systems. In this setting, one may further require that the Bose-symmetric extensions simultaneously include both original subsystems, leading to what is called r*-PPT bosonic exchangeability* [CKMR07] or *PPT extendible with respect to the complete graph* $\mathcal{K}_r$ [ACG+26]. This refinement yields a sharper and still complete hierarchy of tests that interpolate between the PPT and separability conditions. Thanks to the monogamy of entanglement [Ter04], a state passing all these tests behaves as if it could be consistently extended to many identical copies while maintaining only a weak amount of entanglement across any bipartition. Despite the natural formulation of this criterion, explicitly constructing entangled states that satisfy such strong extendibility conditions remains a challenging problem, even for the simplest cases [DPS04].

A powerful approach to understanding cones of maps and states is through *duality*. The cone of positive maps is dual to the cone of separable states, while the cone of decomposable maps is dual to the cone of PPT states [EK00, SSŻ09, Kye23]. Duality also connects map properties to cones of matrices. The cone of *completely positive matrices* CP_n [BSM03], consisting of matrices that can be factored as $XX^\top$ for some entrywise non-negative (rectangular) matrix X, has as its dual the cone of *copositive matrices* COP_n [SMB21]. A real symmetric matrix M is in COP_n if $\langle x, Mx\rangle \geq 0$ for all non-negative vectors $x \in \mathbb{R}^n_+$. Just like the set of positive maps, the cone COP_n is notoriously difficult to characterize, with membership being a co-NP-complete problem [MK87]. The subset of COP_n comprising matrices that are a sum of a positive semidefinite and an entrywise non-negative matrix, denoted SPN_n, is tractable and corresponds to the first level of a sum-of-squares (SOS) hierarchy that approximates COP_n. The strict containment $\mathsf{COP}_n \supsetneq \mathsf{SPN}_n$ for $n \geq 5$, exemplified by the famous Horn matrix [SMB21], mirrors the distinction between positive and decomposable maps. Let us point out here that the use of copositive matrices for entanglement detection dates back to [MATS21], see also [Mar23, RPAR+25, MMRRP+25]. On the dual side, the connection between completely positive matrices and separability dates back to [Yu16, TAQ+18], see also [JM19, SN21, Sin21, Ber23, GNS25, Gul26]. Finally, the dual of (PPT-) bosonic extendibility hierarchy admits a natural interpretation in terms of sum-of-squares (SOS) representations of Hermitian forms [DPS04, FF21]. This duality connects the feasibility of an r-extendibility test to the existence of SOS certificates of block-positivity for corresponding entanglement witnesses. In this context, a fundamental open question was raised in [DPS04, Sec. VI], which we state informally,

Can the cone of entanglement witnesses (i.e. block-positive operators or elements of the dual of the separable set) be obtained as the union of the witnesses of these DPS levels?

We refer to Section 8.8.1 for further details. Any counterexample to this question could be used to detect entanglement of quantum states that are r-PPT bosonic extendible for arbitrarily high $r \geq 1$. While partial results are known (e.g., inclusion of its interior), a full resolution remains open, reflecting the deep interplay between convex geometry, operator algebras, and optimization in the characterization of quantum entanglement.

On the other hand, a fruitful strategy for finding PPT entangled states and positive indecomposable maps is to impose *symmetries* on the states and maps under consideration [VW01, EW01, SN21, PJPY24]. A particularly rich and physically relevant class is that of *diagonal unitary covariant* (DUC) maps [Liu14, SN21], which commute with conjugations by diagonal unitary matrices. Such maps, and their close relatives the *conjugate diagonal unitary covariant* (CDUC) maps, have recently been the subject of intense study due to their structured algebraic properties [SN22b, KMP18, SDN24]. Recent work established a fundamental isomorphism between the space of DUC/CDUC maps and the vector space of *pairs of matrices* (A, B) sharing a common diagonal [JM19, SN21]. Within this framework, a cone of pairwise completely positive matrices PCP_n was introduced, which was shown to correspond precisely to the class of *entanglement breaking* DUC/CDUC maps. This breakthrough provided a complete description of the strongest form of positivity for these maps. However, a corresponding characterization for general positivity was left as a significant open problem. This gap motivates the central questions of this paper:

Q1 Can we define and characterize a cone of matrix pairs that corresponds precisely to the set of all positive DUC/CDUC maps?

Q2 Can we leverage the well-understood theory of classical matrix cones, such as COP_n and SPN_n, to systematically construct elements in these new pairwise cones, similarly to the correspondence between the CP_n and the PCP_n cones?

Q3 Can such a framework be applied to generate vast, explicit families of positive indecomposable maps, thereby providing new tools for entanglement detection?

Q4 Can these findings be further leveraged to construct families of entangled quantum states that nevertheless display separability-like properties, such as being PPT or possessing high-order symmetric extensions? More precisely, are there explicit examples of entangled bosonic states that are $\mathcal{K}_r$-PPT bosonic extendible? On the dual side, can we construct entanglement witnesses that admit no SOS certificate of any finite order?

This paper provides affirmative answers to all these questions. We introduce a comprehensive framework for understanding positivity and decomposability of DUC/CDUC maps by defining and analyzing novel cones of matrix pairs. Our main contributions are as follows:

- The Pairwise Copositive Cone: We introduce in Section 8.3 the cone of *pairwise copositive matrices*, denoted PCOP_n. Our first main result is that this cone is the dual of the PCP_n cone and provides the sought-after characterization: a DUC/CDUC map parameterized by a pair (A, B) is positive if and only if $(A, B) \in \mathsf{PCOP}_n$. This completely resolves the problem of characterizing positivity for this class of maps, answering Q1.

- A bridge between the classical and pairwise cones: We establish a powerful constructive result, Theorem 8.26, which provides a canonical way to "lift" any matrix $M \in \mathsf{COP}_n$ to a family of pairs in PCOP_n. This theorem enables the transfer results about copositive matrices into the domain of operator algebra and quantum information theory. These results, discussed in Section 8.4, and the results discussed in the next point (see Section 8.5) answer Q2.

- Characterization of (in)decomposability: We extend our analysis to decomposability by introducing the cone of *pairwise decomposable matrices*, PDEC_n. We show this cone precisely characterizes decomposable DUC/CDUC maps and prove an analogous constructive theorem (Theorem 8.35) that links PDEC_n to the tractable cone SPN_n. In particular, for each matrix in $\mathsf{COP}_n \setminus \mathsf{SPN}_n$, we construct an $(n^2 - n)/2$-*dimensional family of positive indecomposable linear maps* (Corollary 8.38). Interestingly, we further show that when the underlying copositive matrix is *extremal*, the lifted family translates directly into a family of *optimal* entanglement witnesses, yielding an $(n^2 - n)/2$-dimensional collection of "edge" objects (Corollary 8.39). The gap between PCOP_n and PDEC_n thus corresponds to the domain of indecomposable positive maps, and our results bridge this gap to the one between COP_n and SPN_n, which has been studied extensively in the literature. Markov-Choi maps (discussed in Section 8.6) correspond to LDUI maps having a special form. We characterize positivity, decomposability, and other properties of such maps in Proposition 8.41. In Propositions 8.43 and 8.46, we further provide new conditions for identifying positive indecomposable linear maps within this family. As a consequence, in Section 8.6.1 and Examples 8.44, 8.47, and 8.48, we present several examples of indecomposable Markov–Choi maps that significantly extend the known classes described in [Kye92, CKL92, Ha03].

- Positive maps from graphs: As a primary application of our framework, we introduce in Section 8.7 a one-parameter family of linear maps Φ_t^G associated with any simple graph G. These maps act like the completely depolarizing channel on the diagonal of the input, and as a scaled Schur product on the off-diagonal entries of the input corresponding to edges in G; a similar construction has been proposed in [KMP18]. We derive sharp, analytic thresholds for the parameter t that separate the regimes of complete positivity, decomposability, and positivity. These thresholds are expressed in terms of fundamental graph parameters of the underlying graph G: the *largest eigenvalue* $\lambda(G)$, the *clique number* $\omega(G)$, and a new graph parameter $\sigma(G)$ which we define and relate to the SPN_n cone; see Theorem 8.52. This general constructions serves as a tool for generating new positive indecomposable maps. We prove in Proposition 8.57 that any triangle-free non-bipartite graph yields such maps; this is the case for odd cycles, see Proposition 8.59. More significantly, by exploiting the rich algebraic structure of rank 3 *strongly regular graphs*, we derive an exact formula for the parameter $\sigma(G)$ in Theorem 8.61. This allows us to prove that infinite families of strongly regular graphs, including the classical *Paley graphs* (see Corollary 8.63), generate positive indecomposable maps, providing a wealth of new, highly structured examples and thus answering Q3.

- Connections to quantum state extendibility: In the final part of the paper, we connect our results to hierarchies of quantum state extendibility. We show in Proposition 8.67, Theorems 8.72 and 8.74 that the well-known *sum-of-squares* (SOS) hierarchies for copositive matrices ($\mathsf{K}_n^{(r)}$, see Section 8.7 and also [DKP02, Sch79b]) correspond directly to witnesses for different levels of PPT-bosonic extendibility of quantum states, such as (mixture of) Dicke states. In particular, such connections allow us to construct a surprisingly wide family of entanglement witnesses which do not have SOS properties of any order (Theorem 8.68), thus providing counterexamples to the question dating back to [DPS04]. Furthermore, on the dual side, we completely characterize the PPT bosonic extendibility of Dicke states (with respect to the complete graph $\mathcal{K}_{r+2}$) in terms of the dual set $(\mathsf{K}_n^{(r)})^\circ$ (Theorem 8.79), which allows us to provide explicit examples of bosonic entangled states that are arbitrarily highly extendible whenever the local dimension n is not less than 5. This answers Q4. As a byproduct, we also prove in Corollary 8.81 the existence of r-partite entangled bosonic (Dicke) states of which are PPT with respect to all bipartitions.

The paper is organized as follows. Section 8.2 establishes our notation and reviews the necessary preliminaries on matrix cones and positive maps. Section 8.3 introduces the central object of study, the pairwise copositive cone PCOP_n, and proves its duality with

PCP_n as well as some other basic properties. Section 8.4 establishes the main constructive theorem linking the PCOP_n cone to COP_n, hence providing a characterization of positivity for large classed of (C)DUC linear maps. Section 8.5 develops the analogous theory for the pairwise decomposable cone PDEC_n. In Section 8.6 we discuss Markov-Choi linear maps and their positivity properties. Section 8.7 applies this framework to define the graph-based maps and determines the exact positivity and decomposability thresholds; we also specialize this analysis to the case of strongly regular graphs. Finally, in Section 8.8 we put forward the remarkable connection between hierarchies of quantum state extendibility and hierarchies of sum-of-squares programs for membership in the COP_n cone.

8.2 PRELIMINARIES

8.2.1 *Notation*

We start by defining the notation used throughout this paper. A vector v is an element in either $\mathbb{C}^n$ or $\mathbb{R}^n$. We sometimes also use Dirac's *bra-ket* notation to write vectors. In this notation, column vectors $v \in \mathbb{C}^n$ are written as kets $|v\rangle$ and their dual row vectors (conjugate transposes) $v^* \in (\mathbb{C}^n)^*$ are written as bras $\langle v|$. The standard *inner product* $v^*w = \langle v, w\rangle$ on $\mathbb{C}^n$ is denoted by $\langle v|w\rangle$ and the rank one matrix vw^* is denoted by the *outer product* $|v\rangle\langle w|$. The standard basis in $\mathbb{C}^n$ is denoted by $\{|i\rangle\}_{i\in[n]}$, where $[n] := \{0, 1, \ldots, n-1\}$.

We define $\mathcal{M}_n(\mathbb{C})$ as the set of $n \times n$ complex matrices and $\mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) := \{A \in \mathcal{M}_n(\mathbb{C}) : A = A^*\}$ as the set of $n \times n$ self-adjoint complex matrices, where the conjugate transpose of $A \in \mathcal{M}_n(\mathbb{C})$ is denoted by A^*. $\mathcal{M}_n(\mathbb{R})$ and $\mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ are defined similarly for real matrices. The cone of positive semi-definite (PSD) matrices in $\mathcal{M}_n(\mathbb{C})$ is denoted by $\mathsf{PSD}_n^{\mathbb{C}}$, while the cone of real positive semidefinite matrices in $\mathcal{M}_n(\mathbb{R})$ is denoted by $\mathsf{PSD}_n^{\mathbb{R}}$. The cone of entry-wise non-negative matrices by EWP_n. The set of all linear maps $\Phi : \mathcal{M}_n(\mathbb{C}) \to \mathcal{M}_n(\mathbb{C})$ is denoted by $\mathcal{T}_n(\mathbb{C})$. In this paper, we shall overload the diag notation to denote three different things:

- For a matrix $A \in \mathcal{M}_n(\mathbb{C})$, $\mathrm{diag}(A) \in \mathcal{M}_n(\mathbb{C})$ denotes the diagonal matrix obtained by setting the off-diagonal entries of A to zero. In other words, $\mathrm{diag}(\cdot)$ is the conditional expectation from $n \times n$ matrices to the set of diagonal matrices.
- For a matrix $A \in \mathcal{M}_n(\mathbb{C})$, $\mathrm{diag}[A] \in \mathbb{C}^n$ denotes the vector containing the diagonal elements of the matrix A.
- For a vector $a \in \mathbb{C}^n$, $\mathrm{diag}\{a\} \in \mathcal{M}_n(\mathbb{C})$ denotes the diagonal matrix with the entries of the vector a on the diagonal.

In general, the meaning of the operator can be inferred from the context, but we shall consistently use the appropriate brackets for the sake of clarity. We use I_n to denote the identity matrix, and J_n to denote the matrix with all entries equal to 1. We define the vector of all ones as $|\mathbf{1}_n\rangle := \sum_{i=1}^{n} |i\rangle$ such that $|\mathbf{1}_n\rangle\langle\mathbf{1}_n| = J_n$. Finally, we introduce a specific notation that will be used frequently throughout this paper: *the removal of the diagonal part* of a matrix, denoted by

$$\mathring{A} := A - \mathrm{diag}(A) = \sum_{i \neq j} A_{ij} |i\rangle\langle j|, \quad A \in \mathcal{M}_n(\mathbb{C}).$$

8.2.2 *Convex properties of matrices*

In this section, we discuss some important convex conic subsets of matrices. Recall that the cone of *real positive-semidefinite matrices* can be characterized in two equivalent ways,

$$\mathsf{PSD}_n^{\mathbb{R}} = \mathrm{cone}\left\{ |v\rangle\langle v| \ : \ v \in \mathbb{R}^n \right\} = \left\{ X \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R}) \ : \ \langle v|X|v\rangle \geq 0, \, \forall v \in \mathbb{R}^n \right\}.$$

We use $\mathbb{R}_+^n$ to mean the set of all vectors with non-negative entries in the computational basis. Similarly, we denote by EWP_n the set of entrywise non-negative $n \times n$ matrices

$$\mathsf{EWP}_n := \left\{ X \in \mathcal{M}_n(\mathbb{R}) \ : \ X_{ij} \geq 0, \, \forall i, j \in [n] \right\},$$

as well as its symmetric counterpart $\mathsf{EWP}_n^{\mathrm{sa}} := \mathsf{EWP}_n \cap \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$.

Next, we define set of *completely positive matrices* [BSM03]

$$\mathsf{CP}_n := \mathrm{cone}\left\{ |v\rangle\langle v| \ : \ v \in \mathbb{R}_+^n \right\}.$$

The extremal rays of CP_n are easily characterized:

$$\mathrm{ext}\, \mathsf{CP}_n = \{ \mathbb{R}_+ \, |v\rangle\langle v| \ : \ v \in \mathbb{R}_+^n \}.$$

It is clear from the definition above that completely positive matrices are positive-semidefinite and entrywise positive; we call the latter set *doubly non-negative matrices*. Thus we have the inclusion,

$$\mathsf{CP}_n \subseteq \mathsf{DNN}_n := \mathsf{PSD}_n^{\mathbb{R}} \cap \mathsf{EWP}_n. \tag{50}$$

It is a remarkable fact that the above inclusion is an equality for $n \leq 4$ [BSM03, Theorem 2.4], but it is strict for $n \geq 5$. Below is an example of a doubly non-negative matrix that is not completely positive, see [BSM03, Example 2.4]:

$$X = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 1 & 6 \end{bmatrix}.$$

We also introduce the set of *copositive matrices* [SMB21]

$$\mathsf{COP}_n := \left\{ X \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R}) \,:\, \langle v|X|v\rangle \geq 0,\, \forall v \in \mathbb{R}_+^n \right\}$$

which is dual to the cone of completely positive matrices $\mathsf{CP}_n^\circ = \mathsf{COP}_n$. We recall here that the dual of the cone $C \subseteq \mathbb{R}^N$ is the cone

$$C^\circ := \{x \in \mathbb{R}^N \,:\, \langle x, y\rangle \geq 0,\, \forall y \in C\}.$$

The complete characterization of the extremal rays for copositive matrices is still an open question, and the complete solution has only been found up to dimension 6 [Hil12, AHD21].

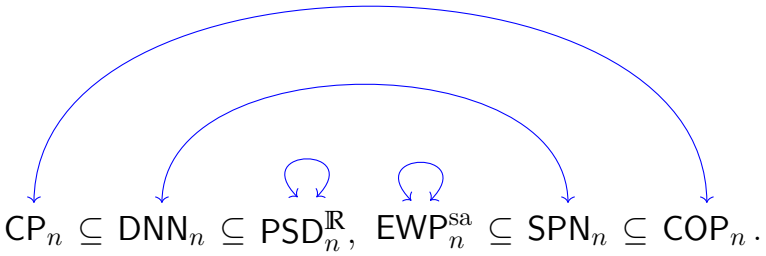
In particular, the cone of positive-semidefinite matrices is self-dual $\mathsf{PSD}_n^\circ = \mathsf{PSD}_n$, as are the cones on entrywise non-negative matrices $\mathsf{EWP}_n^\circ = \mathsf{EWP}_n$, $(\mathsf{EWP}_n^{\mathrm{sa}})^\circ = \mathsf{EWP}_n^{\mathrm{sa}}$. The dual of doubly non-negative matrices is the set

$$\mathsf{SPN}_n := \mathsf{PSD}_n^{\mathbb{R}} + \mathsf{EWP}_n^{\mathrm{sa}}. \tag{51}$$

Applying duality to Eq. (50) we obtain the reversed inclusion $\mathsf{COP}_n \supseteq \mathsf{SPN}_n$, which is an equality for $n = 4$ and strict for $n \geq 5$, see [SMB21, Chapters 2.9, 2.10]. The paradigmatic example of a copositive matrix that cannot be decomposed as the sum of a real positive semidefinite matrix and an entrywise (symmetric) non-negative matrix is the *Horn matrix*

$$H := \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}. \tag{52}$$

Combining all the following observations and dualities, we obtain the following chain of inclusions of cones, where the blue arrows indicate a duality relation:



Note that all the cones above are subsets of $\mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ and are *proper cones*: they are closed, have non-empty interior, and are pointed (they contain no line).

We provide a generalization of the completely positive cone CP_n to matrix pairs recently introduced and studied in [JM19, SN21]. Consider the convex cone of *pairwise completely positive matrices* [JM19, Definition 3.1]:

$$\mathsf{PCP}_n := \operatorname{cone}\left\{\left(\,|v\odot\bar{v}\rangle\langle w\odot\bar{w}|\,,|v\odot w\rangle\langle v\odot w|\,\right)\,:\,v,w\in\mathbb{C}^n\right\}$$

where $\odot$ denotes the Hadamard (or entrywise) product of vectors: $(v\odot w)_i = v_i w_i$. This cone lives in the vector space of pairs of matrices having the same (real) diagonal (see [SN21])

$$\mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) := \left\{(A,B)\in\mathcal{M}_n(\mathbb{R})\times\mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})\,:\,\operatorname{diag}[A]=\operatorname{diag}[B]\right\}.$$

as a *proper cone*. Indeed, we will see later that $(J_n + A, I_n + B) \in \mathsf{PCP}_n$ whenever

$$\|(A,B)\|_2^2 := \|A\|_2^2 + \|\mathring{B}\|_2^2 = \sum_{i,j}|A_{ij}|^2 + \sum_{i\neq j}|B_{ij}|^2 \leq 1,$$

which implies that $(J_n, I_n) \in int(\mathsf{PCP}_n)$, from the correspondence with the separability of diagonal unitary invariant states (Proposition 8.13) and the separability criterion in [GB02, Theorem 1]. Moreover, it is obvious that PCP_n cannot contain any line, proving that it is a proper cone.

The extremal rays of the convex cone PCP_n have been characterized in [SN21, Theorem 5.13]:

$$\operatorname{ext}\mathsf{PCP}_n = \left\{\mathbb{R}_+\left(\,|v\odot\bar{v}\rangle\langle w\odot\bar{w}|\,,|v\odot w\rangle\langle v\odot w|\,\right)\,:\,v,w\in\mathbb{C}^n\right\}. \tag{53}$$

The connection between the sets CP_n and PCP_n is given by the following result, proven in [JM19, Theorem 3.4].

Proposition 8.1. Given a matrix $A \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$, the following equivalence holds:

$$(A, A) \in \mathsf{PCP}_n \iff A \in \mathsf{CP}_n.$$

The convex dual of the cone PCP_n will be introduced and studied in detail in Section 8.3, with the goal of constructing positive maps.

8.2.3 *Convex properties of linear maps*

In this section, we provide a background on properties of linear maps that play a significant role in entanglement theory.

Definition 8.2. We define the following notions of linear maps,

1. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is called *positive* if $\mathcal{E}(X) \in \mathsf{PSD}_n^{\mathbb{C}}$ for all $X \in \mathsf{PSD}_n^{\mathbb{C}}$.
2. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is *k-positive* if the map $\mathrm{id}_k \otimes \mathcal{E} : \mathcal{M}_k \otimes \mathcal{M}_n \to \mathcal{M}_k \otimes \mathcal{M}_n$ is positive, where $\mathrm{id}_k : \mathcal{M}_k(\mathbb{C}) \to \mathcal{M}_k(\mathbb{C})$ is the identity map.

A positive map is trivially 1-positive.

Definition 8.3. Let $\top$ be the transposition map. We define the following properties of linear maps,

1. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is completely positive if it is k-positive for all $k \in \mathbb{N}$.
2. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is called *completely copositive* if $\mathcal{E} \circ \top$ is completely positive, or equivalently, $\mathcal{E} = \mathcal{X} \circ \top$ where $\mathcal{X}$ is completely positive.
3. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is called *PPT* if it is completely positive and completely copositive.
4. A completely positive linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is entanglement breaking if $\mathcal{E} \otimes \mathrm{id}_n(X)$ is separable for all $X \in \mathsf{PSD}(\mathbb{C}^n \otimes \mathbb{C}^n)$

A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ that is n-positive is completely positive. Positive, Completely positive maps, and PPT maps are closed under composition, while the completely copositive maps are not.

Definition 8.4. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is said to be decomposable if it a sum of completely positive and a copositive map, i.e $\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2 \circ \top$ where $\mathcal{E}_1, \mathcal{E}_2$ are completely positive

The paradigmatic examples of decomposable map is the identity map id, the transposition map $\top$, and the depolarizing map $\mathcal{E}(\rho) = \mathrm{Tr}(\rho)I$, and their convex sums. The convex properties of linear maps have dual connection to the convex properties of bipartite matrices. We provide these well-known duality conditions in the next theorem [HHH96, Kye23].

Theorem 8.5. The following duality conditions are true for bipartite quantum states $\rho \in \mathcal{M}_n(\mathbb{C}) \otimes \mathcal{M}_n(\mathbb{C})$ and linear maps in $\mathcal{T}_n(\mathbb{C})$.

- ρ is positive-semidefinite if and only if $\mathcal{E} \otimes \mathrm{id}_n(\rho) \geq 0$ for all completely positive maps $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$.
- ρ is PPT if and only if $\mathcal{E} \otimes \mathrm{id}_n(\rho) \geq 0$ for all decomposable maps $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$.
- ρ is separable if and only if $\mathcal{E} \otimes \mathrm{id}_n(\rho) \geq 0$ for all positive maps $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$.

Remark 8.6. A linear map is positive if it is decomposable, and in $\mathcal{T}_2(\mathbb{C})$ all positive linear maps are decomposable. On the dual side, by Theorem 8.5, it implies that all PPT states are separable.

The convex properties of linear maps can also be understood in terms of the matrix properties with the Choi-Jamiołkowski Isomorphism that provides a bijection between linear maps in matrix algebras to bipartite matrices.

Lemma 8.7 (Choi-Jamiołkowski Isomorphism [Cho75a])**.** Define the linear bijection $J : \mathcal{T}_d(\mathbb{C}) \to \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ as $J(\Phi) = \sum_{i,j=1}^{d} \Phi(|i\rangle\langle j|) \otimes |i\rangle\langle j|$. Then, $\Phi \in \mathcal{T}_d(\mathbb{C})$ is

1. hermiticity preserving if and only if $J(\Phi)$ is self-adjoint,
2. positive if and only if $J(\Phi)$ is block positive, i.e., $\langle x \otimes y|J(\Phi)|x \otimes y\rangle \geq 0 \; \forall \, |x\rangle, |y\rangle \in \mathbb{C}^d$,
3. completely positive if and only if $J(\Phi)$ is positive semi-definite,
4. completely copositive if and only if $J(\Phi)^{\Gamma}$ is positive semi-definite,
5. decomposable if and only if $\exists X_1, X_2 \geq 0 \quad$ such that $\quad J(\Phi) = X_1 + X_2^{\Gamma}$
6. entanglement breaking if and only if $J(\Phi)$ is separable.

In Lemma 8.7, part (5) appears in [Stø82], while part (6) is due to [HSR03].

8.2.4 *Linear maps and matrices with diagonal unitary symmetry*

We provide some background about the class of quantum maps and matrices that play an important role in this paper, because of their nice symmetry properties. Let us denote the group of diagonal unitary matrices with $D\mathcal{U}_n \subseteq \mathcal{U}_n$, i.e the group of matrices with complex phases on the diagonal.

$$D\mathcal{U}_n = \left\{ \mathrm{diag}\{e^{i\theta_1}, \ldots, e^{i\theta_n}\} \;\middle|\; \theta_1, \ldots, \theta_n \in \mathbb{R} \right\}.$$

Now, we introduce two notions of maps covariant with the diagonal unitary symmetries,

Definition 8.8. A linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is called

1. *diagonal unitary covariant (DUC)* if
$$\forall X \in \mathcal{M}_n(\mathbb{C}) \text{ and } \forall U \in D\mathcal{U}_n, \quad \mathcal{E}(UXU^*) = U\mathcal{E}(X)U^*$$
2. *conjugate diagonal unitary covariant (CDUC)* if
$$\forall X \in \mathcal{M}_n(\mathbb{C}) \text{ and } \forall U \in D\mathcal{U}_n, \quad \mathcal{E}(UXU^*) = \overline{U}\mathcal{E}(X)U^{\top}$$

These classes of linear maps were first introduced in [Liu14, LS15]. In [JM19, SN21] , the structure of these channels was characterized completely in terms of matrix pairs, with common diagonals. Let $\mathcal{M}_n(\mathbb{C})^{\times 2}_{\mathbb{C}^n} := \{(A,B) \in \mathcal{M}_d(\mathbb{C})^{\times 2} \mid \mathrm{diag}(A) = \mathrm{diag}(B)\}$ denote the set of such matrix pairs.

Proposition 8.9. The linear space of (conjugate) diagonal unitary covariant channels is isomorphic to matrix pairs, $\mathcal{M}_n(\mathbb{C})^{\times 2}_{\mathbb{C}^n} \cong \mathsf{DUC}_n \cong \mathsf{CDUC}_n$, with the correspondences $(A,B) \mapsto \Phi^{\mathsf{DUC}}_{A,B}$ and $(A,B) \mapsto \Phi^{\mathsf{CDUC}}_{A,B}$:

$$\Phi^{\mathsf{DUC}}_{A,B}(X) = \delta_A(X) + \mathring{B} \odot X,$$
$$\Phi^{\mathsf{CDUC}}_{A,B}(X) = \delta_A(X) + \mathring{B} \odot X^\top$$

for $X \in \mathcal{M}_n(\mathbb{C})$, where $\delta_A(X) := \mathrm{diag}\{A\,\mathrm{diag}[X]\} = \sum_{i,j=1}^n A_{ij}X_{jj}|i\rangle\langle i|$.

Remark 8.10. Note that our naming of DUC/CDUC map is **opposite** to that of [SN21, Definition 6.3]. Also note that,

- the DUC/CDUC maps $\Phi^{(\mathsf{C})\mathsf{DUC}}_{A,B}$ are hermiticity preserving if and only if the matrix pair $(A,B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}^{\mathrm{sa}}_n(\mathbb{C})$.
- the notions of DUC and CDUC maps are connected by the composition with the transpose map, i.e,
$$\Phi^{\mathsf{DUC}}_{A,B} \circ \top = \Phi^{\mathsf{CDUC}}_{A,B}$$

In relation with (C)DUC linear maps, we further introduce the following invariance properties of matrices.

Definition 8.11. A bipartite matrix $X \in \mathcal{M}_n(\mathbb{C}) \otimes \mathcal{M}_n(\mathbb{C})$ is called

1. *local diagonal unitary invariant (LDUI)* if
$$\forall U \in D\mathcal{U}_n, \quad (U \otimes U)X(U \otimes U)^* = X.$$
2. *conjugate local diagonal unitary invariant (CLDUI)* if
$$\forall U \in D\mathcal{U}_n, \quad (U \otimes \overline{U})X(U \otimes \overline{U})^* = X.$$

We denote these linear spaces by LDUI_n and CLDUI_n, following the terminology of [SN21]. We then further identify $\mathcal{M}_n(\mathbb{C})^{\times 2}_{\mathbb{C}^n} \cong \mathsf{LDUI}_n \cong \mathsf{CLDUI}_n$ via the Choi-Jamiołkowski isomorphism (Lemma 8.7) described below (see also Proposition 8.14 for related adapted notation).

Proposition 8.12 ([SN21])**.** For $\Phi \in \mathcal{T}_n(\mathbb{C})$,

- Φ is DUC if and only if $J(\Phi)$ is CLDUI. In particular, we have

$$J(\Phi^{\mathsf{DUC}}_{A,B}) = \sum_{ij} A_{ij} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{i\neq j} B_{ij} \left|ii\right\rangle\!\left\langle jj\right| =: X^{\mathsf{CLDUI}}_{A,B}, \quad (A,B) \in \mathcal{M}_n(\mathbb{C})^{\times 2}_{\mathbb{C}^n}; \tag{54}$$

- Φ is CDUC if and only if $J(\Phi)$ is LDUI. In particular, we have

$$J(\Phi^{\mathsf{CDUC}}_{A,B}) = \sum_{ij} A_{ij} \left|ij\right\rangle\!\left\langle ij\right| + \sum_{i\neq j} B_{ij} \left|ij\right\rangle\!\left\langle ji\right| =: X^{\mathsf{LDUI}}_{A,B}, \quad (A,B) \in \mathcal{M}_n(\mathbb{C})^{\times 2}_{\mathbb{C}^n}. \tag{55}$$

Under the correspondence above, pairs of matrices in PCP_n have been shown in [SN21, Lemmas 6.10, 6.11] to correspond to *entanglement breaking* (conjugate) diagonal unitary covariant maps.

Proposition 8.13. Given a pair of matrices $(A,B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$, we have

$$(A,B) \in \mathsf{PCP}_n \iff \Phi^{(\mathsf{C})\mathsf{DUC}}_{A,B} \text{ is entanglement breaking} \iff X^{(\mathsf{C})\mathsf{LDUI}}_{A,B} \text{ is separable.}$$

We end this section by recalling the following definition and result from [SN21], characterizing the stronger notion of *complete positivity* for $(\mathsf{C})\mathsf{DUC}$ maps.

Proposition 8.14. Consider the following cones:

$$\mathsf{LDUI}^+_n := \left\{ (A,B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) \ : \ A \in \mathsf{EWP}_n,\ A_{ij}A_{ji} \geq |B_{ij}|^2 \,\forall\, i \neq j \right\}.$$
$$\mathsf{CLDUI}^+_n := \left\{ (A,B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) \ : \ A \in \mathsf{EWP}_n,\ B \in \mathsf{PSD}^{\mathbb{C}}_n, \right\}.$$

Then we have

$$\begin{aligned}(A,B)\in \mathsf{LDUI}_n^+ &\iff \Phi_{A,B}^{\mathsf{CDUC}} \text{ is completely positive}\\ &\iff \Phi_{A,B}^{\mathsf{DUC}} \text{ is completely copositive} \iff X_{A,B}^{\mathsf{LDUI}}\geq 0,\\ (A,B)\in \mathsf{CLDUI}_n^+ &\iff \Phi_{A,B}^{\mathsf{DUC}} \text{ is completely positive}\\ &\iff \Phi_{A,B}^{\mathsf{CDUC}} \text{ is completely copositive} \iff X_{A,B}^{\mathsf{CLDUI}}\geq 0.\end{aligned}$$

Proof. The inclusions follows from easily from Definition 8.16, while the equivalence is proven in [SN21, Lemma 2.12], see also [NS21, Lemma 7.6] or [JM19, Theorem 5.2] ■

Proposition 8.15. Consider the following cone of pairwise doubly non-negative matrices:

$$\mathsf{PDNN}_n := \left\{(A,B)\in \mathcal{M}_n(\mathbb{R})\underset{\mathbb{R}^n}{\times}\mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) \,:\, A\in\mathsf{EWP}_n,\, B\in\mathsf{PSD}_n^{\mathbb{C}},\, \forall i,j\ A_{ij}A_{ji}\geq |B_{ij}|^2\right\}.$$

Then we have

$$(A,B)\in\mathsf{PDNN}_n \iff \Phi_{A,B}^{(\mathsf{C})\mathsf{DUC}} \text{ is PPT} \iff X_{A,B}^{(\mathsf{C})\mathsf{LDUI}} \text{ is PPT}.$$

Proof. The equivalence follows from [SN21, Lemma 6.11,6.12] ■

Finally, we introduce a subclass of LDUI states called the (mixture of) Dicke states [Yu16, TAQ+18, SN21], which will be of our main interest in Section 8.8. Recall that the symmetric space $\mathbb{C}^n\vee\mathbb{C}^n\subset(\mathbb{C}^n)^{\otimes 2}$ has an orthonormal basis $\{|\psi_{ij}\rangle\}_{1\leq i\leq j\leq n}$ (called *Dicke basis*) where

$$|\psi_{ij}\rangle := \begin{cases}(|ij\rangle+|ji\rangle)/\sqrt{2} & \text{if } i<j,\\ |ii\rangle & \text{if } i=j.\end{cases}$$

Bipartite positive semidefinite matrices which are diagonal in the Dicke basis

$$X=\sum_{1\leq i\leq j\leq n} Y_{ij}|\psi_{ij}\rangle\langle\psi_{ij}|\in\mathcal{B}(\mathbb{C}^n\vee\mathbb{C}^n),\quad Y_{ij}\in\mathbb{R}_+,$$

are called *Dicke states* (or *diagonal symmetric matrices*). By taking $P\in\mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ as

$$P_{ij}=\begin{cases}Y_{ij}/2 & \text{if } i<j,\\ Y_{ji}/2 & \text{if } j<i,\\ Y_{ii} & \text{if } i=j,\end{cases}$$

we have $X = X^{\mathsf{LDUI}}_{P,P}$. From [SN21, Example 3.4], we conclude that

$$\begin{aligned} X^{\mathsf{LDUI}}_{P,P} \text{ is positive semidefinite} &\iff P \in \mathsf{EWP}^{\mathrm{sa}}_n, \\ X^{\mathsf{LDUI}}_{P,P} \text{ is PPT} &\iff P \in \mathsf{DNN}_n, \\ X^{\mathsf{LDUI}}_{P,P} \text{ is separable} &\iff P \in \mathsf{CP}_n. \end{aligned}$$

In particular, when $n \leq 4$, every bipartite Dicke state is separable if and only if PPT while when $n \geq 5$, every $P \in \mathsf{DNN}_n \setminus \mathsf{CP}_n$ gives rise to a PPT entangled Dicke state $X^{\mathsf{LDUI}}_{P,P}$.

8.3 PAIRWISE COPOSITIVITY

We introduce and study in this section the set of *pairwise copositive matrices*, which is the generalization of the cone of copositive matrices COP_n to the setting of pairs of matrices, in the same way as pairwise completely positive matrices PCP_n generalize completely positive matrices CP_n. Recall that to a matrix X we associate its diagonal-less version $\mathring{X}$

$$\mathring{X} = X - \mathrm{diag}(X) \qquad \text{or} \qquad \mathring{X}_{ij} = \mathbb{1}_{i \neq j} X_{ij}.$$

Definition 8.16. Define the set of *pairwise copositive matrices* as $\mathsf{PCOP}_n :=$

$$\left\{ (A, B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}^{\mathrm{sa}}_n(\mathbb{C}) \,:\, \langle v \odot \bar{v} | A | w \odot \bar{w} \rangle + \langle v \odot w | \mathring{B} | v \odot w \rangle \geq 0,\ \forall v, w \in \mathbb{C}^n \right\}.$$

Proposition 8.17. The set PCOP_n is a proper convex cone, dual to PCP_n:

$$\mathsf{PCOP}_n = \mathsf{PCP}^{\circ}_n.$$

Proof. The convexity property follows immediately from the definition. For the duality claim, let us first write down explicitly the (natural) scalar product on the vector space $\mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}^{\mathrm{sa}}_n(\mathbb{C})$:

$$\langle (A_1, B_1), (A_2, B_2) \rangle = \langle A_1, A_2 \rangle + \langle \mathring{B}_1, \mathring{B}_2 \rangle = \langle \mathring{A}_1, \mathring{A}_2 \rangle + \langle B_1, B_2 \rangle \,, \tag{56}$$

using the Euclidean (or Hilbert-Schmidt) scalar product on $n \times n$ matrices. The duality follows now directly from the from of the extremal rays of the PCP_n cone (53) and from the fact that $\langle \mathring{X}, Y \rangle = \langle \mathring{X}, \mathring{Y} \rangle$ for arbitrary matrices X, Y. Finally, the fact that PCOP_n is a proper cone follows from the established duality and the fact that PCP_n is proper. ∎

Proposition 8.18. Given a pair of matrices $(A, B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$, we have

$$\langle vw|X_{A,B}^{\mathsf{LDUI}}|vw\rangle = \langle v\odot\overline{v}|A|w\odot\overline{w}\rangle + \langle v\odot\overline{w}|\mathring{B}|v\odot\overline{w}\rangle, \tag{57}$$

$$\langle vw|X_{A,B}^{\mathsf{CLDUI}}|vw\rangle = \langle v\odot\overline{v}|A|w\odot\overline{w}\rangle + \langle v\odot w|\mathring{B}|v\odot w\rangle, \tag{58}$$

for $v, w \in \mathbb{C}^n$ and $|vw\rangle := |v\otimes w\rangle$.

Proof. We first consider the *LDUI-twirling*

$$\mathcal{T}_{\mathsf{LDUI}}(X) = \mathcal{T}_{D\mathcal{U}_n^{\otimes 2}}(X) := \int_{D\mathcal{U}_n} (U\otimes U)X(U\otimes U)^* dU, \quad X \in \mathcal{M}_n(\mathbb{C})^{\otimes 2}, \tag{59}$$

where dU denotes the normalized Haar measure on $D\mathcal{U}_n$. Then $\mathcal{T}_{\mathsf{LDUI}}$ can be considered as a orthogonal projection of $\mathcal{M}_n(\mathbb{C})^{\otimes 2}$ onto the linear space LDUI_n (we refer to [SN21, PJPY24] for general properties of twirling maps). Furthermore, we have

$$\begin{aligned}
\forall\, X \in \mathcal{M}_n(\mathbb{C})^{\otimes 2}, &\quad X \in \mathsf{LDUI}_n \iff \mathcal{T}_{\mathsf{LDUI}}(X) = X,\\
\forall\, X, Y \in \mathcal{M}_n(\mathbb{C})^{\otimes 2}, &\quad \mathrm{Tr}(X\mathcal{T}_{\mathsf{LDUI}}(Y)) = \mathrm{Tr}(\mathcal{T}_{\mathsf{LDUI}}(X)Y) = \mathrm{Tr}(\mathcal{T}_{\mathsf{LDUI}}(X)\mathcal{T}_{\mathsf{LDUI}}(Y)),\\
\forall\, v, w \in \mathbb{C}^n, &\quad \mathcal{T}_{\mathsf{LDUI}}(|vw\rangle\langle vw|) = X^{\mathsf{LDUI}}_{|v\odot\bar{v}\rangle\langle w\odot\bar{w}|,|v\odot\bar{w}\rangle\langle v\odot\bar{w}|},
\end{aligned}$$

where the first two facts follows from [PJPY24, Section 2.3] and the last fact is from [SN21, Remark 5.16]. Now we show the proof of the first equation by the following computations.

$$\begin{aligned}
\langle vw \mid X_{A,B}^{\mathsf{LDUI}} \mid vw\rangle &= \mathrm{Tr}\Big(\,|vw\rangle\langle vw|\, X_{A,B}^{\mathsf{LDUI}}\Big)\\
&= \mathrm{Tr}\Big(\,|vw\rangle\langle vw|\, \mathcal{T}_{\mathsf{LDUI}}(X_{A,B}^{\mathsf{LDUI}})\Big)\\
&= \mathrm{Tr}\Big(\,\mathcal{T}_{\mathsf{LDUI}}(|vw\rangle\langle vw|)\, X_{A,B}^{\mathsf{LDUI}}\Big)\\
&= \mathrm{Tr}\Big(X^{\mathsf{LDUI}}_{|v\odot\overline{v}\rangle\langle w\odot\overline{w}|,|v\odot\overline{w}\rangle\langle v\odot\overline{w}|}\, X_{A,B}^{\mathsf{LDUI}}\Big)\\
&= \langle v\odot\overline{v}|A|w\odot\overline{w}\rangle + \langle v\odot\overline{w}|\mathring{B}|v\odot\overline{w}\rangle.
\end{aligned}$$

The second formula can be shown similarly via the *CLDUI-twirling*

$$\mathcal{T}_{\mathsf{CLDUI}}(X) := \int_{D\mathcal{U}_n} (U\otimes\overline{U})X(U\otimes\overline{U})^* dU, \quad X \in \mathcal{M}_n(\mathbb{C})^{\otimes 2}, \tag{60}$$

which is left to the reader. ∎

In [SN21, Theorem 6.6] it was shown that elements in PCOP corresponds to *positive* conjugate diagonal unitary covariant maps, a dual result to Proposition 8.13.

Proposition 8.19. Given a pair of matrices $(A, B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$, we have

$$(A, B) \in \mathsf{PCOP}_n \iff \Phi_{A,B}^{\mathsf{(C)DUC}} \text{ is positive} \iff X_{A,B}^{\mathsf{(C)LDUI}} \text{ is block-positive.}$$

Proof. Assume that $(A, B) \in \mathsf{PCOP}_n$. Then, by Proposition 8.18, we get

$$\forall v, w \in \mathbb{C}^n \quad \langle vw|X_{A,B}^{\mathsf{LDUI}}|vw\rangle = \langle v \odot \overline{v}|A|w \odot \overline{w}\rangle + \langle v \odot \overline{w}|\mathring{B}|v \odot \overline{w}\rangle \geq 0$$

This is equivalent to the condition that that $X_{A,B}^{\mathsf{LDUI}}$ is block-positive $\iff$ $\Phi_{A,B}^{\mathsf{CDUC}}$ is positive [EK00]. ∎

We further collect in the following proposition some simple results about the convex cone PCOP.

Proposition 8.20. For every pair $(A, B) \in \mathsf{PCOP}_n$, the following implications hold:

1. $A \in \mathsf{EWP}_n$.
2. $\forall i \neq j \in [n] \quad \sqrt{A_{ii}A_{jj}} + \sqrt{A_{ij}A_{ji}} - |B_{ij}| \geq 0$.
3. $(A + \mathring{B}) + (A + \mathring{B})^\top = A + A^\top + 2\,\mathrm{Re}(\mathring{B}) \in \mathsf{COP}_n$.
4. $(D_1^* D_1 A D_2^* D_2, D_1^* D_2^* B D_1 D_2) \in \mathsf{PCOP}_n$ for any complex diagonal matrices D_1 and D_2.

Regarding diagonal elements of the pair and the connection to the PCP cone, we have:

5. $(A, \mathrm{diag}(A)) \in \mathsf{PCOP}_n \iff A \in \mathsf{EWP}_n \iff (A, \mathrm{diag}(A)) \in \mathsf{PCP}_n$.
6. $(\mathrm{diag}(B), B) \in \mathsf{PCOP}_n \iff B \in \mathsf{PSD}_n^{\mathbb{C}}$.
7. $(\mathrm{diag}(B), B) \in \mathsf{PCP}_n \iff B = \mathrm{diag}\, B$.

Regarding identical elements in the pair, we have:

8. $(A, A) \in \mathsf{PCOP}_n \iff A \in \mathsf{EWP}_n^{\mathrm{sa}} \iff X_{A,A}^{\mathsf{LDUI}} \geq 0$.

Proof. From the definition of PCOP_n we have

$$\langle v \odot \bar{v}|A|w \odot \bar{w}\rangle + \langle v \odot w|\mathring{B}|v \odot w\rangle \geq 0, \ \forall v, w \in \mathbb{C}^n. \tag{61}$$

For Items 1 and 2, we refer to [SN21, Proposition 6.7].

To show Item 3, we replace in Eq. (61), $v = z, w = \bar{z} \in \mathbb{C}^n$.We get

$$\langle z \odot \bar{z}|A + \mathring{B}|z \odot \bar{z}\rangle \geq 0, \quad \forall z \in \mathbb{C}^n \iff \langle p|(A + \mathring{B}) + (A + \mathring{B})^\top|p\rangle \geq 0, \quad \forall p \in \mathbb{R}^n_+. \tag{62}$$

This implies $(A + \mathring{B}) + (A + \mathring{B})^\top = A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{COP}_n$.

Item 4 follows from the substitution $v \mapsto D_1 v = \mathrm{diag}[D_1] \odot v$ and $w \mapsto D_2 w = \mathrm{diag}[D_2] \odot w$ in Eq. (61), in which case $D_1 v \odot \overline{D_1 v} = D_1^* D_1 (v \odot \overline{v})$ and $D_1 v \odot D_2 w = D_1 D_2 (v \odot w)$.

Item 5 follows immediately since $\mathring{B} = 0$, while Item 6 and Item 7 follow from $\mathring{A} = 0$.

Finally, Item 8 follows from Item 1 and Proposition 8.14. ■

Remark 8.21. The results regarding pairs of matrices (A, B) where either A or B are diagonal can be understood in terms of the corresponding linear maps as follows.

- Item 5: A "classical" map $\Phi^{(\mathsf{C})\mathsf{DUC}}_{A,\mathrm{diag}(A)}(X) = \mathrm{diag}\{A\,\mathrm{diag}[X]\}$ is positive $\iff$ it is completely positive $\iff$ it is entanglement breaking.
- Item 6: A (transpose-)Schur product map $\Phi^{\mathsf{DUC}}_{\mathrm{diag}(B),B}(X) = B \odot X$ (resp. $\Phi^{\mathsf{CDUC}}_{\mathrm{diag}(B),B}(X) = B \odot X^\top$) is positive $\iff$ it is completely positive (resp. completely co-positive).
- Item 7: A (transpose-)Schur product map $\Phi^{\mathsf{CDUC}}_{\mathrm{diag}(B),B}(X) = B \odot X^\top$ is entanglement breaking $\iff$ it is "classical" (i.e. only takes into account the diagonal of the input).

Remark 8.22. We have seen in Proposition 8.1 that $(A, A) \in \mathsf{PCP}_n \iff A \in \mathsf{CP}_n$. From Item 8 above, it follows that a similar property does not hold for PCOP_n and COP_n. In the language of linear maps, the result from Item 8 translates to the fact that the linear DUC map

$$\Phi^{\mathsf{DUC}}_{A,A}(X) = \mathrm{diag}\{A\,\mathrm{diag}[X]\} + \mathring{A} \odot X$$

is positive if and only if it is completely positive.

Recall that $\Phi^{\mathsf{DUC}}_{A,B}$ (resp. $\Phi^{\mathsf{DUC}}_{A,B}$) is completely positive (resp. completely copositive), if $(A,B) \in \mathsf{CLDUI}^+_n$. An important example of element in the PCOP cone, different that the ones one might construct using Proposition 8.14, is given below.

Example 8.23. We have $(\mathring{N}, -\mathring{N}) \in \mathsf{PCOP}_n$ for any $N \in \mathsf{EWP}^{\mathrm{sa}}_n$. Indeed, for $v, w \in \mathbb{C}^n$, one has

$$\begin{aligned}\langle v \odot \bar{v}|\mathring{N}|w \odot \bar{w}\rangle - \langle v \odot w|\mathring{N}|v \odot w\rangle &= \sum_{i\neq j} N_{ij}|v_i|^2|w_j|^2 - \sum_{i\neq j} N_{ij}\bar{v}_i\bar{w}_i v_j w_j \\ &= \sum_{i<j} N_{ij}(|v_i|^2|w_j|^2 + |v_j|^2|w_i|^2 - \bar{v}_i\bar{w}_i v_j w_j - \bar{v}_j\bar{w}_j v_i w_i) \\ &= \sum_{i<j} N_{ij}|v_i\bar{w}_j - v_j\bar{w}_i|^2 \geq 0.\end{aligned}$$

In particular, $(\mathring{J}_n, -\mathring{J}_n) \in \mathsf{PCOP}_n$. Note that since $-\mathring{N} \notin \mathsf{PSD}^{\mathbb{C}}_n$ unless $\mathring{N} = 0$, we have

$$(\mathring{N}, -\mathring{N}) \in \mathsf{PCOP}_n \setminus \mathsf{CLDUI}^+_n.$$

This example is the main motivation for the rest of the paper: we shall consider perturbations of the $\mathring{N}$ matrix appearing the first and in the second slot of the pair, yielding interesting examples of PCOP pairs, and in effect, positive maps.

We complete this section by providing the characterizations of pairwise copositivity in terms of copositivity, which generalize Item 3 of Proposition 8.20. First, for $A \in \mathsf{EWP}_n$, let us denote by

$$\tilde{A} := (A \odot A^\top)^{\odot 1/2} = (\sqrt{A_{ij}A_{ji}})_{1\leq i,j\leq n}.$$

Theorem 8.24. If a pair $(A,B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}^{\mathrm{sa}}_n(\mathbb{C})$ satisfies $A \in \mathsf{EWP}_n$ and $\tilde{A} + \mathrm{Re}(U^*\mathring{B}U) \in \mathsf{COP}_n$ for every $U \in D\mathcal{U}_n$, then $(A,B) \in \mathsf{PCOP}_n$. In particular, for $A \in \mathcal{M}^{\mathrm{sa}}_n(\mathbb{R})$ *real symmetric*,

$$(A,B) \in \mathsf{PCOP}_n \iff A \in \mathsf{EWP}_n \text{ and } A + \mathrm{Re}(U^*\mathring{B}U) \in \mathsf{COP}_n \ \ \forall U \in D\mathcal{U}_n$$

Proof. For $v, w \in \mathbb{C}^n$, let us write $v \odot w = Up$ where $p \in \mathbb{R}^n_+$ and $U \in D\mathcal{U}_n$. Then we have

$$\begin{aligned}\langle v \odot \bar{v}|A\Big|w \odot \bar{w}\rangle + \langle v \odot w|\mathring{B}|v \odot w\rangle &= \sum_{i,j} A_{ij}|v_i|^2|w_j|^2 + \langle p|U^*\mathring{B}U|p\rangle \\ &= \sum_{i<j}(A_{ij}p_j^2\frac{|v_i|^2}{|v_j|^2} + A_{ji}p_i^2\frac{|v_j|^2}{|v_i|^2}) + \langle p|U^*BU|p\rangle \\ &\geq \sum_{i<j} 2\sqrt{A_{ij}A_{ji}}p_ip_j + \langle p|U^*BU|p\rangle \\ &= \langle p\Big|\tilde{A} + \mathrm{Re}(U^*\mathring{B}U)\Big|p\rangle \geq 0,\end{aligned}$$

where in the second inequality, we use that $\mathrm{diag}(A) = \mathrm{diag}(B) = U^* \mathrm{diag}(B)U$ and in the next step the AM-GM inequality. This shows the first assertion.

The direction ($\Longleftarrow$) of the second assertion now follows from the first by noting that $\tilde{A} = A$ since A is a real symmetric matrix. For the other direction ($\Longrightarrow$), note that $(A, U^*BU) \in \mathsf{PCOP}_n$ for all $U \in D\mathcal{U}_n$ from Proposition 8.20, Item 4, with $D_1 = U$ and $D_2 = I_n$. Therefore, we conclude by applying Proposition 8.20, Item 3. ■

The corollary below would play a key role in the next section. Let us first denote by $D\mathcal{O}_n := \left\{O \in D\mathcal{U}_n : \mathrm{diag}[O] \in \{\pm 1\}^n\right\}$ the finite group of *diagonal orthogonal matrices*.

Corollary 8.25. If (A, B) satisfies $A \in \mathsf{EWP}_n$, $B \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$, and $\tilde{A} + O\mathring{B}O \in \mathsf{COP}_n$ for every $O \in D\mathcal{O}_n$, then $(A, B) \in \mathsf{PCOP}_n$. In particular, for $A, B \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ *real symmetric*,

$$(A, B) \in \mathsf{PCOP}_n \iff A \in \mathsf{EWP}_n \text{ and } A + O\mathring{B}O \in \mathsf{COP}_n \ \forall O \in D\mathcal{O}_n.$$

Proof. We only need to show the first assertion. First of all, for all D real diagonal, we can write $D = OP = PO$ for some P a nonnegative diagonal matrix and $O \in D\mathcal{O}_n$. Then $|D| := \sqrt{D^*D} = P$ and hence the assumption implies that

$$|D|\tilde{A}|D| + D\mathring{B}D = P(\tilde{A} + O\mathring{B}O)P \in \mathsf{COP}_n. \tag{63}$$

Now for $U \in D\mathcal{U}_n$, let us write $U = D_1 + iD_2 \in D\mathcal{U}_n$ with D_1, D_2 real diagonal (hence $D_1^2 + D_2^2 = I_n$). We claim that for all $A \in \mathsf{EWP}_n$, we have $\tilde{A} - |D_1|\tilde{A}|D_1| - |D_2|\tilde{A}|D_2| \in \mathsf{EWP}_n^{\mathrm{sa}}$. To show this, we use the AM-GM inequality and the fact that $D_1^2 + D_2^2 = I_n$:

$$\forall i, j \in [n], \qquad |D_1|_{ii}|D_1|_{jj} + |D_2|_{ii}|D_2|_{jj} \leq \frac{|D_1|_{ii}^2 + |D_1|_{jj}^2}{2} + \frac{|D_2|_{ii}^2 + |D_2|_{jj}^2}{2} = 1. \tag{64}$$

Then, since B is real, we have

$$\begin{aligned}\widetilde{A} + \mathrm{Re}(U^*\mathring{B}U) &= \widetilde{A} + D_1\mathring{B}D_1 + D_2\mathring{B}D_2 \\ &= \underbrace{\left(|D_1|\widetilde{A}|D_1| + D_1\mathring{B}D_1\right)}_{\mathsf{COP}_n \text{ by Eq. (63)}} + \underbrace{\left(|D_2|\widetilde{A}|D_2| + D_2\mathring{B}D_2\right)}_{\mathsf{COP}_n \text{ by Eq. (63)}} \\ &+ \underbrace{\left(\widetilde{A} - |D_1|\widetilde{A}|D_1| - |D_2|\widetilde{A}|D_2|\right)}_{\mathsf{EWP}_n^{\mathrm{sa}} \text{ by Eq. (64)}}\end{aligned}$$

This shows that $\widetilde{A} + \mathrm{Re}(U^*\mathring{B}U)$ is copositive, and then the first claim follows now from Theorem 8.24. ■

8.4 LIFTING COPOSITIVITY TO PAIRWISE COPOSITIVITY

In this section, we study the membership problem for the cone PCOP in the case of several classes of pairs of matrices. Many of the results in this section are focused on establishing an equivalence with the membership problem for the cone of copositive matrices COP. Another motivation is the generalization of Example 8.23 to pairs where we perturb the second component by small amount of matrix, which turns out to be copositive.

More precisely, we apply Corollary 8.25 to obtain the following main result of this section, an efficient method to generate a wide family of pairs in PCOP_n lifted from a *single* copositive matrix.

Theorem 8.26. Suppose $M, N \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ satisfy $\mathrm{diag}(N) = \mathrm{diag}(M)$, $N \in \mathsf{EWP}_n^{\mathrm{sa}}$, and $N_{ij} \geq \frac{1}{2}M_{ij}$ for all $i \neq j \in [n]$. Then

$$M \in \mathsf{COP}_n \iff (N, M - \mathring{N}) \in \mathsf{PCOP}_n.$$

In particular, denoting $(M_+)_{ij} := \max(M_{ij}, 0)$ and $(M_-)_{ij} := -\min(M_{ij}, 0)$, we have

$$\begin{aligned}M \in \mathsf{COP}_n &\iff \frac{1}{2}(M_+ + \mathrm{diag}(M), M_+ - 2M_- + \mathrm{diag}(M)) \in \mathsf{PCOP}_n \\ &\iff (M_+, \mathrm{diag}(M) - M_-) \in \mathsf{PCOP}_n.\end{aligned}$$

In a similar vein, for all $\lambda \geq \frac{1}{2}\max(0, \max(\mathring{M}))$, we have

$$M \in \mathsf{COP}_n \iff (\mathrm{diag}(M) + \lambda\mathring{J}_n, M - \lambda\mathring{J}_n) \in \mathsf{PCOP}_n.$$

Proof. The direction ($\Longleftarrow$) of the first statement follows from Item 3 from Proposition 8.20 as

$$N + N^\top + 2\,\mathrm{Re}(\mathring{M} - \mathring{N}) = 2M \in \mathsf{COP}_n.$$

For the direction ($\Longrightarrow$), let $O \in D\mathcal{O}_n$ and let us decompose $O = O_+ - O_-$ such that both $O_\pm$ are diagonal matrices with entries either 0 or 1 and $O_+O_- = 0$. Also, note that $O_+ + O_- = I_n$. Then since $2N - M \in \mathsf{EWP}_n^{\mathrm{sa}}$, we have the following decomposition into sum of copositive matrices

$$\begin{aligned} N + O(\mathring{M} - \mathring{N})O &= (N - ONO) + OMO = 2(O_+NO_- + O_-NO_+) + OMO \\ &= \underbrace{\big(O_+(2N - M)O_- + O_-(2N - M)O_+\big)}_{\mathsf{EWP}_n^{\mathrm{sa}} \subseteq \mathsf{COP}_n} + \underbrace{O_+MO_+}_{\mathsf{COP}_n} + \underbrace{O_-MO_-}_{\mathsf{COP}_n} \in \mathsf{COP}_n. \end{aligned}$$

Since this is true for all $O \in D\mathcal{O}_n$, we have by Corollary 8.25 that $(N, M - \mathring{N}) \in \mathsf{PCOP}_n$.

Now the second and third assertions simply follows from the first statement with $N = \frac{1}{2}(M_+ + \mathrm{diag}(M))$, $N = M_+$ (note that $\mathrm{diag}(M_+) = \mathrm{diag}(M)$, $\mathrm{diag}(M_-) = 0$, and $M = M_+ - M_-$), and $N = \mathrm{diag}(M) + \lambda\mathring{J}$, respectively. ∎

Remark 8.27. The first statement of Theorem 8.26 can be interpreted as follows: for any fixed copositive matrix M, one can generate the family

$$\mathcal{F}_M = \Big\{(N, M - \mathring{N}) : N \in \mathsf{EWP}_n^{\mathrm{sa}},\ \mathrm{diag}(N) = \mathrm{diag}(M),\ \text{and } N_{ij} \geq \frac{1}{2}M_{ij}\ \forall\, i \neq j\Big\}$$

of pairs in PCOP_n. In other words, any pair $(N, M - \mathring{N}) \in \mathcal{F}_M$ defines positive linear maps $\Phi^{(\mathsf{C})\mathsf{DUC}}_{N, M-\mathring{N}}$. Note that this family is both simple and rich, in the sense that it allows for $(n^2 - n)/2$ *degrees of freedom* in the choice of the upper off-diagonal entries $(N_{ij})_{1 \leq i < j \leq n}$. In the remainder of the paper, we will show that this construction indeed generates a broad class of *positive indecomposable* linear maps and *entanglement witnesses* capable of detecting entanglement in PPT states that are arbitrarily close to separable ones.

Example 8.28. For the Horn matrix H defined in Eq. (52), the last assertion in Theorem 8.26 implies that

$$(I_5 + \lambda\mathring{J}_5, H - \lambda\mathring{J}_5) \in \mathsf{PCOP}_5 \text{ whenever } \lambda \geq \tfrac{1}{2}.$$

We show that the condition $\lambda \geq \frac{1}{2}$ is also necessary (see also Example 8.37), which implies that the lower bound $\lambda \geq \frac{1}{2}\max(0, \max(\mathring{M}))$ in the previous theorem

is *tight* as a multiple of $\max(0, \max(\mathring{M}))$. Indeed, for $t \geq 0$ we may choose $v = (1, 0, t, t, 0)^\top$ and $w = (-1, 0, t, t, 0)^\top$ to compute that

$$\langle v^{\odot 2} | I_5 + \lambda \mathring{J}_5 | w^{\odot 2} \rangle + \langle v \odot w | \mathring{H} - \lambda \mathring{J}_5 | v \odot w \rangle = 1 + 4t^2(2\lambda - 1).$$

Thus, the condition $(I_5 + \lambda \mathring{J}_5, H - \lambda \mathring{J}_5) \in \mathsf{PCOP}_5$ implies that $2\lambda - 1 \geq -\frac{1}{4t^2}$ for all $t > 0$. By taking $t \to \infty$, we obtain $\lambda \geq 1/2$.

On the other hand, the bound $\lambda \geq \frac{1}{2} \max(0, \max(\mathring{M}))$ from Theorem 8.26 is *not tight* in another perspective: if $M \in \mathsf{PSD}_n^{\mathbb{R}}$, then $(\operatorname{diag}(M) + \lambda \mathring{J}, M - \lambda \mathring{J}) \in \mathsf{PCOP}_n$ for all $\lambda \geq 0$ (see Item 6 in Proposition 8.20) while $\max(\mathring{M}) > 0$ whenever M has positive off-diagonal elements.

The simple corollary below will be used later in Section 8.7 to establish the positivity of linear maps defined by graphs.

Corollary 8.29. Let $A \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ such that $I - A \in \mathsf{EWP}_n$. Then

$$(\operatorname{diag}(A) + \mathring{J}_n, A) \in \mathsf{PCOP}_n \quad \iff \quad A + \mathring{J}_n \in \mathsf{COP}_n.$$

8.5 PAIRWISE DECOMPOSABILITY

Between the class of positive linear maps and the one of completely positive maps lies the important intermediate class of decomposable maps. We study in this section the corresponding cone of pairs of matrices and connect it to decomposable maps in operator algebra. Recall that a linear map $\mathcal{E} \in \mathcal{T}_n(\mathbb{C})$ is called decomposable if we can write $\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2 \circ \top$, for some CP maps $\mathcal{E}_1$ and $\mathcal{E}_2$. To study decomposable diagonal unitary covariant linear maps, we introduce the following set:

Definition 8.30. Define the set of *pairwise decomposable matrices* PDEC_n as the set of pairs $(A, B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$ having the following properties:

- $A \in \mathsf{EWP}_n$
- $B = B^{(1)} + B^{(2)}$ with $B^{(1)} \in \mathsf{PSD}_n^{\mathbb{C}}$ and $B^{(2)} \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$ such that $B^{(2)}_{ii} \geq 0$ for all $i \in [n]$ and $|B^{(2)}_{ij}|^2 \leq A_{ij} A_{ji}$ for all $i \neq j \in [n]$.

Note from the definition that

$$(A,B)\in\mathsf{PDEC}_n \iff (\tilde{A},B)=\left((A\odot A^\top)^{\odot 1/2},B\right)\in\mathsf{PDEC}_n, \tag{65}$$

which is not true in general for $(A,B)\in\mathsf{PCOP}_n$ (we refer to Section 8.6).

We first characterize the decomposability property of (conjugate) diagonal unitary covariant maps.

Proposition 8.31. The following statements are equivalent:

1. $\Phi_{A,B}^{(\mathsf{C})\mathsf{DUC}}$ is decomposable.
2. $(A,B)\in\mathsf{PDEC}_n$.

Proof. Since $\Phi_{A,B}^{\mathsf{DUC}}\circ\top=\Phi_{A,B}^{\mathsf{CDUC}}$ and since decomposability is invariant under the composition with transposition, we may only consider $\Phi_{A,B}^{\mathsf{DUC}}$.

((1)⇒(2)) Assume $\Phi_{A,B}^{\mathsf{DUC}}$ is a decomposable linear map, $\Phi_{A,B}^{\mathsf{DUC}}=\mathcal{E}_1+\mathcal{E}_2$ where $\mathcal{E}_1,\mathcal{E}_2$ are (resp.) completely positive and completely copositive maps. We use the DUC-twirling map

$$\mathcal{T}_{\mathsf{DUC}}(\mathcal{E})(\cdot):=\int_{\mathcal{DU}_n}U^*\mathcal{E}(U\cdot U^*)U\,dU$$

on both sides, and we have by [PJPY24, Proposition 2.1],

$$\mathcal{T}_{\mathsf{DUC}}(\Phi_{A,B}^{\mathsf{DUC}})=\mathcal{T}_{\mathsf{DUC}}(\mathcal{E}_1)+\mathcal{T}_{\mathsf{DUC}}(\mathcal{E}_2)\implies\Phi_{A,B}^{\mathsf{DUC}}=\Phi_{A_1,B_1}^{\mathsf{DUC}}+\Phi_{A_2,B_2}^{\mathsf{DUC}} \tag{66}$$

for CP map $\Phi_{A_1,B_1}^{\mathsf{DUC}}$ and a co-CP map $\Phi_{A_2,B_2}^{\mathsf{DUC}}$. Now it is straightforward to verify that $B^{(i)}=B_i$, $i=1,2$, satisfy the conditions above. For the reverse direction **((2)⇒(1))**, we construct a decomposition

$$(A,B)=(\operatorname{diag}B^{(1)},B^{(1)})+(A-\operatorname{diag}B^{(1)},B^{(2)})$$

which gives us a decomposition into completely positive and a completely copositive map. ∎

Below, the implications in the first row can be either verified by hand from the definitions, or obtained from Proposition 8.19, 8.14, and 8.31 from the obvious implications in the second row.

$$
\begin{array}{ccccccc}
(A,B) \in \mathsf{PCP}_n & \Longrightarrow & \begin{cases} (A,B) \in \mathsf{LDUI}_n^+ \text{ or} \\ (A,B) \in \mathsf{CLDUI}_n^+ \end{cases} & \Longrightarrow & (A,B) \in \mathsf{PDEC}_n & \Longrightarrow & (A,B) \in \mathsf{PCOP} \\
\Updownarrow & & \Updownarrow & & \Updownarrow & & \Updownarrow \\
\Phi_{A,B}^{(\mathsf{C})\mathsf{DUC}} \text{ is EB} & \Longrightarrow & \begin{cases} \Phi_{A,B}^{\mathsf{CDUC}} \text{ is CP or} \\ \Phi_{A,B}^{\mathsf{DUC}} \text{ is CP} \end{cases} & \Longrightarrow & \Phi_{A,B}^{(\mathsf{C})\mathsf{DUC}} \text{ is dec.} & \Longrightarrow & \Phi_{A,B}^{(\mathsf{C})\mathsf{DUC}} \text{ is positiv}
\end{array}
$$

We start with an example directly strengthening Example 8.23, obtained by taking $A = \mathring{N}$, $B^{(1)} = 0$, and $B^{(2)} = \pm\mathring{N}$ in Definition 8.30.

Example 8.32. For any matrix $N \in \mathsf{EWP}_n^{\mathrm{sa}}$, we have $(\mathring{N}, \pm\mathring{N}) \in \mathsf{PDEC}_n$.

We rephrase next [SN21, Proposition 6.8] to provide a useful necessary condition for membership in the cone PDEC_n.

Proposition 8.33. Let $A \in \mathcal{M}_n(\mathbb{R})$ and $B \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$. Then, we have

$$\forall i \neq j \in [n] \qquad \frac{1}{n-1}\sqrt{A_{ii}A_{jj}} + \sqrt{A_{ij}A_{ji}} - |B_{ij}| \geq 0 \implies (A,B) \in \mathsf{PDEC}_n$$

Recall now the definition of the SPN cone: these are real matrices that can be written as a sum of a real positive semidefinite matrix and a symmetric entrywise non-negative matrix:

$$\mathsf{SPN}_n = \mathsf{PSD}_n^{\mathbb{R}} + \mathsf{EWP}_n^{\mathrm{sa}},$$

We have the following analogue of Item 3 of Proposition 8.20.

Proposition 8.34. If $(A,B) \in \mathsf{PDEC}_n$, then $\widetilde{A} + \mathrm{Re}(\mathring{B}) \in \mathsf{SPN}_n$.

Proof. We can write $B = B^{(1)} + B^{(2)}$ satisfying the conditions listed in Definition 8.30. Then, since $|\mathrm{Re}(B_{ij}^{(2)})| \leq \sqrt{A_{ij}A_{ji}} = \widetilde{A}_{ij}$ for all $i \neq j \in [n]$, we can show the following inclusion:

$$\widetilde{A} + \mathrm{Re}(\mathring{B}) = \underbrace{(\widetilde{A} + \mathrm{Re}(\mathring{B}^{(2)}))}_{\mathsf{EWP}_n^{\mathrm{sa}}} + \underbrace{\mathrm{Re}(\mathring{B}^{(1)})}_{\mathsf{PSD}_n^{\mathbb{R}}} \in \mathsf{SPN}_n.$$

■

Note that the condition $\widetilde{A} + \mathrm{Re}(\mathring{B}) \in \mathsf{SPN}_n$ above also implies the direct analogue of Proposition 8.20, Item 3:

$$(A + \mathring{B}) + (A + \mathring{B})^\top = A + A^\top + 2\,\mathrm{Re}(\mathring{B}) \in \mathsf{SPN}_n,$$

since $(A + A^\top)/2 - \widetilde{A} \in \mathsf{EWP}_n^{\mathrm{sa}}$.

We now establish the main result of this section, a theorem that should be compared with the "lifting" theorem for copositivity, Theorem 8.26 from the previous section.

Theorem 8.35. Let $M \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ and let $N \in \mathsf{EWP}_n^{\mathrm{sa}}$ with $\mathrm{diag}(M) = \mathrm{diag}(N)$, and suppose $N_{ij} \geq \frac{1}{2}M_{ij} + \frac{1}{4}(M_{ii} + M_{jj})$ for all $i \neq j \in [n]$. Then, we have

$$M \in \mathsf{SPN}_n \quad \Longleftrightarrow \quad (N, M - \mathring{N}) \in \mathsf{PDEC}_n.$$

Furthermore, if M is positive semidefinite (resp. entrywise non-negative), then the condition $N \in \mathsf{EWP}_n^{\mathrm{sa}}$ (resp. $N \in \mathsf{EWP}_n^{\mathrm{sa}}$ such that $N - M/2 \in \mathsf{EWP}_n$) is enough to obtain $(N, M - \mathring{N}) \in \mathsf{PDEC}_n$.

Proof. The condition $(N, M - \mathring{N}) \in \mathsf{PDEC}_n$ implies $M \in \mathsf{SPN}_n$ from Proposition 8.34. For the converse, let us assume $M \in \mathsf{SPN}_n$ and write $M = A^{(1)} + A^{(2)}$ where $A^{(1)} \in \mathsf{PSD}_n^{\mathbb{R}}$ and $A^{(2)} \in \mathsf{EWP}_n^{\mathrm{sa}}$. Then

- $(\mathrm{diag}(A^{(1)}), A^{(1)}) \in \mathsf{PDEC}_n$ and $(\mathring{N}, -\mathring{N}) \in \mathsf{PDEC}_n$ whenever $N \in \mathsf{EWP}_n^{\mathrm{sa}}$;
- $(\mathrm{diag}(A^{(2)}) + \mathring{N}, A^{(2)} - \mathring{N}) \in \mathsf{PDEC}_n$ whenever $N - A^{(2)}/2 \in \mathsf{EWP}_n$. Indeed, $N_{ij}^2 \geq (A_{ij}^{(2)} - N_{ij})^2$ holds whenever $N_{ij} \geq A_{ij}^{(2)}/2$, and hence the decomposition $A^{(2)} - \mathring{N} = B^{(1)} + B^{(2)}$ with $B^{(1)} = 0$ satisfies the conditions in Definition 8.30.

Consequently, we have

$$(N, M - \mathring{N}) = (\mathrm{diag}(A^{(1)}), A^{(1)}) + (\mathrm{diag}(A^{(2)}) + \mathring{N}, A^{(2)} - \mathring{N}), \in \mathsf{PDEC}_n$$

if $N - A^{(2)}/2 \in \mathsf{EWP}_n$. On the other hand, if $i \neq j \in [n]$, then

$$A_{ij}^{(2)} \leq M_{ij} + |A_{ij}^{(1)}| \leq M_{ij} + \sqrt{A_{ii}^{(1)} A_{jj}^{(1)}} \leq M_{ij} + \frac{A_{ii}^{(1)} + A_{jj}^{(1)}}{2} \leq M_{ij} + \frac{M_{ii} + M_{jj}}{2}.$$

Therefore, $N - A^{(2)}/2 \in \mathsf{EWP}_n$ is satisfied whenever $N_{ij} \geq \frac{1}{2}M_{ij} + \frac{1}{4}(M_{ii} + M_{jj})$ for all $i \neq j$. ■

Remark 8.36. The proof above actually shows that, if $M = A^{(1)} + A^{(2)} \in \mathsf{SPN}_n$ with $A^{(1)} \in \mathsf{PSD}_n^{\mathbb{R}}$ and $A^{(2)} \in \mathsf{EWP}_n^{\mathrm{sa}}$, then

$$\big(\operatorname{diag}(A^{(1)}), A^{(1)}\big) + \frac{1}{2}\big(A^{(2)} + \operatorname{diag}(A^{(2)}), A^{(2)} + \operatorname{diag}(A^{(2)})\big) \in \mathsf{PDEC}_n,$$

by choosing $N = \operatorname{diag}(M) + \frac{1}{2}\mathring{A}^{(2)}$. This precisely recovers [MATS21, Theorem 2.2]:

$$W = X^{\mathsf{LDUI}}_{\operatorname{diag}(A^{(1)}),A^{(1)}} + \Pi_S X^{\mathsf{LDUI}}_{\operatorname{diag}(A^{(2)}),A^{(2)}} \Pi_S \in \mathsf{PPT}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$$

(i.e. W is *decomposable*), where $\Pi_S := \frac{1}{2}(I_{d^2} + F_d) = \frac{1}{2}(I_{d^2} + \sum_{i,j=1}^d |ij\rangle\langle ji|)$ is the projection onto the symmetric subspace $\mathbb{C}^n \vee \mathbb{C}^n \subset (\mathbb{C}^n)^{\otimes 2}$. Indeed, the relations from [SN21, Proposition 4.3] imply that

$$\Pi_S X^{\mathsf{LDUI}}_{A,B} \Pi_S = X^{\mathsf{LDUI}}_{(A+B)/2,(A+B)/2}$$

whenever $A, B \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ with $\operatorname{diag}(A) = \operatorname{diag}(B)$.

Example 8.37. For the matrix

$$\widetilde{H} := \begin{bmatrix} 1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 \end{bmatrix} = |v\rangle\langle v| + \begin{bmatrix} 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \end{bmatrix} \in \mathsf{SPN}_4, \quad v = (1,-1,1,-1)^\top,$$

Theorem 8.35 implies that $(I_4 + \lambda \mathring{J}_4, \widetilde{H} - \lambda \mathring{J}_4) \in \mathsf{PDEC}_4$ if $\lambda \geq 1$. We claim that this condition is also necessary. Note that $\widetilde{H}$ is a principal 4×4 submatrix of the Horn matrix H, and thus the argument in Example 8.28 implies

$$(I_5 + \lambda \mathring{J}_5, H - \lambda \mathring{J}_5) \in \mathsf{PCOP}_5 \ \ \forall\, \lambda \geq \frac{1}{2} \implies (I_4 + \lambda \mathring{J}_4, \widetilde{H} - \lambda \mathring{J}_4) \in \mathsf{PCOP}_4 \ \ \forall\, \lambda \geq \frac{1}{2}.$$

In particular, we have $(I_4 + \lambda \mathring{J}_4, \widetilde{H} - \lambda \mathring{J}_4) \in \mathsf{PCOP}_4 \setminus \mathsf{PDEC}_4$ in the interval $\lambda \in [1/2, 1)$, which leads to the *positive indecomposable linear maps* $\Phi^{\mathsf{(C)DUC}}_{I_4+\lambda \mathring{J}_4, \widetilde{H}-\lambda \mathring{J}_4}$.

To show the claim, suppose $\widetilde{H} - \lambda \mathring{J}_4 = B^{(1)} + B^{(2)}$ where $B^{(1,2)}$ satisfy the conditions in Definition 8.30, i.e., $B^{(2)} \in \mathcal{M}_4^{\mathrm{sa}}(\mathbb{C})$, $B^{(2)}_{ii} \geq 0$, $|B^{(2)}_{ij}| \leq \lambda$, for $i \neq j$, and

$$B^{(1)} = \begin{bmatrix} 1 & -1-\lambda & 1-\lambda & 1-\lambda \\ -1-\lambda & 1 & -1-\lambda & 1-\lambda \\ 1-\lambda & -1-\lambda & 1 & -1-\lambda \\ 1-\lambda & 1-\lambda & -1-\lambda & 1 \end{bmatrix} - B^{(2)} \in \mathsf{PSD}_4^{\mathbb{C}}.$$

First, the psd condition for each of 2×2 principal submatrices of $B^{(1)}$ implies that $\mathrm{diag}(B^{(2)}) = 0$ and $B^{(2)}_{ij} = -\lambda$ for all $i, j \in [4]$ with $|i - j| = 1$. Next, the condition for 3×3 principal submatrix

$$\begin{bmatrix} 1 & -1 & 1-\lambda-B^{(2)}_{13} \\ -1 & 1 & -1 \\ 1-\lambda-\overline{B^{(2)}_{13}} & -1 & 1 \end{bmatrix} \geq 0 \implies \begin{vmatrix} 1 & -1 & 1-\lambda-B^{(2)}_{13} \\ -1 & 1 & -1 \\ 1-\lambda-\overline{B^{(2)}_{13}} & -1 & 1 \end{vmatrix} = -|\lambda + B^{(2)}_{13}|^2 \geq 0$$

forces that $B^{(2)}_{13} = B^{(2)}_{31} = -\lambda$, and similarly $B^{(2)}_{24} = B^{(2)}_{42} = -\lambda$. Finally, the last condition $B^{(1)} \geq 0$ would force that $1 - \lambda - B^{(2)}_{14} = -1$, i.e., $B^{(2)}_{14} = 2 - \lambda$. Since $|B^{(2)}_{14}| \leq \lambda$, this implies $\lambda \geq 1$.

Finally, the following corollary allows us to provide a $(n^2 - n)/2$-*dimensional region* of positive indecomposable linear maps within the classes of DUC and CDUC linear maps.

Corollary 8.38. If $M \in \mathsf{COP}_n \setminus \mathsf{SPN}_n$, then both the maps $\Phi^{(\mathsf{C})\mathsf{DUC}}_{N, M - \mathring{N}}$ are *positive and non-decomposable* for all $N \in \mathsf{EWP}_n^{\mathrm{sa}}$ such that $\mathrm{diag}(N) = \mathrm{diag}(M)$ and $N_{ij} \geq \frac{1}{2} M_{ij}$ for all $i > j$. Moreover, if $P \in \mathsf{DNN}_n$ with $\langle P, M \rangle < 0$, then the Dicke state $X^{\mathsf{LDUI}}_{P,P}$ is PPT entangled with

$$\Phi^{\mathsf{CDUC}}_{N, M - \mathring{N}}(X^{\mathsf{LDUI}}_{P,P}) \not\geq 0.$$

In other words, the entanglement in the state $X^{\mathsf{LDUI}}_{P,P}$ can be detected by the witness map $\Phi^{\mathsf{DUC}}_{N, M - \mathring{N}}$.

In Section 8.8.1, we strengthen Corollary 8.38 by providing a broad family of *entanglement witnesses* capable of detecting entanglement in quantum states with arbitrarily high levels of *PPT extendibility*.

As a final remark, it is natural to ask which is the most efficient among these large classes of entanglement witnesses. In this context, [LKCH00] introduced the notion of *optimality*. A nonzero entanglement witness $W \in \mathrm{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$ is called *optimal* if it detects the maximal set of entangled states, i.e., if another nonzero entanglement witness $W' \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$ satisfies

$$\mathrm{Tr}(W\rho) < 0 \implies \mathrm{Tr}\big(W'\rho\big) < 0$$

for every (entangled) state ρ, then $W' = cW$ for some $c > 0$ (we refer to [LKCH00, Lemma 1 and Corollary 1]). It is shown [LKCH00, Theorem 1] that the optimality of W is equivalent to, for arbitrary nonzero positive semidefinite matrix $X \in (M_n \otimes M_n)^+$, we have $W - X \notin \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$. In other words, any decomposition $W = W' + X$ where $W' \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$ and $X \geq 0$ implies $X = 0$. Therefore, optimal witnesses can be regarded as *edge objects* as discussed in [BCH+02]. A necessary condition for optimality of W is that, there exists a separable state ρ_{sep} such that $\mathrm{Tr}(W\rho_{sep}) = 0$, meaning that W is on the *boundary* of $\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$ (every such W is on an *exposed face* of $\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$ according to [Kye13]). However, the converse is not true: using the flip operator F, define the witness $W := F + |11\rangle\langle 11|$. Clearly, since F is also an entanglement witness, W is not optimal, but it satisfies

$$\mathrm{Tr}(W|12\rangle\langle 12|) = \langle 12|F_d|12\rangle = 0,$$

proving that it is on the boundary of $\mathsf{Sep}(\mathbb{C}^2 \otimes \mathbb{C}^2)^\circ$.

In the following statement, we show that the previous construction again provides a wide ($(n^2-n)/2$-dimensional) class of optimal entanglement witnesses.

Corollary 8.39. Let M be an extremal copositive matrix which is also exceptional, i.e., $M \notin \mathsf{SPN}_n$. Then for any $N \in \mathsf{EWP}_n^{\mathrm{sa}}$ with $\mathrm{diag}(N) = \mathrm{diag}(M)$ and $N_{ij} \geq \frac{1}{2}M_{ij}$ for all $i \neq j$, the CLDUI matrix $X^{\mathsf{CLDUI}}_{N,M-\mathring{N}}$ is optimal and indecomposable.

Proof. Suppose we have a decomposition $X^{\mathsf{CLDUI}}_{N,M-\mathring{N}} = X_1 + X_2$ where X_1 is block-positive and X_2 is a positive semidefinite matrix. By taking the *CLDUI-twirling* as in Eq. (60), we have $X^{\mathsf{CLDUI}}_{N,M-\mathring{N}} = X_1' + X_2'$ where $X_i' = \mathcal{T}_{\mathsf{CLDUI}} X_i =: X^{\mathsf{CLDUI}}_{A_i,B_i}$. Then [PJPY24, Proposition 2.1] implies that X_1' is block-positive and $X_2 \geq 0$, and

hence $(A_1, B_1) \in \mathsf{PCOP}_n$, $A_2 \in \mathsf{EWP}_n$, and $B_2 \in \mathsf{PSD}_n^{\mathbb{C}}$. Now let us focus on the decomposition

$$(N, M - \mathring{N}) = (A_1, B_1) + (A_2, B_2) = (A_1, B_1) + (\mathring{A}_2, 0) + (\mathrm{diag}(B_2), B_2),$$

which yields the following decomposition

$$M = ((A_1 + A_1^\top)/2 + \mathrm{Re}(\mathring{B}_1)) + ((\mathring{A}_2 + \mathring{A}_2^\top)/2 + \mathrm{Re}(B_2))$$

of the copositive matrix M. Since $(\mathring{A}_2 + \mathring{A}_2^\top)/2 + \mathrm{Re}(B_2) \in \mathsf{SPN}_n$, the extremality and exceptionality of M forces $(\mathring{A}_2 + \mathring{A}_2^\top)/2 + \mathrm{Re}(B_2) = 0$. By comparing both sides, we further have $(\mathring{A}_2 + \mathring{A}_2^\top)/2 = \mathrm{Re}(B_2) = 0$, and hence $A_2 = B_2 = 0$. Finally, since the CLDUI-twirling $\mathcal{T}_{\mathsf{CLDUI}}$ is trace-preserving, we have $X_2 = 0$, which concludes the optimality of $X^{\mathsf{LDUI}}_{N, M-\mathring{N}}$. ■

Remark 8.40.

1. The condition $M \notin \mathsf{SPN}_n$ is essential above. Indeed, $M = 3(|i\rangle\langle j| + |j\rangle\langle i|)$ is an extremal copositive matrix [SMB21, Theorem 2.29], and the choice $N = 2M/3$ gives a copositive pair $\frac{1}{3}(2M, M) \in \mathsf{PCOP}_n \setminus \mathsf{CLDUI}_n^+$. However, we have a decomposition

   $$(2M, M) = (M, M) + (M, 0),$$

   where $(M, M) \in \mathsf{PCOP}_n$ and $(M, 0) \in \mathsf{CLDUI}_n^+$.

2. If $N_{ij} \geq \frac{1}{2}\max(0, M_{ij})$ for some $i \neq j$, then the LDUI matrix $X^{\mathsf{LDUI}}_{N, M-\mathring{N}}$ is not optimal. Indeed, We can decompose the pair into

   $$(N, M - \mathring{N}) = (N - N', M - \mathring{N} + N') + (N', -N'),$$

   where $N' = (N_{ij} - \frac{1}{2}\max(M_{ij}, 0))(|i\rangle\langle j| + |j\rangle\langle i|)$ and $(N', -N') \in \mathsf{LDUI}_n^+$.

8.6 MARKOV-CHOI MAPS

In this section, we consider another variant of Example 8.23 obtained by perturbing the first element of the pair $(\mathring{J}, -\mathring{J})$ with an arbitrary real matrix $A - \mathring{J}$ (with A nonnega-

tive entries), while keeping the second element of the form $\operatorname{diag}(A) - \mathring{J}$. This class of examples yields DUC maps that are very important in the literature, such as the Choi map [Cho75c] and many of its generalizations [CL77, TT88, Kye92, CKL92, Ha03, CMR18, BSSC25, SBSC24]. These maps are of the form

$$\Phi^{\mathsf{DUC}}_{A,\operatorname{diag}(A)-\mathring{J}}(Z) = \operatorname{diag}\{A \operatorname{diag}[Z]\} - \mathring{Z} = \sum_{i,j=1}^{n} (A_{ij} + \mathbb{1}_{i=j}) Z_{jj} |i\rangle\langle i| - Z.$$

We will call such maps *Markov-Choi* because of their precise form: on the diagonal, the map acts like a classical Markov matrix A, while on the off-diagonal elements, the map flips the sign of the entry, exactly like the celebrated Choi map [Cho75c].

Let us first gather several positivity properties of such maps in the following proposition.

Proposition 8.41. Let $A \in \mathsf{EWP}_n$. Then:

1. $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n$ if and only if $\sum_{i=1}^{n} \frac{p_i}{p_i + (Ap)_i} \leq 1 \quad \forall\, p \in \mathbb{R}^n_{>0}$.
2. $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n$ if and only if $\operatorname{diag}(A) - \mathring{J} + S \in \mathsf{PSD}_n^{\mathbb{R}}$ for some $S \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ with $\operatorname{diag}(S) = 0$ and $|S_{ij}|^2 \leq A_{ij} A_{ji}\ \forall\, i \neq j \in [n]$.
3. $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{CLDUI}_n^+$ if and only if $\sum_{i=1}^{n} \frac{1}{1 + A_{ii}} \leq 1$.
4. $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{LDUI}_n^+$ if and only if $A_{ij} A_{ji} \geq 1\ \forall\, i \neq j \in [n]$.
5. $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCP}_n$ if and only if $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDNN}_n = \mathsf{CLDUI}_n^+ \cap \mathsf{LDUI}_n^+$ if and only if $\sum_{i=1}^{n} \frac{1}{1 + A_{ii}} \leq 1$ and $A_{ij} A_{ji} \geq 1\ \forall\, i \neq j \in [n]$.

Proof. For the first point, $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n$ if and only if the Markov-Choi map

$$\Phi^{\mathsf{DUC}}_{A,\operatorname{diag} A-\mathring{J}}(Z) = \operatorname{diag}\{A \operatorname{diag}[Z]\} - \mathring{Z} = \operatorname{diag}\{(I + A) \operatorname{diag}[Z]\} - Z$$

is positive. For an arbitrary vector $v \in \mathbb{C}^n$, where $v_i \neq 0$ for all $i \in [n]$, we have

$$\Phi(|v\rangle\langle v|) \geq 0 \iff \operatorname{diag}\{(I + A) \operatorname{diag}[|v\rangle\langle v|]\} \geq |v\rangle\langle v|$$

We define $D_v := \operatorname{diag}\{(I + A)\operatorname{diag}[|v\rangle\langle v|]$, ane hence it follows that,

$$\begin{aligned}\Phi(|v\rangle\langle v|) \geq 0 &\iff D_v^{-1/2}\,|v\rangle\langle v|\,D_v^{-1/2} \leq I \\ &\iff \left\|D_v^{-1/2}\,|v\rangle\right\| \leq 1 \\ &\iff \left\|\left(\frac{v_i}{\sqrt{\sum_{j=1}^n A_{ij} + \mathbb{1}_{i=j})|v_j|^2}}\right)_{i\in[n]}\right\|^2 \leq 1 \\ &\iff \sum_{i=1}^n \frac{|v_i|^2}{|v_i|^2 + (A|v.|^2)_i} \leq 1,\end{aligned}$$

which is the condition in the statement for $p_i := |v_i|^2 > 0$. Conversely, the condition implies that $\Phi^{\mathsf{DUC}}_{A,\operatorname{diag} A - \mathring{J}}(|v\rangle\langle v|) \geq 0$ for all $v \in \mathbb{C}^n$ with non-zero entries, and thus the positivity of $\Phi^{\mathsf{DUC}}_{A,\operatorname{diag} A - \mathring{J}}$ by a density argument.

For the second point, $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n$ if and only if $\operatorname{diag}(A) - \mathring{J} = B^{(1)} + B^{(2)}$ where $B^{(1,2)}$ satisfies the conditions in Definition 8.30. Note that we may assume that $B^{(1,2)}$ are real symmetric, by taking (entrywise) real part, and $\operatorname{diag}(B^{(2)}) = 0$ by choosing $\widetilde{B}^{(1)} = B^{(1)} + \operatorname{diag}(B^{(2)})$ and $\widetilde{B}^{(2)} = \mathring{B}^{(2)}$ if necessary. Therefore, we have the advertised condition by setting $S = -\widetilde{B}^{(2)}$.

For the third point, by Proposition 8.14, the condition on the LHS is equivalent to $\operatorname{diag}(A) - \mathring{J} \in \mathsf{PSD}_n^{\mathsf{C}}$. Therefore, similarly as in the proof of the first point,

$$\begin{aligned}\operatorname{diag}(A) \geq \mathring{J} &\iff \operatorname{diag}(I + A) \geq J = |\mathbf{1}\rangle\langle\mathbf{1}| \iff \left\|(\operatorname{diag}(I + A))^{-1/2}\,|\mathbf{1}\rangle\right\| \leq 1 \\ &\iff \left\|\left(\frac{1}{\sqrt{1 + A_{ii}}}\right)_{i\in[n]}\right\|^2 = \sum_{i=1}^n \frac{1}{1 + A_{ii}} \leq 1.\end{aligned}$$

The fourth point is straightforward from the condition in Proposition 8.14. Finally, last fifth point follows from the *comparison matrix* argument from [SN21, Lemma 2.11] since $M(\operatorname{diag}(A) - \mathring{J}) = \operatorname{diag}(A) - \mathring{J}$. ∎

Note that the last statement of Proposition 8.41 implies that

$$X^{(\mathsf{C})\mathsf{LDUI}}_{A,\operatorname{diag}(A) - \mathring{J}} \text{ is separable if and only if PPT,}$$

by Propositions 8.13 and 8.15. In other words, it is impossible to find PPT entanglement directly from pairs of the form $(A, \operatorname{diag}(A) - \mathring{J})$.

It is in general challenging to solve analytically the conditions in Proposition 8.41 (1) and (2) (we refer to [CKL92, Yam93, Ha03, BSSC25] for exact solutions in several special cases). Since our main interest lies in finding *exceptional* pairs $(A, \operatorname{diag}(A) - \mathring{J})$ in $\mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ (equivalently, those for which the corresponding Markov–Choi map $\Phi^{\mathsf{DUC}}_{A,\operatorname{diag} A - \mathring{J}}$ is positive and indecomposable), we shall further restrict our attention to

several special classes of matrices A for which membership in the cones PCOP_n or PDEC_n can be explicitly obtained, and accordingly, examples of positive indecomposable maps can be readily constructed.

8.6.1 *Markov-Choi maps from exceptional copositive matrices*

In relation with copositivity, we first record some simple necessary and, respectively, sufficient conditions for $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n$.

Proposition 8.42. Let $A \in \mathsf{EWP}_n$ and let $\widetilde{A} := (A \odot A^\top)^{\odot 1/2} = (\sqrt{A_{ij}A_{ji}})_{i,j\in[n]}$. Then we have the following implications:

$$\widetilde{A} - \mathring{J} \in \mathsf{COP}_n \implies (A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \implies (A + A^\top)/2 - \mathring{J} \in \mathsf{COP}_n.$$

Proof. If $\widetilde{A} - \mathring{J} \in \mathsf{COP}_n$, then the first statement of Theorem 8.26 with $N = \widetilde{A}$ and $M = \widetilde{A} - \mathring{J}$ implies that $(\widetilde{A}, \mathrm{diag}(\widetilde{A}) - \mathring{J}) \in \mathsf{PCOP}_n$. By Proposition 8.20 (4) , this implies that $\widetilde{A} - O\mathring{J}O \in \mathsf{COP}_n$ for all $O \in D\mathcal{O}_n$ and hence, by Corollary 8.25, we have that $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n$. This shows the first implication. The second implication is straightforward from Proposition 8.20 (3). ∎

Note that if A is further assumed to be *symmetric*, i.e., $A \in \mathsf{EWP}_n^{\mathrm{sa}}$, then we have

$$(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \iff A - \mathring{J} \in \mathsf{COP}_n. \tag{67}$$

which is a special case of Theorem 8.26 by choosing $N = A, M = A - \mathring{J}$.

On the other hand, a necessary condition for $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n$ in Proposition 8.34 is $\widetilde{A} - \mathring{J} \in \mathsf{SPN}_n$. Therefore, one can construct the matrix pair as follows: for any *exceptional* copositive matrix $M \in \mathsf{COP}_n \setminus \mathsf{SPN}_n$, we have $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ whenever

$$\widetilde{A} = (A \odot A^\top)^{\odot 1/2} = \lambda M + \mathring{J}$$

for $0 < \lambda < (\max(M_-))^{-1}$ (note that $M_- \neq 0$ since $M \notin \mathsf{EWP}_n$). Note that when $A = \lambda M + \mathring{J} = \tilde{A}$, the corresponding positive indecomposable Markov-Choi maps

$$\Phi^{\mathsf{DUC}}_{A,\mathrm{diag}(A)-\mathring{J}}(Z) = \lambda \sum_{i,j} M_{ij} Z_{jj} |i\rangle\langle i| + \mathrm{Tr}(Z) I_n - Z, \quad Z \in \mathcal{M}_n(\mathbb{C}),$$

already provides us with a new class of constructions. To our knowledge, all the previous results in the literature assumed A to be *asymmetric* to construct examples of positive-indecomposable maps. Note that in the cases they consider, $\widetilde{A} - \mathring{J}$ is also not necessarily

copositive. This shows that, this is not a necessary condition for PCOP_n, and shift our focus on this case in the remainder of the section.

8.6.2 *Markov-Choi maps from non-copositive matrices*

Here we discuss two cases where the exceptional pair $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ is obtained from a matrix A such that $\widetilde{A} - \mathring{J} \notin \mathsf{COP}_n$. Both cases would result in generalizing previous examples of positive indecomposable Markov-Choi maps from [Kye92, CKL92, Ha03].

The first case is when $\widetilde{A} = (A \odot A^\top)^{\odot 1/2}$ is diagonal. In this case, it is shown that

$$\widetilde{A} - \mathring{J} \in \mathsf{COP}_n \iff \widetilde{A} - \mathring{J} \in \mathsf{SPN}_n \iff \widetilde{A} - \mathring{J} \in \mathsf{PSD}_n^{\mathbb{R}} \iff \sum_{i=1}^n \frac{1}{1 + A_{ii}} \leq 1,$$

from [SMB21, Theorem 2.102].

We show below that this is also equivalent to the membership in PDEC_n.

Proposition 8.43. Suppose $A \in \mathsf{EWP}_n$ satisfies $A_{ij}A_{ji} = 0$ for all $i \neq j \in [n]$. Then we have

$$(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n \iff \sum_{i=1}^n \frac{1}{1 + A_{ii}} \leq 1 \iff (A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{CLDUI}_n^+.$$

In particular, we have $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ whenever A satisfies $\sum_{i=1}^n \frac{1}{1+A_{ii}} > 1$ and $\sum_{i=1}^n \frac{p_i}{p_i + (Ap)_i} \leq 1$ for all $p \in \mathbb{R}^n_{>0}$.

Proof. Since $A_{ij}A_{ji} \equiv 0$, the condition in Proposition 8.41 (2) forces that $S = 0$, and hence $\mathrm{diag}(A) - \mathring{J} \in \mathsf{PSD}_n^{\mathbb{R}}$, which is equivalent to $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{CLDUI}_n^+$ as in Proposition 8.41 (3). ∎

Example 8.44. For a 3×3 matrix $A = \begin{bmatrix} a_1 & 0 & c_1 \\ c_2 & a_2 & 0 \\ 0 & c_3 & a_3 \end{bmatrix} \in \mathsf{EWP}_3$, it is shown [Kye92, CMR18] that $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_3$ whenever $a_1, a_2, a_3 \geq a$ and $(c_1c_2c_3)^{1/3} \geq 2 - a$ for some $a \geq 1$. More generally, for $A \in \mathsf{EWP}_n$, the result of [Ha03, Theorem 2.4] implies that $(A, \mathrm{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n$ if, for some $k = 1, \ldots, n-1$ and $a \geq n - 2$, we have $A_{ii} \geq a$ for all $i \in [n]$ and

$\left(\prod_{i=1}^n A_{i,i+k}\right)^{1/n} \geq n-a-1$ where the sum in the index is in modulo n. Indeed, we may add an entrywise positive matrix to setting in [Ha03, Theorem 2.4], namely, $A = N + A^{\mathrm{H}a}$ with $N \in \mathsf{EWP}_n$ and

$$A^{\mathrm{H}a}_{ii} \equiv a \text{ and } A^{\mathrm{H}a}_{ij} = c_i \delta_{j,i+k}, \quad a \geq n-2, \quad (c_1 \cdots c_n)^{1/n} \geq n-a-1,$$

and using the cone property of PCOP_n. Therefore, one can construct the exceptional pair $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ under the conditions

$$A_{ij}A_{ji} = 0, \quad a \leq A_{ii} < n-1 \text{ for all } i \neq j \in [n], \text{ and } \left(\prod_{i=1}^n A_{i,i+k}\right)^{1/n} \geq n-a-1$$

for some $k = 1, \ldots, n-1$ and $n-2 \leq a < n-1$.

Remark 8.45. In [Ha03], the author showed a stronger form of indecomposability in the previous map: when $A_{ii} \equiv a$ and $A_{ij} = c_i\, \delta_{j,i+k}$ with $(c_1 \cdots c_n)^{1/n} \geq n-a-1$, the corresponding map $\Phi^{\mathsf{DUC}}_{A,\operatorname{diag}(A)-\mathring{J}}$ is *atomic*, i.e., it cannot be a sum of a 2-positive and a 2-copositive linear map.

Next, let us consider the case where $\widetilde{A} = (A \odot A^T)^{\odot 1/2} = aI_n + \lambda \mathring{J}_n$ for some $a, \lambda \geq 0$. As in the previous case, we can show $\widetilde{A} - \mathring{J} \in \mathsf{COP}_n$ if and only if $\widetilde{A} - \mathring{J} \in \mathsf{SPN}_n$, which also characterizes pairwise decomposability of $(A, \operatorname{diag}(A) - \mathring{J})$.

Proposition 8.46. Suppose $A \in \mathsf{EWP}_n$ satisfies $A_{ii} \equiv a$ and $\sqrt{A_{ij}A_{ji}} \equiv \lambda$ for all $i \neq j \in [n]$. Then we have

$$\begin{aligned}(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n \iff \widetilde{A} - \mathring{J} \in \mathsf{COP}_n \iff \widetilde{A} - \mathring{J} \in \mathsf{SPN}_n \\ \iff \lambda \geq 1 - \frac{a}{n-1}.\end{aligned}$$

In particular, we have $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ whenever $0 \leq a < n-1$, $0 \leq \lambda < 1 - \frac{a}{n-1}$, and A satisfies $\sum_{i=1}^n \frac{p_i}{p_i + (Ap)_i} \leq 1$ for all $p \in \mathbb{R}^n_{>0}$.

Proof. The condition $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n$ is equivalent to $(aI_n + \lambda \mathring{J}, aI_n - \mathring{J}_n) \in \mathsf{PDEC}_n$, thanks to Eq. (65). The decomposability of the corresponding Markov-Choi map

$$\Phi^{\mathsf{DUC}}_{aI_n+\lambda\mathring{J}, aI_n-\mathring{J}_n}(Z) = \lambda \operatorname{Tr}(Z) I_n + (a+1-\lambda)\operatorname{diag}(Z) - Z, \quad Z \in \mathcal{M}_n(\mathbb{C}),$$

has been characterized in [PJPY24, Section 4], where it is shown that it is equivalent to its positivity. This shows that

$$(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n \iff (\tilde{A}, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \iff \tilde{A} - \mathring{J} \in \mathsf{COP}_n,$$

where the last equivalence follows from Theorem 8.26. Now if $\lambda \geq 1$, then clearly $\tilde{A} - \mathring{J}_n = aI_n + (\lambda - 1)\mathring{J}_n \in \mathsf{EWP}_n^{\mathrm{sa}}$. If $\lambda < 1$, then by [Ber23, Theorem 2.102],

$$\begin{aligned} \tilde{A} - \mathring{J} = aI_n + (\lambda - 1)\mathring{J}_n \in \mathsf{COP}_n &\iff aI_n + (\lambda - 1)\mathring{J}_n \in \mathsf{SPN}_n \\ &\iff aI_n + (\lambda - 1)\mathring{J}_n \in \mathsf{PSD}_n^{\mathbb{R}} \\ &\iff a + (n-1)(\lambda - 1) \geq 0, \end{aligned}$$

which shows the remaining equivalences in the statement. ∎

Example 8.47. Consider a 3×3 matrix $A = \begin{bmatrix} a & b_1 & c_1 \\ c_2 & a & b_2 \\ b_3 & c_3 & a \end{bmatrix} \in \mathsf{EWP}_3$ satisfying

$$\sqrt{b_1 c_2} = \sqrt{b_2 c_3} = \sqrt{c_1 b_3} = \lambda, \quad a + (b_1 b_2 b_3)^{1/3} + (c_1 c_2 c_3)^{1/3} \geq 2, \quad \text{and} \quad a + \lambda \geq 1.$$

If $b_* := (b_1 b_2 b_3)^{1/3}$ and $c_* := (c_1 c_2 c_3)^{1/3}$, the last two conditions are equivalent to $a + b_* + c_* \geq 2$ and $a + \sqrt{b_* c_*} = a + \lambda \geq 1$. Therefore, we may apply the result from [CMR18, Corollary 2.4], which is mainly based on [CKL92, Theorem 2.1], to obtain that $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_3$. On the other hand, Proposition 8.46 implies that $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PDEC}_n$ if and only if $a + 2\lambda \geq 2$, which depends only on a and λ. Consequently, we can obtain positive indecomposable Markov-Choi maps $\Phi^{\mathsf{DUC}}_{A, \operatorname{diag}(A) - \mathring{J}}$ under the conditions $0 \leq a < 2$ and $1 - a \leq \lambda < 1 - \frac{a}{2}$, thereby recovering and generalizing the construction in [CKL92].

Finally, we provide another family of positive indecomposable maps in all dimensions.

Example 8.48. Let us consider a *circulant matrix* $A = circ(a, c_1, \ldots, c_{n-1}) \in \mathsf{EWP}_n$, i.e.,

$$A_{ii} \equiv a \text{ and } A_{i,i+k} \equiv c_k; \quad i = 1, \ldots, n, \quad k = 1, \ldots, n-1, \tag{68}$$

with $a, c_j \geq 0$ and $\sqrt{c_j c_{n-j}} = \lambda$ for all $j = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. Then by taking $c := \max_{1 \leq j \leq n-1} c_j$, the argument in Example 8.44 based on [Ha03] implies that $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n$ whenever $a \geq n - 2$ and $c \geq n - a - 1$. There-

fore, Proposition 8.46 implies that $(A, \operatorname{diag}(A) - \mathring{J}) \in \mathsf{PCOP}_n \setminus \mathsf{PDEC}_n$ under the conditions

$$n-2 \leq a < n-1, \quad c \geq n-a-1, \quad \text{and} \quad 0 \leq \lambda < 1 - \frac{a}{n-1}.$$

8.7 MAPS ASSOCIATED TO GRAPHS

In this section, we define a one-parameter family of maps using adjacency matrix of a graph. Recall that for every graph G we can define its *adjacency matrix*

$$A_G(i,j) = \begin{cases} 1 & \text{if } (i,j) \text{ is an edge in } G \\ 0 & \text{otherwise.} \end{cases}$$

Throughout this and the next section, we assume that G is a simple, undirected, and loopless graph with n vertices, in which case we always have $A_G \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ and $A_G = \mathring{A}_G$. We introduce the following quantities:

- $\lambda(G)$ the *maximal eigenvalue* of its adjacency matrix A_G. For a non-empty graph, $\lambda(G) \geq 1$;
- $\omega(G)$ its *clique number*, i.e. the size of the largest clique in G;
- $\alpha(G)$ the *stable or independence number* of G, i.e. the size of its largest stable set; clearly $\alpha(G) = \omega(\bar{G})$, where $\bar{G}$ is the complementary graph of G.

We refer the reader to [GR13] for more details about algebraic graph theory and graph parameters.

For a graph G on n vertices, we also introduce the quantity

$$\sigma(G) := \max\{t \in \mathbb{R} \,:\, J - tA_G \in \mathsf{SPN}_n\}, \tag{69}$$

where we recall that SPN_n is the set of real symmetric matrices that can be written as a sum of a positive semidefinite real matrix and an entrywise non-negative matrix. In particular, $\sigma(G) \geq 1 + \frac{1}{n-1}$ for all graphs G since

$$J_n - \left(1 + \frac{1}{n-1}\right) A_G = \frac{1}{n-1}(nI_n - J_n) + \frac{n}{n-1}(J_n - I_n - A_G) \in \mathsf{PSD}_n^{\mathbb{R}} + \mathsf{EWP}_n^{\mathrm{sa}} = \mathsf{SPN}_n.$$

Note that the value $\sigma(G)$ as defined is a property of the isomorphism class of the graph G because the set SPN_n is invariant under permutations. Moreover, given a graph G,

the value $\sigma(G)$ can be computed using semidefinite programming [BV04]. Moreover, it turns out that $\sigma(G)$ is related to a *hierarchy of semidefinite programs* that approximates the independence number of G [DKP02, Sch79b] that we review next; this hierarchy will also play an important role in Section 8.8. First, we recall the following result casting the independence number as a copositive program.

Theorem 8.49 ([DKP02, Corollary 2.4])**.** For any graph G on n vertices,

$$\alpha(G) = \min\{t \,:\, t(I + A_G) - J \in \mathsf{COP}_n\}.$$

Since membership in the copositive cone is a computationally hard problem [MK87], the following hierarchy of semidefinite program has been introduced. We recall that a polynomial P in n variables $x_1, \ldots, x_n$ is a sum of squares (SOS) if it can be decomposed as a

$$P(x) = \sum_{i=1}^{d} Q_i(x)^2$$

for some polynomials $Q_1, \ldots, Q_d$; SOS polynomials are clearly non-negative, but the converse is false in general [Ble12, BPT12].

Definition 8.50 ([DKP02, Definition 3.1 and Eq. (20)])**.** For any graph G on n vertices, define

$$\vartheta^{(r)}(G) := \min\{t \,:\, t(I + A_G) - J \in \mathsf{K}_n^{(r)}\},$$

where

$$\mathsf{K}_n^{(r)} := \{A \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R}) \,:\, x \in \mathbb{R}^n \mapsto \langle x^{\odot 2}|A|x^{\odot 2}\rangle \|x\|_2^{2r} \text{ is SOS}\}.$$

We gather next some important and relevant results regarding the parameters $\vartheta^{(r)}(G)$ and the corresponding sets $\mathsf{K}_n^{(r)}$ [DKP02, GL07, LV23, SV24]. First, for $r = 0$ the sum of squares decomposition for the polynomial $\langle x^{\odot 2}|A|x^{\odot 2}\rangle$ corresponds precisely to decomposing $A = P + E$ with a real positive semidefinite matrix P and a matrix E having non-negative entries [Par00]; we have thus

$$\mathsf{K}_n^{(0)} = \mathsf{SPN}_n.$$

The fundamental result here is that the numbers $\vartheta^{(r)}(G)$ provide increasingly good approximations for the independence number [DKP02]:

$$\alpha(G) \xleftarrow{r\to\infty} \vartheta^{(r)}(G) \leq \cdots \leq \vartheta^{(1)} \leq \vartheta^{(0)}(G).$$

It has been recently shown [SV24] that the sequence $(\vartheta^{(r)}(G))_{r\geq 0}$ is actually finite: for every graph G there exists a finite r_0 such that $\alpha(G) = \vartheta^{(r_0)}(G)$, while the conjecture [DKP02] that $\vartheta^{(\alpha(G)-1)}(G) = \alpha(G)$, proven for $\alpha(G) \leq 8$, remains open in the general case.

Since $J - tA_G = J - t(J - I - A_{\bar{G}}) = (t-1)(\frac{t}{t-1}(I + A_{\bar{G}}) - J)$ and since $\sigma(G) > 1$, it is now clear that the quantity σ from Eq. (69) is related to the value $\vartheta^{(0)}$ from Definition 8.50:

$$\sigma(G) = \frac{\vartheta^{(0)}(\bar{G})}{\vartheta^{(0)}(\bar{G}) - 1}.$$

Since $\vartheta^{(0)}(\bar{G}) \geq \alpha(\bar{G}) = \omega(G)$, we have the following upper bound:

$$\sigma(G) \leq \frac{\omega(G)}{\omega(G)-1} = 1 + \frac{1}{\omega(G)-1}. \tag{70}$$

Lemma 8.51. For every graph G, we have the following lower bound:

$$\sigma(G) \geq 1 + \frac{1}{\lambda(G)}.$$

Proof. The claim follows from the decomposition

$$J - \Big(1 + \frac{1}{\lambda(G)}\Big)A_G = \underbrace{I - \frac{1}{\lambda(G)}A_G}_{\in \mathsf{PSD}^{\mathbb{R}}} + \underbrace{J - I - A_G}_{=A_{\bar{G}} \in \mathsf{EWP}} \in \mathsf{SPN}_n.$$

■

We come now to the main result of this section, characterizing the different positivity properties of a linear map defined by a graph. More precisely, given a graph G and $t \geq 0$, let us consider the pair $(J, I - tA_G) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$.

Theorem 8.52. Let G be a graph with at least one edge, and consider, for a non-negative parameter $t \geq 0$, the linear map

$$\Phi_t^G(Z) := (\operatorname{Tr} Z)I - tA_G \odot Z, \quad Z \in \mathcal{M}_n(\mathbb{C}) \tag{71}$$

Then, the map $\Phi_t^G(Z)$ is

1. completely positive $\iff$ PPT $\iff$ EB $\iff$ $t \leq 1/\lambda(G)$;
2. completely copositive $\iff$ $t \leq 1$;
3. decomposable $\iff$ $t \leq \sigma(G)$;
4. positive $\iff$ $t \leq 1 + 1/(\omega(G) - 1)$;

Proof. The map Φ_t^G is a DUC map corresponding to the pair $(J, I - tA_G)$. Hence, many of the properties in the statement can be addressed using the theory developed in this work and in [SN21].

Complete positivity. We have

$$(J, I - tA_G) \in \mathsf{CLDUI}_n^+ \iff \begin{cases} J \in \mathsf{EWP}_n \\ I - tA_G \in \mathsf{PSD}_n^{\mathbb{R}} \iff t\lambda(G) \leq 1. \end{cases}$$

Note that $I - tA_G \in \mathsf{PSD}_n$ if and only if $I - tA_G$ is a *correlation matrix*. By [SN21, Proposition 3.7], we have

$$\Phi_t^G \text{ is EB} \iff (J, I - tA_G) \in \mathsf{PCP}_n \iff \Phi_t^G \text{ is PPT} \iff I - tA_G \in \mathsf{PSD}_n^{\mathbb{R}} \iff \Phi_t^G \text{ is CP.}$$

Complete copositivity. This is very similar to the previous case:

$$(J, I - tA_G) \in \mathsf{LDUI}_n^+ \iff \begin{cases} J \in \mathsf{EWP}_n \\ \forall i \neq j,\ (I - tA_G)_{ij}^2 \leq 1 \iff t \leq 1. \end{cases}$$

Decomposability. Since $\max(J - tA_G) = 1$, the map Φ_t^G is decomposable, i.e., $(J, I - tA_G) \in \mathsf{PDEC}_n$, if and only if $A = J - tA_G \in \mathsf{SPN}_n$ by Theorem 8.35 with $N = J$, and thus $t \leq \sigma(G)$ by the definition of the σ.

Positivity. With $Y := I - tA_G$, we are in the setting of Corollary 8.29:

$$\Phi_t^G \text{ is positive} \iff Y + \mathring{J} \in \mathsf{COP}_n \iff J - tA_G \in \mathsf{COP}_n.$$

We are are now going to switch to the complement $\bar{G}$ of the graph G and use the fact that $A_{\bar{G}} = \mathring{J} - A_G$. The condition becomes now

$$J - tA_G \in \mathsf{COP}_n \iff t(A_{\bar{G}} + I) + (1 - t)J \in \mathsf{COP}_n.$$

If $t \leq 1$, then the matrix above is doubly non-negative, as the sum of a entrywise positive matrix ($t(A_{\bar{G}} + I)$) and a positive semidefinite matrix ($(1-t)J$), and thus copositive. This settles the case $t \leq 1$. If $t > 1$, let us rewrite

$$t(A_{\bar{G}} + I) + (1-t)J = (t-1)\left[\frac{t}{t-1}(A_{\bar{G}} + I) - J\right]$$

and then use Theorem 8.49:

$$\frac{t}{t-1}(A_{\bar{G}}+I) - J \in \mathsf{COP}_n \iff \frac{t}{t-1} \geq \alpha(\bar{G}) = \omega(G) \iff t \leq \frac{\omega(G)}{\omega(G)-1} = 1 + \frac{1}{\omega(G)-1},$$

proving the claim in the statement.

■

We summarize all the bounds in the theorem above in Fig. 27. Importantly, the construction above yields:

1. *positive but not completely positive maps*, for all values of the parameter

$$t \in \left(\frac{1}{\lambda(G)}, 1 + \frac{1}{\omega(G)-1}\right] \neq \emptyset.$$

   For example, the value $t = 1$ yields such a map, for all non-empty graphs G.

2. *positive indecomposable maps*, when $G \neq \mathcal{K}_n$, for all values of the parameter

$$t \in \left(\sigma(G), 1 + \frac{1}{\omega(G)-1}\right], \quad \text{whenever } \sigma(G) < 1 + \frac{1}{\omega(G)-1}.$$

   We shall discuss several examples of graphs for which the interval above is non-empty in the following subsections.

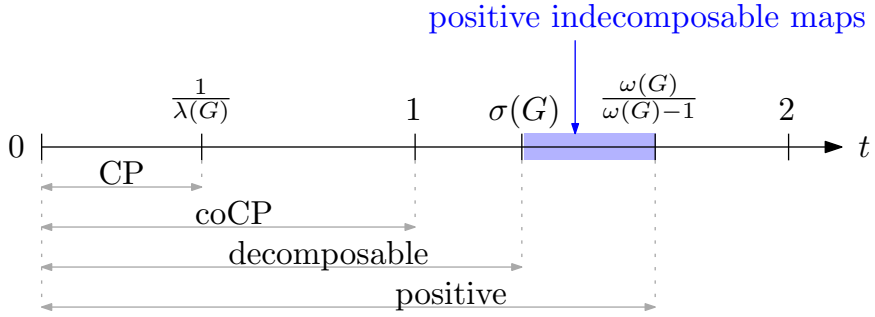


Figure 27: The positivity properties of the linear maps Φ_t^G from (71) as the parameter t varies. The blue region corresponds to the important case of positive indecomposable maps.

Remark 8.53. Linear maps having a similar structure as the ones in (71) been studied in [KMP18, Section 4]:

$$\Psi_t^G(Z) = \frac{t}{n}(\operatorname{Tr} Z)I_n + A_G \odot Z, \quad Z \in \mathcal{M}_n(\mathbb{C}).$$

The main difference between the maps Φ_t^G and Ψ_t^G is the sign in front of the Hadamard product term $A_G \odot Z$. This leads to very different structural properties of the maps, the two regimes being complementary. Note that the fact that the PPT^2 conjecture holds for the maps Ψ_t^G, see [KMP18, Corollary 4.4], is a special case of the more general proof for DUC maps from [SN22b, Theorem 4.5]. Note that the PPT^2 conjecture for the maps Φ_t^G trivially holds, since these maps are automatically PPT and EB as soon as they are completely positive, by the first point of Theorem 8.52.

Remark 8.54. While $\sigma(G)$ can be computed with a SDP, computing the parameter $\omega(G)$ is NP-complete. This makes it challenging to characterize whether the map Φ_t^G is indecomposable for an arbitrary graph.

In the next sections we focus on the parameter $\sigma(G)$ and $\omega(G)$ with the aim of exhibiting large families of graph-induced linear maps Φ_t^G that are positive indecomposable. To this end, we first gather some basic general properties of the quantity $\sigma(\cdot)$.

Proposition 8.55. The quantity $\sigma(\cdot)$ has the following properties:

1. We have the following dual formulation for the quantity σ:

$$\sigma(G) = \min\{\operatorname{Tr}(JX) \,:\, X \in \mathsf{SPN}_n^\circ \text{ s.t. } \operatorname{Tr}(A_G X) = 1\}. \tag{72}$$

2. $\sigma(G \sqcup H) = \min(\sigma(G), \sigma(H))$.

Proof. *Dual formulation.* The computation of the dual semidefinite program of Eq. (69) is straightforward. Note that the dual set of SPN_n can be readily computed using Eq. (51):

$$\mathsf{SPN}_n^\circ = \mathsf{PSD}_n^{\mathbb{R}} \cap \mathsf{EWP}_n^{\mathrm{sa}} = \mathsf{DNN}_n$$

The reader should also refer to [DKP02, Lemma 5.2], where several formulations for the dual of the $\vartheta^{(0)}$ quantity are discussed and a connection to Schrijver's ϑ' function [Sch79b] is put forward.

Disjoint union of graphs. First, note that if $G' \subseteq G$ is an induced subgraph of G, by taking submatrices we obviously have

$$\sigma(G') \geq \sigma(G).$$

This fact establishes the inequality $\sigma(G \sqcup H) \leq \min(\sigma(G), \sigma(H))$. For the reverse inequality, let $t := \min(\sigma(G), \sigma(H))$. There exist positive semidefinite matrices $R_{1,2}$ and entrywise positive matrices $E_{1,2}$ such that

$$J - tA_G = R_1 + E_1 \quad \text{and} \quad J - tA_H = R_2 + E_2.$$

We write then

$$J - t(A_G \oplus A_H) = (R_1 \oplus R_2) + (E_1 \oplus E_2 + \underbrace{J - J \oplus J}_{\in \mathsf{EWP}_n}),$$

finishing the proof. ∎

We now study a way to compute the value $\sigma(G)$ for graphs with symmetries. To simplify this problem, we consider the set of $n \times n$ matrices commuting with the automorphisms of a graph G:

$$\mathsf{C}_G := \{X \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R}) \,:\, [X, P_\pi] = 0 \quad \forall \pi \in \mathrm{Aut}(G)\}. \tag{73}$$

Above, P_π denotes the permutation matrix associated to a permutation $\pi \in S_n$, and elements in $\mathrm{Aut}(G) := \{\pi \in S_n : [A_G, P_\pi] = 0\}$ are called *automorphisms* of G.

Now consider the *twirling map* $\mathcal{T}_G : \mathcal{M}_n(\mathbb{C}) \to \mathsf{C}_G$ defined by

$$\mathcal{T}_G(X) := \frac{1}{|\mathrm{Aut}(G)|} \sum_{\pi \in \mathrm{Aut}(G)} P_\pi X P_\pi^{-1}.$$

The fact that the range of this map lies inside C_G is standard. Introduce

$$\mathsf{SPN}_G := \{R + E \,:\, R \in \mathsf{PSD}_n^{\mathbb{R}} \cap \mathsf{C}_G \text{ and } E \in \mathsf{EWP}_n^{\mathrm{sa}} \cap \mathsf{C}_G\}$$

and

$$\hat{\sigma}(G) := \max\{t \in \mathbb{R} \,:\, J - tA_G \in \mathsf{SPN}_G\}.$$

Proposition 8.56. For any graph G, we have $\sigma(G) = \hat{\sigma}(G)$.

Proof. Since $\mathsf{SPN}_G \subseteq \mathsf{SPN}_n$, we have $\hat{\sigma}(G) \leq \sigma(G)$. For the reverse inequality, let $\sigma(G) = t$ and $X = J - tA_G$. Since $X \in \mathsf{SPN}_n$, we have $X = R + E$ with $R \in \mathsf{PSD}_n^{\mathbb{R}}$ and $E \in \mathsf{EWP}_n^{\mathrm{sa}}$. Write

$$X = \mathcal{T}_G(X) = \underbrace{\mathcal{T}_G(R)}_{=:\hat{R}} + \underbrace{\mathcal{T}_G(E)}_{=:\hat{E}}.$$

We have $\hat{R}, \hat{E} \in \mathsf{C}_G$. Moreover, it is clear that the twirling operation preserves positive semidefiniteness and entrywise positivity, hence $\hat{R} \in \mathsf{PSD}_n^{\mathbb{R}}$ and $\hat{E} \in \mathsf{EWP}_n^{\mathrm{sa}}$, showing that $X \in \mathsf{SPN}_G$ and concluding the proof. ■

8.7.1 *Triangle-free and cyclic graphs*

A graph G is called *triangle-free* if it does not contain any three-cycles, i.e., there exists no sequence of 3 edges $(a, b), (b, c), (c, a)$ of G with $a \neq b \neq c \in [n]$. The triangle-free property of a graph G with at least one edge is alternatively characterized by $\omega(G) = 2$. In the first result of this section, we completely characterize the set of triangle-free graphs G such that $\sigma(G) = \omega(G)/(\omega(G) - 1)$, i.e. the upper bound in (70) is saturated.

Proposition 8.57. If a graph G is triangle free, then $\sigma(G) = 2 = \omega(G)/(\omega(G) - 1)$ if and only if G is bipartite.

Proof. If the graph G is bipartite on $n + m$ vertices, then its adjacency matrix is of the form

$$A_G = \begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix}$$

for some $n \times m$ matrix B. We have now

$$J - 2A_G = \begin{bmatrix} J_n & J_{n\times m} - 2B \\ J_{m\times n} - 2B^\top & J_m \end{bmatrix} = \underbrace{\begin{bmatrix} J & -J \\ -J & J \end{bmatrix}}_{\in \mathsf{PSD}_{n+m}^{\mathbb{R}}} + 2\underbrace{\begin{bmatrix} 0 & +J - B \\ J - B^\top & 0 \end{bmatrix}}_{\in \mathsf{EWP}_{n+m}} \in \mathsf{SPN}_{n+m}.$$

For the reverse implication, we first consider the case of *connected* triangle-free graphs. Now assume that for a connected triangle-free graph G on n vertices, we have $\sigma(G) = 2$, i.e., $J - 2A_G \in \mathsf{SPN}_n$. We conclude using [SMB21, Theorem 2.140], stating that if $A = (A_{ij}) \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$ satisfies $diag(A) = I_n$, $A_{ij} \geq -1$ for all i, j, and if $G_{-1}(A)$ is connected, then $A \in \mathsf{SPN}_n$ if and only if $G_{-1}(A)$ is bipartite. (Here $G_{-1}(A)$ denotes the graph with n vertices such that $A_{G_{-1}(A)}(i, j) = 1$ if and only if $A_{ij} = -1$). Indeed,

the entries of the matrix $A = J - 2A_G$ are all larger than or equal to -1 and the graph associated to the -1 values $G_{-1}(J - 2A_G) = G$ is connected. Hence, the graph G is bipartite. If the graph has more than m connected components G_i, by Proposition 8.55, we have $\min(\sigma(G_i)) = 2$. Also note that $\sigma(G_i) \leq \omega(G_i)/((\omega(G_i) - 1) \leq 2$. This implies that $\forall i \ (\sigma(G_i)) = 2$ implying that the connected graph G_i is bipartite. Hence $G = \bigsqcup G_i$ is bipartite. ■

As a corollary, every triangle-free non-bipartite graph G yields positive indecomposable maps.

Corollary 8.58. Let G be a triangle-free non-bipartite graph. Then, for every value of the parameter t in the non-empty interval $(\sigma(G), 2]$, the linear map Φ_t^G is positive and indecomposable.

The smallest triangle-free non-bipartite graph is the cycle graph on 5 vertices, denoted as C_5 (also known as a pentagon).

Recall that the *cycle graph* on n vertices is the graph C_n having edges

$$\{(i, j) \ : \ |i - j| = 1 \ (\text{mod } n)\}.$$

Cycle graphs with $n \geq 4$ are clearly triangle-free, and C_n is bipartite if and only if n is even; in this case, by Proposition 8.57, we have $\sigma(C_n) = 2 = \omega(C_n)$, hence there are no positive indecomposable maps associated to even cycles. For odd $n \geq 5$, we compute in what follows $\sigma(C_n)$.

Proposition 8.59. For odd $n \geq 5$, $\sigma(C_n) = 1 + \cos(\pi/n)$. Hence, for all

$$t \in (1 + \cos(\pi/n), 2],$$

the linear map $\Phi_t^{C_n}$ is positive indecomposable.

Proof. For the cyclic graph C_n, the group of automorphisms is the dihedral group of permutations, D_n [Rod14]. The set of $n \times n$ matrices that commute with the automorphisms, C_G are real, symmetric and circulant matrices. Since the circulant matrices are parametrized by the vector $a \in \mathbb{R}^n$ with $a_i = A_{0i}$, we use the map $\text{circ}(a) = A$ for any circulant matrix A associated to the vector a (we refer to Eq. (68) for the definition of circulant matrices). A

circulant matrix has eigenvalues given by a multiple of the *discrete Fourier transform* of this vector [Dav79]

$$\forall k \in [n]\,;\, \lambda_k = \sqrt{n}(\mathcal{F}a)_k = \sum_l a_l \exp\left(\frac{2\pi i}{n} kl\right)$$

hence the positive-semidefinite of matrix A is equivalent to $\forall i \;:\; (\mathcal{F}a)_i \geq 0$. Then, by using Proposition 8.56, we have

$$\sigma(C_n) := \max\{t \in \mathbb{R} \;:\; J - tA_{C_n} \in \mathsf{SPN}_{C_n}\}.$$

such that

$$\mathsf{SPN}_{C_n} = \{R + E \;:\; R \in \mathsf{PSD}_n^{\mathbb{R}} \cap \mathsf{C}_{C_n} \text{ and } E \in \mathsf{EWP}_n^{sa} \cap \mathsf{C}_{C_n}\}$$

Using $R = \mathrm{circ}(r)$ and $E = \mathrm{circ}(e)$ and noting that $J - tA_{C_n} = \mathrm{circ}(1, 1-t, 1, \ldots, 1, 1-t)$, we can recast this as a linear program in the entries,

$$\begin{aligned}
\sigma(C_n) = \max \quad & t \\
\text{s.t.} \quad & r_{\pm 1} + e_{\pm 1} = 1 - t \\
\forall i \notin \{0, \pm 1\} \quad & r_i + e_i = 1 \\
& \mathcal{F}r \geq 0 \\
& e \geq 0 \\
& e_i = e_{-i} \\
& e, r \in \mathbb{R}^n
\end{aligned}$$

Assume the maximum is at $t = t^*$ with the values $r = r^*$ and $e = e^*$.

1. Define, $r' = r + e_0 |0\rangle$ and $e' = e - e_0 |0\rangle$. Clearly $\mathcal{F}r' = \mathcal{F}r + e_0 \mathcal{F} |0\rangle \geq 0$ and $e = e - e_0 |0\rangle \geq 0$. Also, $r' + e' = r + e$, therefore this change of variables gives the same value for t while having $e'_0 = 0$ and satisfying all the constraints. Therefore, we can assume $e^*_0 = 0$.

2. Assume that $e^*_{\pm 1} > 0$, then, since we have, $|\mathbf{1}_n\rangle - t^* a_G = r^* + e^*$, it implies that $|\mathbf{1}_n\rangle - (t^* + e^*_1)a_g = r^* + (e^* - e_1 |1\rangle - e_{-1} |-1\rangle)$, contradicting the fact that t^* is the optimum value. Hence, we also assume $e^*_{\pm 1} = 0$.

The arguments above simplifies the optimization problem to the following one,

$$\begin{aligned} \sigma(C_n) = \max \quad & t \\ \text{s.t.} \quad & r_0 = 1 \\ & r_{\pm 1} = 1 - t \\ \forall i \notin \{0, \pm 1\} \quad & r_i + e_i = 1 \\ & \mathcal{F} r \geq 0 \\ \forall i \notin \{0, \pm 1\} \quad & e_i \geq 0 \\ & e_i = e_{-i} \\ & e, r \in \mathbb{R}^n \end{aligned}$$

We show that $e_i \geq 0$ follows from the other constraints. The constraints, $\mathcal{F} r \geq 0$ and $r_0 = 1$ imply that $\forall i,\ |r_i| \leq 1$. Also, have $\forall i \notin \{0, \pm 1\},\ r_i + e_i = 1$. Therefore, it holds that $e_i = 1 - r_i \geq 0$. Moreover, we can these e_i freely such that $r_i + e_i = 1$. A quick calculation shows that,

$$\sigma(C_n) = 1 - \min\{r_1 \in \mathbb{R} : r_0 = 1,\ \mathcal{F} r \geq 0, r \in \mathbb{R}^n\}$$

Since the set $\{r \in \mathbb{R}^n : r_0 = 1, \mathcal{F} r \geq 0\}$ is convex, we may examine its extreme points, namely $\mathcal{F}^{-1}|0\rangle = \sqrt{n} \sum_{j=0}^{n-1} |j\rangle$ and $\frac{1}{2}\mathcal{F}^{-1}(|k\rangle + |-k\rangle) = \sqrt{n} \sum_{j=0}^{n-1} \cos\left(\frac{2\pi jk}{n}\right)|j\rangle$ ($k \neq 0$), as candidates for optimal solutions to the above problem. Consequently, we can compute the value

$$\sigma(C_n) = 1 - \min_k \cos(2\pi k/n) = \begin{cases} 1 + \cos(\pi/n) & \text{for } n \text{ odd}, \\ 2 & \text{for } n \text{ even}. \end{cases}$$

■

Finally, we remark that as $n \to \infty$, $\sigma(C_n) \to 2$ which is equal to $1 + \frac{1}{\omega(C_n)-1}$ for all n.

8.7.2 *Small graphs*

In this section we list graphs with a small number of vertices n which lead to positive indecomposable maps via the strict inequality

$$\sigma(G) < 1 + \frac{1}{\omega(G) - 1},$$

where $\sigma(G)$ is the quantity defined in Eq. (69) and $\omega(G)$ is the clique number of G.

For $n \leq 4$ there are no graphs for which the inequality above holds since $\mathsf{SPN}_n = \mathsf{COP}_n$. For $n = 5$, the 5-cycle is the only such graph, see Proposition 8.59. For $n = 6$, there are three such graphs, that we list below, see also Fig. 28.

- the *square + path* graph, with $\sigma(G) = (5+\sqrt{5})/4$ and $\omega(G) = 2$
- the *tadpole graph* $T_{5,1}$, with $\sigma(G) = (5+\sqrt{5})/4$ and $\omega(G) = 2$
- the *wheel graph* W_6, with $\sigma(G) = 1 + 1/\sqrt{5}$ and $\omega(G) = 3$.

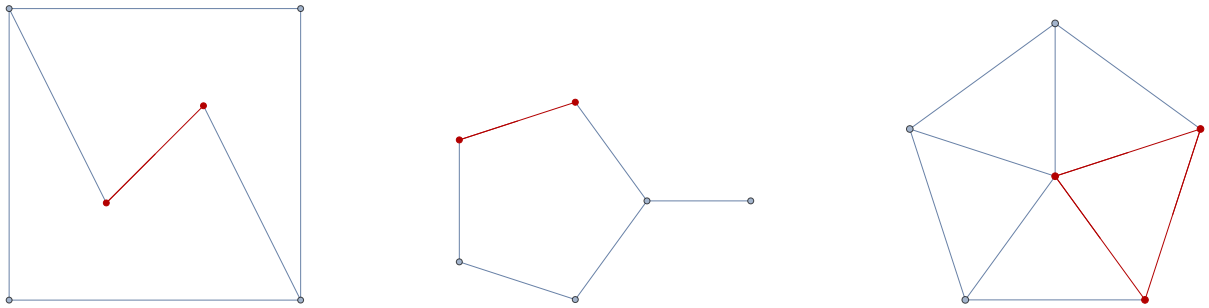


Figure 28: Graphs on 6 vertices leading to positive indecomposable maps. From left to right, the square + path graph, the tadpole graph, and the wheel graph. A maximal clique of each graph is highlighted in red. Note that the wheel graph is the first graph not covered by the Proposition 8.57 as it is not triangle-free.

Let us prove that $\sigma(G) = 1 + 1/\sqrt{5}$ for the wheel graph $G = W_6$, leaving the other two cases for the reader. We shall exhibit primal and dual feasible points for the semidefinite programs from Eq. (69) and Eq. (72) that correspond to lower, resp. upper bounds for $\sigma(G)$. Assigning the last index (6) to the center of the wheel, the adjacency matrix of G is given by

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}.$$

For the primal feasible point, consider the decomposition $J - (1 + 1/\sqrt{5})A = P + E$, where

$$P = \frac{1}{\sqrt{5}}J + \left(1 - \frac{1}{\sqrt{5}}\right)I - \frac{2}{\sqrt{5}}A \quad \text{and } E = \left(1 - \frac{1}{\sqrt{5}}\right)(J - I - A).$$

Clearly $E \in \mathsf{EWP}_6$, while a simple computation shows that the eigenvalues of P are $(2, 2, 2, 0, 0, 0)$, thence $P \in \mathsf{PSD}_6^{\mathbb{R}}$, proving that $\sigma(G) \geq 1 + 1/\sqrt{5}$ by using Eq. (69).

For the upper bound, consider the matrix

$$X = \begin{bmatrix} b & a & 0 & 0 & a & b \\ a & b & a & 0 & 0 & b \\ 0 & a & b & a & 0 & b \\ 0 & 0 & a & b & a & b \\ a & 0 & 0 & a & b & b \\ b & b & b & b & b & c \end{bmatrix}, \qquad \text{with } \begin{cases} a = \dfrac{3-\sqrt{5}}{20} \\ b = \dfrac{\sqrt{5}-1}{20} \\ c = \dfrac{5-\sqrt{5}}{20}. \end{cases}$$

One can show that the eigenvalues of X are $\big((5-\sqrt{5})/10, (3\sqrt{5}-5)/20, (3\sqrt{5}-5)/20, 0, 0, 0\big)$, proving that $X \in \mathsf{DNN}_6$. We also have $\mathrm{Tr}(AX) = 10(a+b) = 1$ and $\mathrm{Tr}(JX) = 10a + 15b + c = 1 + 1/\sqrt{5}$, hence $\sigma(G) \leq 1 + 1/\sqrt{5}$ by Eq. (72), finishing the proof.

For $n = 7$, we have numerically found 33 such graphs using an SDP solver. The code is available at [GNP25a].

8.7.3 *Strongly regular graphs*

A *strongly regular graph* (SRG) is a graph that exhibits a specific kind of regularity [BVM22], [GR13, Chapter 10]. Beyond being k-regular, the number of common neighbors between any two distinct vertices depends only on whether they are adjacent or not. In this section we shall use the symmetry properties of SRG to compute the decomposability parameter σ from (69) in order to put forward large families of positive indecomposable maps Φ_t^G associated to strongly regular graphs.

The structural properties of an SRG G are precisely captured by four parameters (n, k, λ, μ):

- n is the number of vertices of G
- every vertex of G is of degree k (G is k-regular)
- every pair of *adjacent* vertices in G have λ common neighbors
- every pair of *non-adjacent* vertices in G have μ common neighbors.

Strongly regular graphs are fascinating objects that appear in various branches of mathematics, including combinatorics (e.g. in the study of combinatorial designs and error-correcting codes), group theory (often arising as orbital graphs of permutation groups), and algebraic graph theory, where their highly symmetric structure leads to interesting spectral properties. The existence and the number of non-isomorphic SRG for given parameters

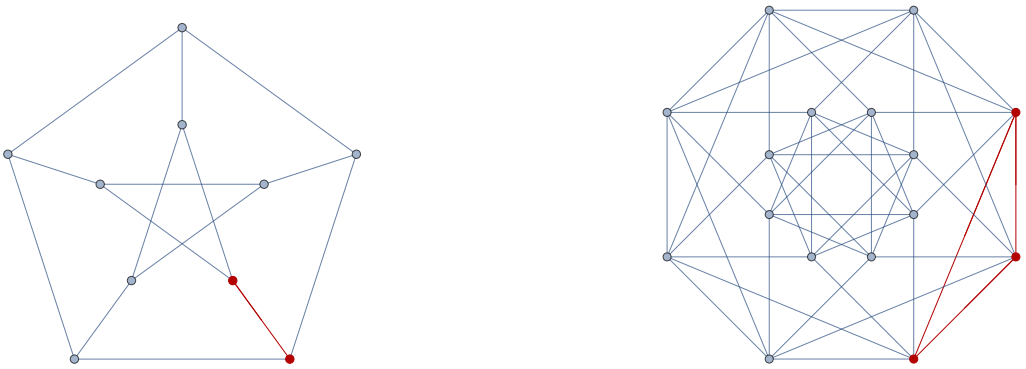


Figure 29: The Petersen (left) and the Shrikhande (right) are SRG with respective parameters $(10, 3, 0, 1)$ and $(16, 6, 2, 2)$. Maximal cliques are highlighted in red.

is subject to ongoing research [BVM22, Bro]. See Fig. 29 for two famous strongly regular graphs.

By definition, the adjacency matrix A of a SRG satisfies the following properties:

- $AJ = JA = kJ$, since each vertex has degree k;
- $A^2 = kI + \lambda A + \mu(\mathring{J} - A)$. This equation follows from considering the number of paths of length 2 between any two vertices.

If G is connected, its adjacency matrix A typically has three distinct eigenvalues [GR13, Chapter 10.2]. The largest eigenvalue is k, the degree of each vertex. This eigenvalue has multiplicity 1 (if G is connected and $n > 1$) and its corresponding eigenvector is the all-ones vector $\mathbf{1}$. The other two eigenvalues, commonly denoted r and s, are given by the formula:

$$r, s = \frac{\lambda - \mu \pm \sqrt{(\lambda - \mu)^2 + 4(k - \mu)}}{2}.$$

By convention, r is taken with the '$+$' sign, so $r \geq 0 \geq s$. For example, the two graphs in Fig. 29 have the following spectra:

- the Petersen graph has eigenvalues $k = 3$ with multiplicity 1, $r = 1$ with multiplicity 5, and $s = -2$ with multiplicity 4;
- the Shrikhande graph has eigenvalues $k = 6$ with multiplicity 1, $r = 2$ with multiplicity 6, and $s = -2$ with multiplicity 9.

Let us also note that if G is a SRG with parameters (n, k, λ, μ), then the complementary graph $\bar{G}$ is also strongly regular, with parameters

$$\bar{n} = n, \quad \bar{k} = n - k - 1, \quad \bar{\lambda} = n + \mu - 2(k + 1), \quad \bar{\mu} = n + \lambda - 2k.$$

The matrices A_G and $A_{\bar{G}}$ commute, with $A_{\bar{G}}$ having non-trivial eigenvalues corresponding to those of A_G:

$$\bar{r} = -r - 1 \quad \text{and} \quad \bar{s} = -s - 1; \tag{74}$$

we refer to [GR13, Chapter 10] for the spectral properties of SRGs.

We now show how the symmetry properties of certain SRGs enable us to compute exactly the decomposability parameter σ defined in Eq. (69). Recall the matrix space C_G considered previously in Eq. (73)

$$\mathsf{C}_G := \{X \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R}) \,:\, [X, P_\pi] = 0 \quad \forall \pi \in \mathrm{Aut}(G)\}.$$

Clearly, $I, J, A_G \in \mathsf{C}_G$ and $A_{\bar{G}} = J - I - A_G \in \mathsf{C}_G$. We are interested in SRGs for which these 3 matrices form a basis of the vector space C_G.

Definition 8.60. A strongly regular graph G is said to be *rank 3* if the automorphism group $\mathrm{Aut}(G)$ acts on the vertex set of G as a rank 3 permutation group. In other words, the action of $\mathrm{Aut}(G)$ on $V(G) \times V(G)$ partitions it into exactly 3 orbits:

- the diagonal $\{(v, v) \,:\, v \in V(G)\}$
- adjacent vertices $\{(u, v) \,:\, u \sim v,\, u \neq v\}$
- non-adjacent vertices $\{(u, v) \,:\, u \nsim v,\, u \neq v\}$.

There has been considerable effort in characterizing rank 3 SRGs, see [BVM22, Chapter 11]. For example, the Petersen graph from Fig. 29 is rank 3, while the Shrikhande graph has rank 4: non-adjacent vertices have 2 common neighbors that can be either adjacent or non-adjacent (see [BVM22, Chapter 10.6]).

For rank 3 SRGs, the vector space C_G is isomorphic to $\mathbb{R}^3$:

$$\mathsf{C}_G = \{X_{\alpha\beta\gamma} := \alpha I + \beta A_G + \gamma A_{\bar{G}} \,:\, \alpha, \beta, \gamma \in \mathbb{R}\}. \tag{75}$$

We shall now use the symmetry properties of (rank 3) SRGs to provide a simpler characterization of the parameter σ. By Proposition 8.56, we have $\sigma(G) = \hat{\sigma}(G)$ where

$$\hat{\sigma}(G) := \max\{t \in \mathbb{R} \,:\, J - tA_G \in \mathsf{SPN}_G\}.$$

and

$$\mathsf{SPN}_G := \{R + E \,:\, R \in \mathsf{PSD}_n^{\mathbb{R}} \cap \mathsf{C}_G \text{ and } E \in \mathsf{EWP}_n^{\mathrm{sa}} \cap \mathsf{C}_G\}$$

We now have all the ingredients for the main result of this section, an explicit formula for $\sigma(G)$ in the case of rank 3 SRGs.

Theorem 8.61. For a rank 3 SRG G with parameters (n, k, λ, μ), we have

$$\sigma(G) = \frac{n(r+1)}{r(n-1)+k}.$$

Proof. Using Proposition 8.56 and Eq. (75), we have

$$\begin{aligned}\sigma(G) = \max\{t \in \mathbb{R} \ : J - tA_G = X_{\alpha'\beta'\gamma'} + X_{\alpha''\beta''\gamma''} \text{ with} \\ X_{\alpha'\beta'\gamma'} \in \mathsf{PSD}_n^{\mathbb{R}} \text{ and } X_{\alpha''\beta''\gamma''} \in \mathsf{EWP}_n^{\mathrm{sa}}\}.\end{aligned}$$

Note that $J - tA_G = X_{1,1-t,1}$ and, using the eigenvalue formulas for the complementary graph (74)

$$\begin{aligned} X_{\alpha'\beta'\gamma'} \in \mathsf{PSD}_n^{\mathbb{R}} &\iff \begin{cases} \alpha' + \beta' k + \gamma'(n-k-1) \geq 0 \\ \alpha' + \beta' r - \gamma'(r+1) \geq 0 \\ \alpha' + \beta' s - \gamma'(s+1) \geq 0 \end{cases} \\ X_{\alpha''\beta''\gamma''} \in \mathsf{EWP}_n^{sa} &\iff \alpha'', \beta'', \gamma'' \geq 0. \end{aligned}$$

We can now recast the semidefinite program definition of $\sigma(G)$ as a much simpler linear program:

$$\begin{aligned} \sigma(G) = \max \quad & t \\ \text{s.t.} \quad & \alpha' + \alpha'' = 1 \\ & \beta' + \beta'' = 1 - t \\ & \gamma' + \gamma'' = 1 \\ & \alpha' + \beta' k + \gamma'(n-k-1) \geq 0 \\ & \alpha' + \beta' r - \gamma'(r+1) \geq 0 \\ & \alpha' + \beta' s - \gamma'(s+1) \geq 0 \\ & \alpha'', \beta'', \gamma'' \geq 0. \end{aligned}$$

A simple analysis shows that one can take $\alpha'' = \beta'' = 0$ and $\alpha' = 1$ and rewrite the optimization problem as follows:

$$\begin{aligned} \sigma(G) = 1 - \min \quad & \beta' \\ \text{s.t.} \quad & 1 + \beta' k + \gamma'(n-k-1) \geq 0 && (76) \\ & 1 + \beta' r - \gamma'(r+1) \geq 0 && (77) \\ & 1 + \beta' s - \gamma'(s+1) \geq 0 && (78) \\ & \gamma' \leq 1. && (79) \end{aligned}$$

Using $s \leq 0 \leq r$ one can show that (77) and (78) $\implies$ (79). Hence the feasible set is a triangle determined by the three vertices obtained by solving pairs of equations from Eqs. (76), (77), (78). Intersecting the equalities from (77) and (78) yields $\beta' = 1$, while intersecting (76) with (77) and (78) respectively yields

$$\beta' = -\frac{n-k+r}{r(n-1)+k} \quad \text{and} \quad \beta' = -\frac{n-k+s}{s(n-1)+k}.$$

The first value above is smaller, and a simple computation gives the announced result. ■

Corollary 8.62. For the complete graph $\mathcal{K}_n$, we have

$$\sigma(\mathcal{K}_n) = \omega(\mathcal{K}_n)/(\omega(\mathcal{K}_n) - 1) = n/(n-1).$$

Proof. The complete graph $\mathcal{K}_n$ is a rank 2 SRG with parameters $(n, n-1, n-2, \mu)$, with an undefined parameter μ. The result above still applies, with the positive eigenvalue $r = \lambda_{\max}(J - I) = n - 1$. ■

We present in Table 15 a table of all non-isomorphic rank 3 strongly regular graphs with less than 20 vertices, following [BVM22, Chapter 11.6]. We refer to [BVM22, Bro] for the families of graphs appearing in the table. We highlight in the last column the graphs G for which positive indecomposable maps of the form Φ_t^G exist; these graphs are identified by the strict inequality

$$\sigma(G) < \frac{\omega(G)}{\omega(G) - 1},$$

where $\sigma(G)$ is computed using Theorem 8.61. Note that the Hamming graph of parameters (2,4), which is the direct product of two complete graphs $\mathcal{K}_4$, is a strongly regular graph of rank 3 having parameters $(16, 6, 2, 2)$; these parameters are identical to those of the Shrikhande graph from Fig. 29, proving that these two SRGs having the same parameters are non-isomorphic.

Let us conclude this section by providing an infinite family of SRGs which yield positive indecomposable maps. Recall that *Paley graphs* of order q are defined for prime powers q such that $q = 1 \pmod 4$. The vertex set of $\mathrm{Paley}(q)$ is the finite field $\mathbb{F}_q$, and two vertices are adjacent if their difference is a (non-zero) square in $\mathbb{F}_q$. $\mathrm{Paley}(q)$ is a strongly regular graphs with parameters

$$\left(q, \frac{q-1}{2}, \frac{q-5}{4}, \frac{q-1}{4}\right)$$

having eigenvalues

$$r, s = \frac{-1 \pm \sqrt{q}}{2}$$

with multiplicities $(q-1)/2$. Importantly, Paley graphs are self-complementary, and vertex- and edge-transitive; hence they are rank 3. We refer the reader to [BVM22, Chapter 7.4]. Theorem 8.61 gives

$$\sigma(\mathrm{Paley}(q)) = 1 + \frac{1}{\sqrt{q}-1} = \frac{q+\sqrt{q}}{q-1}.$$

Computing the clique (or independence) number of Paley graphs is a very difficult problem [BVM22, Chapter 7.4.4]. The Hoffman spectral bound gives

$$\omega(\mathrm{Paley}(q)) \leq \sqrt{q}, \tag{80}$$

which is known in the literature as the "trivial bound". This is relevant for the existence of positive indecomposable maps given by Paley graphs, since

$$\sigma(\mathrm{Paley}(q)) < 1 + \frac{1}{\omega(\mathrm{Paley}(q))-1} \iff \omega(\mathrm{Paley}(q)) < \sqrt{q}.$$

In other words, a Paley graph G provides positive indecomposable maps Φ_t^G for some values of t if and only if it does not saturate the trivial bound for the clique number! It is known that if q is an even prime power, then the trivial bound (80) is saturated [BDR88]. However, if $q = p$ is prime, it has been shown in [HP21] that

$$\omega(\mathrm{Paley}(p)) \leq \frac{\sqrt{2p-1}+1}{2} < \sqrt{p},$$

which provides us with the following corollary.

Corollary 8.63. For any prime number p, and every

$$t \in \left(1 + \frac{1}{\sqrt{p}-1}, 1 + \frac{2}{\sqrt{2p-1}-1}\right],$$

the linear map $\Phi_t^{\mathrm{Paley}(p)}$ is positive and indecomposable.

Note that the considerations above match the data from Table 15: the Paley graphs with parameters $q = 5, 13, 17$ have a gap, while the perfect square $q = 9$ does not.

8.8 BOSONIC EXTENDIBILITY AND SOS HIERARCHIES

In this section, we will shift our focus to detect the extendibility properties of quantum states. This notion is closely connected to the problem of entanglement detection as

it provides useful necessary criteria for separability of quantum states. We introduce various different notions of quantum extensions, and make interesting connections to the hierarchies that have been well-studied for copositive matrices. This allows us to apply known results from polynomial optimization to the problem of entanglement detection.

It is known that checking copositivity is a co-NP complete problem [MK87, DG14]. Hierarchies of polynomially-sized semidefinite programs (SDP) or sum-of-squares (SOS) programs can be used to approximate the cone COP_n. These hierarchies either provide inner and outer approximations that converge to the actual cone. See, for example, the works of [DKP02] and [SV24] for details on such approximation schemes. First of all, we recall the hierarchy of inner approximations to COP_n based on sum of squares [Par00]:

$$\mathsf{K}_n^{(r)} = \{X \in \mathcal{M}_n^{sa}(\mathbb{R}) : x \in \mathbb{R}^n \mapsto \langle x^{\odot 2}|X|x^{\odot 2}\rangle \|x\|_2^{2r} \text{ is SOS}\}.$$

The following results are known about this hierarchy:

- [Par00] $\mathsf{K}_n^{(0)} = \mathsf{SPN}_n = \mathsf{PSD}_n^{\mathbb{R}} + \mathsf{EWP}_n^{\mathrm{sa}}$. In particular we have, $\mathsf{COP}_n = \mathsf{K}_n^{(0)}$ for $n \leq 4$.

- [Par00, DDGH13] If $n \geq 5$, $\mathsf{K}_n^{(0)} \subsetneq \mathsf{K}_n^{(1)} \subseteq \cdots \subseteq \mathsf{K}_n^{(r)} \subsetneq \mathsf{COP}_n$.

- [LV23, SV24] $\bigcup_{r\geq 0} \mathsf{K}_5^{(r)} = \mathsf{COP}_5$ and $int(\mathsf{COP}_n) \subsetneq \bigcup_{r\geq 0} \mathsf{K}_n^{(r)} \subsetneq \overline{\bigcup_{r\geq 0} \mathsf{K}_n^{(r)}} = \mathsf{COP}_n$ for $n \geq 6$.

Let us mention that connection between hierarchies of semidefinite programs for polynomial optimization and hierarchies of separability tests in quantum information has been previously considered in [DPS04, FF21], where the well-known Doherty-Parrilo-Spedalieri (DPS) hierarchy for detecting entanglement has been shown to be dual to a sum-of-squares (SOS) representations for certain Hermitian polynomials. This duality has been used to establish quantitative bounds on the convergence rate of the DPS hierarchy. In this section, we establish hierarchies for LDUI/CLDUI witnesses that detect both PPT-bosonic extendibility [DPS04, NOP09] and complete graph extendibility [ACG+26], and we provide a complete characterization of such witnesses using the copositive hierarchy. In particular, we provide surprisingly wide family of entanglement witnesses which are not certifiable by any level of the DPS hierarchy, thus providing counterexamples to the question dating back to [DPS04]. We also conjecture (see Question 8.70) that the copositive hierarchy can be lifted to provide explicit witnesses for the DPS extendibility hierarchy interpolating the "lifting" in Theorem 8.26 and Theorem 8.35.

8.8.1 *DPS hierarchy*

We use $\bigvee^r \mathbb{C}^n$ to denote the r-fold symmetric subspace of $(\mathbb{C}^n)^{\otimes r}$. We start by defining the DPS hierarchy, or the hierarchy of bosonic (or bose-symmetric) extendibility

Definition 8.64. A state $\rho \in \mathsf{PSD}(\mathbb{C}^n \otimes \mathbb{C}^n)$ is called r-bosonic extendible if there exists a positive operator $\tilde{\rho} \in \mathsf{PSD}(\mathbb{C}^n \otimes \bigvee^r \mathbb{C}^n)$ such that for all $1 \leq i \leq r$, the marginal state of system $\{0, i\}$ is ρ:

$$\forall\, 1 \leq i \leq r \quad \rho_{0i} := \mathrm{I}_n \otimes \mathrm{Tr}_{[r]\setminus\{i\}}\left(\tilde{\rho}\right) = \rho,$$

where we label the subsystems of $\mathbb{C}^n \otimes \bigvee^r \mathbb{C}^n$ by $0, 1, \ldots, r$. Similarly, we call a state r-PPT bosonic extendible, if such an extension is also required to be PPT across all bipartitions. We will denote the set of r-bosonic extendible and its PPT version as $\mathsf{BExt}_n^{(r)}$ and $\mathsf{PPTBExt}_n^{(r)}$ respectively.

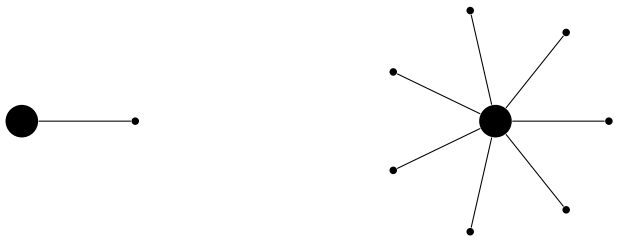


Figure 30: On the left, we denote the state a bipartite ρ, and on the right, the the notion of r-extension that we consider in Definition 8.64. The marginal over any edges of the graph should be equal to ρ. Moreover, we demand that the systems corresponding to the nodes of the star graph together live in the bosonic subspace $\mathsf{BExt}_n^{(r)}$, and for PPT extendible states $\mathsf{PPTBExt}_n^{(r)}$, we impose the PPT condition across all bipartitions.

We have the following inclusion and convergence relations between the sets,

$$\begin{array}{ccccccccc}
\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n) & \subseteq & \mathsf{BExt}_n^{(r)} & \subseteq & \cdots & \subseteq & \mathsf{BExt}_n^{(1)} & = & \mathsf{PSD}(\mathbb{C}^n \otimes \mathbb{C}^n) \\
\| & & \cup| & & & & \cup| & & \cup| \\
\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n) & \subseteq & \mathsf{PPTBExt}_n^{(r)} & \subseteq & \cdots & \subseteq & \mathsf{PPTBExt}_n^{(1)} & = & \mathsf{PPT}(\mathbb{C}^n \otimes \mathbb{C}^n)
\end{array}$$

$$\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n) = \bigcap_{r\geq 1} \mathsf{BExt}_n^{(r)} = \bigcap_{r\geq 1} \mathsf{PPTBExt}_n^{(r)},$$

where the last fact follows from [DPS04].

Remark 8.65. Note that the separable states have a r-bosonic extension and an r-PPT bosonic extension for all $r \geq 2$. For a separable state $\rho = \sum_k |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k|$ we have the following extension that is also PPT across all bipartitions,

$$\tilde{\rho} = \sum_k |v_k\rangle\langle v_k| \otimes |w_k\rangle\langle w_k|^{\otimes r}$$

Let us first recall the following remarkable characterization of *bosonic extendibility witnesses* in terms of the SOS hierarchy for a certain Hermitian form. The precise connection was implicit in [DPS04, Doh14] and later made explicit in [FF21].

Theorem 8.66. Let $W \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) \otimes \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$ be a bipartite Hermitian operator. Then for $r \geq 1$,

1. $W \in (\mathsf{BExt}_n^{(r)})^\circ$ if and only if there exists a positive semidefinite matrix $Z \in \mathcal{M}_n(\mathbb{C})^{\otimes(r+1)}$ such that, for all vectors $v, w \in \mathbb{C}^n$,

$$\langle vw \,|\, W \,|\, vw\rangle \cdot \|w\|_2^{2(r-1)} \;=\; \langle vw\cdots w \,|\, Z \,|\, vw\cdots w\rangle. \tag{81}$$

2. $W \in (\mathsf{PPTBExt}_n^{(r)})^\circ$ if and only if there exist psd matrices $Z_0, Z_1, \ldots, Z_r \in \mathcal{M}_n(\mathbb{C})^{\otimes(r+1)}$ such that, for all vectors $v, w \in \mathbb{C}^n$,

$$\begin{aligned}\langle vw|W|vw\rangle\|w\|_2^{2(r-1)} &= \langle vw\cdots w|Z_0 + Z_1^{\Gamma_{[1]}} + \cdots + Z_r^{\Gamma_{[r]}}|vw\cdots w\rangle \\ &= \langle vw^{\otimes r}|Z_0|vw^{\otimes r}\rangle + \sum_{j=1}^{r}\langle v\bar{w}^{\otimes j}w^{\otimes r-j}|Z_j|v\bar{w}^{\otimes j}w^{\otimes r-j}\rangle,\end{aligned} \tag{82}$$

   where $\Gamma_{[j]}$ is the partial transpose operation with respect to the tensor bipartition $\{1,\ldots,j\} : \{0, j+1, \ldots, r\}$.

Note that for all $r \geq 0$, we have the following inclusions:

$$(\mathsf{PPTBExt}_n^{(r)})^\circ \subseteq \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ = \{W \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})^{\otimes 2} : \langle vw|W|vw\rangle \geq 0 \;\forall v, w \in \mathbb{C}^n\},$$

where the last set is the cone of *block-positive* matrices. We also remark that Eqs. (81) and (82) indeed provide SOS decompositions of the Hermitian form $(v,w)\mapsto \langle vw|W|vw\rangle \|w\|_2^{2(r-1)}$ since they are conic combinations of Hermitian forms of the type

$$v,w\in\mathbb{C}^n \mapsto \left|\langle\psi|v\bar{w}^{\otimes j}w^{\otimes r-j}\rangle\right|^2,\quad \psi\in(\mathbb{C}^n)^{\otimes r+1},\ \ j=0,1,\ldots,r.$$

Now following the previous arguments in Propositions 8.20 and 8.34, we further provide a *necessary* condition for the LDUI/CLDUI operators to witness r-extendibility based on the copositive SOS hierarchy $(\mathsf{K}_n^{(r)})_{r\geq 0}$.

Proposition 8.67. Let $(A,B)\in \mathcal{M}_n(\mathbb{R})\underset{\mathbb{R}^n}{\times}\mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$. If $r\geq 1$ and $X_{A,B}^{(\mathsf{C})\mathsf{LDUI}}\in(\mathsf{PPTBExt}_n^{(r)})^\circ$, then

$$(A+\mathring{B})+(A+\mathring{B})^\top = A+A^\top+2\mathrm{Re}(\mathring{B})\in\mathsf{K}_n^{(r-1)}.$$

Proof. From Theorem 8.66, there exist PSD matrices $Z_0,\ldots,Z_r\in\mathcal{M}_n(\mathbb{C})^{\otimes r+1}$ such that

$$h(v,w):=\langle vw|X_{A,B}^{(\mathsf{C})\mathsf{LDUI}}|vw\rangle\|w\|_2^{2(r-1)}=\sum_{j=0}^r\langle v\bar{w}^{\otimes j}w^{\otimes r-j}|Z_j|v\bar{w}^{\otimes j}w^{\otimes r-j}\rangle,\quad v,w\in\mathbb{C}^n.$$

Setting $v=w=x\in\mathbb{R}^n$ and by the relations Eqs. (57) and (58), we have that the polynomial

$$h(x,x)=\langle x^{\odot 2}|A+\mathring{B}|x^{\odot 2}\rangle\|x\|_2^{2(r-1)}=\frac{1}{2}\langle x^{\odot 2}|A+A^\top+2\mathrm{Re}(\mathring{B})|x^{\odot 2}\rangle\|x\|_2^{2(r-1)}$$

is SOS. This concludes $A+A^\top+2\mathrm{Re}(\mathring{B})\in\mathsf{K}_n^{(r-1)}$. ∎

Later in Theorem 8.74, we will establish the precise correspondence between $X_{A,B}^{\mathsf{LDUI}}$ satisfying $A+A^\top+2\mathrm{Re}(\mathring{B})\in\mathsf{K}_n^{(r-1)}$ and the notion of *complete graph extendibility*.

On the other hand, it was questioned in [DPS04, Section VI] whether the set $\mathsf{Sep}(\mathbb{C}^n\otimes\mathbb{C}^n)^\circ$ can be saturated by the cones $(\mathsf{PPTBExt}_n^{(r)})^\circ$, i.e., whether the equality

$$\mathsf{Sep}(\mathbb{C}^n\otimes\mathbb{C}^n)^\circ=\bigcup_{r\geq 1}(\mathsf{PPTBExt}_n^{(r)})^\circ \tag{83}$$

holds. Since $\mathsf{Sep}(\mathbb{C}^n\otimes\mathbb{C}^n)^\circ=\left(\cap_{r\geq 1}\mathsf{PPTBExt}_n^{(r)}\right)^\circ=\overline{\cup_{r\geq 1}(\mathsf{PPTBExt}_n^{(r)})^\circ}$, the question mathematically asks whether the closure is essential or not. It was shown in [DPS04, Theorem 2] that the interior of $\mathsf{Sep}(\mathbb{C}^n\otimes\mathbb{C}^n)^\circ$ is contained in $\cup_{r\geq 1}(\mathsf{PPTBExt}_n^{(r)})^\circ$. In other words, every entanglement witness W which is "strictly" block-positive,

$$\langle vw|W|vw\rangle>0,\quad \forall\, v,w\neq 0,$$

is certifiable by r-SOS property for some finite r. Conversely, any witness $W \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ \setminus \cup_{r\geq 1}(\mathsf{PPTBExt}_n^{(r)})^\circ$, if exists, could be used to detect entanglement of quantum states that are r-PPT bosonic extendible for each $r \geq 1$. Moreover, W would be on the boundary in the sense that $\mathrm{Tr}(W\rho) = 0$ for some $\rho \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)$, as discussed in [DPS04]. Note that the set $\cup_{r\geq 1}(\mathsf{PPTBExt}_n^{(r)})^\circ$ is not precisely the interior of $\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$: $W = X^{\mathsf{LDUI}}_{J_4,\widetilde{H}-\mathring{J}_4} \in \mathsf{PPT}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ = (\mathsf{PPTBExt}_n^{(1)})^\circ$ from Example 8.37 while we have

$$\mathrm{Tr}\big(W\,|v\rangle\langle v|^{\otimes 2}\big) = \langle v^{\otimes 2}|X^{\mathsf{LDUI}}_{J_4,\widetilde{H}-\mathring{J}_4}|v^{\otimes 2}\rangle = \langle v^{\odot 2}|\widetilde{H}|v^{\odot 2}\rangle = 0$$

for $v = \frac{1}{\sqrt{2}}(0,1,1,0)^\top \in \mathbb{C}^4$, and hence $W \notin int\big(\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ\big)$.

Now we provide the following *explicit ($(n^2-n)/2$-dimensional) counterexamples* to the question in Eq. (83) which strengthens Corollary 8.38.

Theorem 8.68. Suppose $n \geq 6$ and let M be a copositive matrix which does not have r-SOS property for any r, i.e., $M \in \mathsf{COP}_n \setminus \cup_{r\geq 0}\mathsf{K}_n^{(r)}$. Then for any $N \in \mathsf{EWP}_n^{\mathrm{sa}}$ with $\mathrm{diag}(N) = \mathrm{diag}(M)$ and $N_{ij} \geq \frac{1}{2}M_{ij}\ \forall\, i \neq j \in [n]$, we have

$$X^{(\mathsf{C})\mathsf{LDUI}}_{N,M-\mathring{N}} \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ \setminus \bigcup_{r\geq 1}(\mathsf{PPTBExt}_n^{(r)})^\circ.$$

Furthermore, all these entanglement witnesses are on the boundary of $\mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$.

Proof. The fact $X^{(\mathsf{C})\mathsf{LDUI}}_{N,M-\mathring{N}} \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ$ follows from Lemma 8.7, Proposition 8.19, and Theorem 8.26. Furthermore, Proposition 8.67 implies that $X^{(\mathsf{C})\mathsf{LDUI}}_{N,M-\mathring{N}} \notin (\mathsf{PPTBExt}_n^{(r)})^\circ$ for any $r \geq 0$. The last assertion follows a priori from [DPS04, Theorem 2], as mentioned earlier. ∎

Remark 8.69. The existence of copositive matrices in $\mathsf{COP}_n \setminus \cup_{r\geq 0}\mathsf{K}_n^{(r)}$ for arbitrary $n \geq 6$ was first shown in [LV23]. One such example is

$$M = H \oplus 0_{(n-5)\times(n-5)} \in \mathsf{COP}_n \setminus \bigcup_{r\geq 0}\mathsf{K}_n^{(r)}, \quad n \geq 6,$$

where $H \in \mathsf{COP}_5$ is the Horn matrix defined in Eq. (52). For other examples, we refer to [LV23, Theorem 3, Example 1 and 3]. In particular, this implies that

$$X^{(\mathsf{C})\mathsf{LDUI}}_{J_n, M-\mathring{J}_n} \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ \setminus \bigcup_{r\geq 1} (\mathsf{PPTBExt}^{(r)}_n)^\circ,$$
$$X^{(\mathsf{C})\mathsf{LDUI}}_{J_5\oplus 0_{(n-5)\times(n-5)}, (H-\mathring{J}_5)\oplus 0_{(n-5)\times(n-5)}} \in \mathsf{Sep}(\mathbb{C}^n \otimes \mathbb{C}^n)^\circ \setminus \bigcup_{r\geq 1} (\mathsf{PPTBExt}^{(r)}_n)^\circ.$$

Note that the latter matrix is a (trivial) lifting of $5 \otimes 5$ Hermitian matrix $X^{(\mathsf{C})\mathsf{LDUI}}_{J_5, H-\mathring{J}_5}$ into $n \otimes n$ system (we also refer to [SN21, Proposition 4.8]). Since

$$\begin{aligned}&\langle vw| X^{\mathsf{LDUI}}_{J_5\oplus 0_{(n-5)\times(n-5)}, (H-\mathring{J}_5)\oplus 0_{(n-5)\times(n-5)}} |vw\rangle \|w\|_2^{2(r-1)} \\ &= \Big(\sum_{1\leq i<j\leq 5} |v_i \overline{w}_j - v_j \overline{w}_i|^2 + \sum_{i,j=1}^{5} (v_i \overline{v}_j w_i \overline{w}_j H_{ij}) \Big) \Big(\sum_{j=1}^{n} |w_j|^2 \Big)^{r-1}\end{aligned}$$

is SOS for no $n \geq 6$ and $r \geq 1$, this actually shows that

$$\mathsf{Sep}(\mathbb{C}^{n_A} \otimes \mathbb{C}^{n_B})^\circ \supsetneq \bigcup_{r\geq 1} (\mathsf{PPTBExt}^{(r)}_{n_A, n_B})^\circ$$

whenever $n_A \geq 5$ and $n_B \geq 6$, by embedding $X^{\mathsf{LDUI}}_{J_5, H-\mathring{J}_5}$ into proper spaces.

Recall that we constructed positive maps by lifting copositive matrices to the matrix pairs of the form $(N, M - \mathring{N})$ in Theorem 8.26. We leave open the question whether a similar "lifting" construction of r-extendibility witnesses can be carried out from the hierarchies of copositive matrices.

Question 8.70. For $r \geq 2$ and $M \in \mathsf{K}^{(r-1)}_n$, do we have $X^{(\mathsf{C})\mathsf{LDUI}}_{N, M-\mathring{N}} \in (\mathsf{PPTExt}^{(r)}_n)^\circ$ for some choice of $N \in \mathsf{EWP}^{sa}_n$? Moreover, is it possible to choose $\mathring{N} = \max(M)\mathring{J}$ similar to the construction in Theorem 8.26?

Note that the above assertion for $r = 1$ already follows from Theorem 8.35. Although the complete answer to the above question remains unclear, we show in the next section that another type of hierarchy of extensions, called *complete graph extendibility*, can be fully characterized in terms of the copositive sum of squares hierarchy, generalizing some results from the literature.

8.8.2 *Complete extendibility*

Let $\mathcal{K}_r$ denotes the complete graph with r vertices. A bosonic quantum state is called *$\mathcal{K}_r$-PPT bosonic extendible* (or *r-PPT bosonic exchangeable*) if there exists a bosonic operator $\tilde{\rho} \in \mathsf{PSD}\left(\bigvee^r \mathbb{C}^n\right)$ such that $(\mathrm{I}_n^{\otimes 2} \otimes \mathrm{Tr}^{\otimes r-2})(\tilde{\rho}) = \rho$ and $\tilde{\rho}$ is also PPT across every bipartition of the r systems. We refer to [ACG+26] for general notion of graph extendibility.

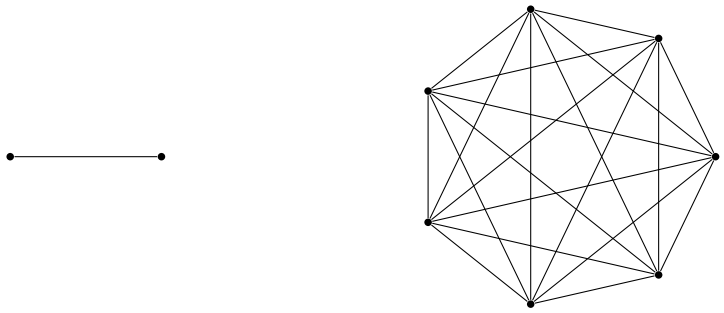
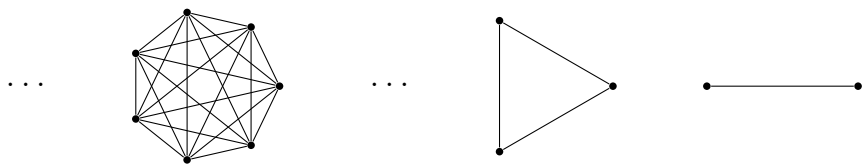


Figure 31: On the left, we denote a bipartite bosonic state ρ, and on the right, the the notion of r-extension that we consider in Definition 8.64. The marginal over every edge of the graph should be equal to ρ. Moreover, we demand that the global state corresponding to the complete graph should live in the bosonic subspace. For PPT extendible states $\mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$, we impose the PPT condition across all bipartitions.

For $r \geq 2$, let us denote by $\mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$ the convex cone of $n \otimes n$ bosonic positive-semidefinite operators ρ which are $\mathcal{K}_r$-PPT bosonic extendible. It is clear that $\mathsf{PPTBExt}_n^{(\mathcal{K}_2)}$ is simply the set of PPT bipartite bosonic operators $\mathsf{PPT}(\mathbb{C}^n \vee \mathbb{C}^n)$, and we also have an inclusion chain for $\mathcal{K}_r$-bosonic extendible states.

$$\mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n) \subseteq \mathsf{PPTBExt}_n^{(\mathcal{K}_r)} \subseteq \cdots \subseteq \mathsf{PPTBExt}_n^{(\mathcal{K}_3)} \subseteq \mathsf{PPTBExt}_n^{(\mathcal{K}_2)} = \mathsf{PPT}(\mathbb{C}^n \vee \mathbb{C}^n). \tag{84}$$



Indeed, the set of separable bosonic states are exactly equal the cone generated by product bosonic states [ISTY08], i.e

$$\mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n) = \mathrm{cone}\{|v\rangle\langle v| \otimes |v\rangle\langle v|\}$$

Therefore a separable bosonic state $\rho = \sum_k |v_k\rangle\langle v_k| \otimes |v_k\rangle\langle v_k|$ has a $\mathcal{K}_r$-bosonic extension $\sum_k |v_k\rangle\langle v_k|^{\otimes r}$ for all $r \geq 2$.

Furthermore, $\mathsf{PPTBExt}_n^{(\mathcal{K}_{r+1})} \subseteq \mathsf{PPTBExt}_n^{(r)} \subseteq \mathsf{BExt}_n^{(r)}$ for $r \geq 1$. Thus, from the previous hierarchy of $(\mathsf{PPTBExt}_n^{(r)})_{r\geq 1}$ or simply from *Quantum de Finetti theorem* [CFS02, CKMR07], we again have

$$\mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n) = \bigcap_{r\geq 2} \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}.$$

It is natural to ask whether the inclusion in Eq. (84) would be finite or not. That is, given some local Hilbert space dimension n, is there a finite $r \geq 2$ such that

$$\mathsf{PPTBExt}_n^{(\mathcal{K}_r)} = \mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)?$$

If $n = 2$ the question is obvious: $\mathsf{PPTBExt}_2^{(\mathcal{K}_2)} = \mathsf{PPT}(\mathbb{C}^2 \vee \mathbb{C}^2) = \mathsf{Sep}(\mathbb{C}^2 \vee \mathbb{C}^2)$. When $n \geq 3$, it is shown that $\mathsf{PPT}(\mathbb{C}^n \vee \mathbb{C}^n) \supsetneq \mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)$ [TG09, MATS21]. However, explicit construction of examples beyond this, i.e., entangled bose-symmetric states having high degree of extendibility, remains to be a challenging problem.

This section is mainly devoted to finding an explicit element in $\mathsf{PPTBExt}_n^{(\mathcal{K}_r)} \setminus \mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)$ for every $n \geq 5$ and $r \geq 2$, that is, an extendible and highly symmetric PPT entangled state. We also show that such a state exists within the class of (mixtures of) bipartite *Dicke states*, [Yu16, TAQ+18]. Our result also allows us to construct r-partite entangled bosonic states of which are PPT with respect to all bipartitions, by looking at the bosonic extension of a matrix $\mathsf{PPTBExt}_n^{(r-1)} \setminus \mathsf{Sep}_n$. Due to the fact that it is an extension, the entanglement of this bosonic state can be even verified by checking that the *two-body* marginals are entangled.

Remark 8.71. Any r-partite bosonic state $\rho \in \mathsf{PSD}(\bigvee^r \mathbb{C}^n)$ have only two types of entanglement [ATSL12, TG09]:

1. ρ is *fully separable*, i.e., $\rho = \sum_i |v_i\rangle\langle v_i|^{\otimes r}$ for some vectors $v_i \in \mathbb{C}^n$,
2. ρ is *genuine entangled* i.e., ρ cannot be written as a convex combination of states which are separable with respect to (possibly different) bipartitions.

In particular, any bosonic state which is not fully separable is entangled across any bipartitions of the system. Hence, we do not make a distinction within various notions of multipartite entanglement for this class of states.

Simiarly as in Theorem 8.66, we first derive a SOS correspondence to the dual of $\mathcal{K}_r$-PPT bosonic extendibility (i.e the set of witnesses for $\mathcal{K}_r$-PPT bosonic extendibility), which we prove later has a correspondence with the SOS hierarchy for LDUI/CLDUI witnesses.

Theorem 8.72. For a Hermitian operator $W \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C}) \otimes \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$ and for $r \geq 2$, the following are equivalent.

1. $W \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$;
2. There exist positive semidefinite matrices $Z_0, Z_1, \ldots, Z_{\lfloor r/2 \rfloor} \in \mathcal{M}_n(\mathbb{C})^{\otimes r}$ such that, for all vectors $v \in \mathbb{C}^n$,

$$\begin{aligned}\langle v^{\otimes 2}|W|v^{\otimes 2}\rangle \|v\|_2^{2(r-2)} &= \langle v^{\otimes r}|Z_0 + Z_1^{\Gamma_{[1]}} + \cdots + Z_{\lfloor r/2 \rfloor}^{\Gamma_{[\lfloor r/2 \rfloor]}}|v^{\otimes r}\rangle \\ &= \sum_{j=0}^{\lfloor r/2 \rfloor} \langle \overline{v}^{\otimes j} v^{\otimes r-j}|Z_j|\overline{v}^{\otimes j} v^{\otimes r-j}\rangle,\end{aligned}$$

   where $\Gamma_{[j]} = \top^{\otimes j} \otimes \mathrm{I}_n^{\otimes r-j}$ is the partial transpose operation with respect to the tensor bipartition $\{[j], [r] \setminus [j]\}$.

Proof. **((1)⇒(2))** If $W \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$, then by definition we have

$$\mathrm{Tr}\left((W \otimes I_n^{\otimes r-2})\tilde{\rho}\right) = \mathrm{Tr}(W\rho) \geq 0,$$

where $\rho \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$ and $\tilde{\rho}$ is any $\mathcal{K}_r$-PPT bosonic extension of ρ. Note that $\tilde{\rho} \in \mathcal{B}\left(\vee^r \mathbb{C}^n\right)^+$ can be chosen to have a constraint that $\tilde{\rho}^{\top_{[j]}} \geq 0$ for all $j = 1, \ldots, \lfloor r/2 \rfloor$, that is indeed the the condition that $\tilde{\rho}$ is PPT with respect to every bipartition. We claim that there exist PSD operators $Z_0, \ldots, Z_{\lfloor r/2 \rfloor} \in \mathcal{M}_n(\mathbb{C})^{\otimes r}$ such that

$$\Pi_S(W \otimes I_n^{\otimes r-2})\Pi_S = \Pi_S\Big(Z_0 + \sum_{j=1}^{\lfloor r/2 \rfloor} Z_j^{\Gamma_{[j]}}\Big)\Pi_S,$$

where Π_S is a projection of $(\mathbb{C}^n)^{\otimes r}$ onto the symmetric space $(\mathbb{C}^n)^{\vee r}$. This will imply that

$$\langle v^{\otimes 2}|W|v^{\otimes 2}\rangle \|v\|_2^{2(r-2)} = \langle v^{\otimes r}|\Pi_S(W \otimes I_n^{\otimes r-2})\Pi_S|v^{\otimes r}\rangle = \langle v^{\otimes r}|Z_0 + Z_1^{\Gamma_{[1]}} + \cdots + Z_{r-1}^{\Gamma_{[\lfloor r/2 \rfloor]}}|v^{\otimes r}\rangle$$

for $v \in \mathbb{C}^n$. Note that the extension $\tilde{\rho} \in \bigcap_{j=0}^{\lfloor r/2 \rfloor} \mathcal{C}_j$ where $\mathcal{C}_0 = \mathsf{PSD}\left(\vee^r \mathbb{C}^n\right)$ and

$$\mathcal{C}_j = \{X \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})^{\otimes r} : X^{\Gamma_{[j]}} \geq 0\}.$$

Therefore, the required condition says that $W \otimes I_n^{\otimes r-2} \in \left(\bigcap_{j=0}^{\lfloor r/2 \rfloor} \mathcal{C}_j\right)^\circ = \overline{\sum_{j=0}^{\lfloor r/2 \rfloor} \mathcal{C}_j^\circ}$. In other words, there exists $Z_0, \ldots, Z_{\lfloor r/2 \rfloor}$ such that

$$W \otimes I_n^{\otimes r-2} = Z_0 + \sum_{j=1}^{\lfloor r/2 \rfloor} Z_j^{\Gamma_{[j]}}$$

where $\Pi_S Z_0 \Pi_S \geq 0$, $Z_j \geq 0$ for $j \geq 1$ (since $Z_j^{\top[j]} \in \mathcal{C}_j^\circ$), showing the claim (The closure can be ignored as we can show that the set of Hermitian polynomials of the type

$$h_{Z_0,\ldots,Z_{\lfloor r/2 \rfloor}}(z) = \sum_{j=0}^{\lfloor r/2 \rfloor} \langle \overline{z}^{\otimes j} z^{\otimes r-j} | Z_j | \overline{z}^{\otimes j} z^{\otimes r-j} \rangle, \quad z \in \mathbb{C}^n,$$

is closed. Indeed, this set is the conic hull of the set of Hermitian forms $z \mapsto |\langle \varphi | \overline{z}^{\otimes j} z^{\otimes r-j} \rangle|^2$ for $\varphi \in (\mathbb{C}^n)^{\otimes r}$ and $j = 0, 1, \ldots, \lfloor r/2 \rfloor$.)

((2)⇒(1)) The condition in **??** is equivalent to

$$\langle v^{\otimes r} | \Big(W \otimes I_n^{\otimes r-2} - (Z_0 + \sum_{j=1}^{\lfloor r/2 \rfloor} Z_j^{\Gamma[j]}) \Big) | v^{\otimes r} \rangle = 0 \quad \forall\, v \in \mathbb{C}^n$$

$$\iff \operatorname{Tr}\Big(X \Big(W \otimes I_n^{\otimes r-2} - (Z_0 + \sum_{j=1}^{\lfloor r/2 \rfloor} Z_j^{\Gamma[j]}) \Big) \Big) = 0 \quad \forall\, X \in span\{ |v^{\otimes r}\rangle\langle v^{\otimes r}| : v \in \mathbb{C}^n \}.$$

It is well-known that $span\{ |v^{\otimes r}\rangle\langle v^{\otimes r}| : v \in \mathbb{C}^n \} = \mathcal{B}\big(\bigvee^r \mathbb{C}^n \big)$ [Chi10, Har13], and hence one has

$$\Pi_S (W \otimes I_n^{\otimes r-2}) \Pi_S = \Pi_S (Z_0 + Z_1^{\Gamma[1]} + \cdots Z_{\lfloor r/2 \rfloor}^{\Gamma[\lfloor r/2 \rfloor]}) \Pi_S.$$

Now for $\rho \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$ and for $\tilde{\rho}$ a $\mathcal{K}_r$-PPT bosonic extension of ρ, it is straightforward that

$$\operatorname{Tr}(W\rho) = \operatorname{Tr}\left(\Pi_S (Z_0 + Z_1^{\top[1]} + \cdots Z_{\lfloor r/2 \rfloor}^{\Gamma[\lfloor r/2 \rfloor]}) \Pi_S \tilde{\rho} \right) = \operatorname{Tr}(Z_0 \tilde{\rho}) + \sum_{j=1}^{\lfloor r/2 \rfloor} \operatorname{Tr}\left(Z_j \tilde{\rho}^{\Gamma[j]} \right) \geq 0,$$

and therefore, $W \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$. ■

Next, let us recall the following characterization of SOS polynomials from [ZVP06, Proposition 9].

Proposition 8.73. Let $p(x)$ be a real homogeneous polynomial in $x \in \mathbb{R}^n$ of degree r such that $p(x^{\odot 2})$ is a sum of squares. Then p admits a decomposition of the form

$$p(x) = \sum_{j=0}^{\lfloor r/2 \rfloor} \sum_{\substack{\alpha \in \mathbb{N}_0^n \\ |\alpha| = r-2j}} x^\alpha \psi_{j,\alpha}(x)^2 \tag{85}$$

where $|\alpha| := \alpha_1 + \cdots + \alpha_n$, $x^\alpha := x_1^{\alpha_1} \cdots x_n^{\alpha_n}$, and each $\psi_{j,\alpha}$ is a homogeneous polynomial of degree j.

Recall from Proposition 8.67 that a necessary condition for $X^{\mathsf{LDUI}}_{A,B} \in (\mathsf{PPTBExt}^{(r-1)}_n)^\circ$ is

$$A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{K}^{(r-2)}_n.$$

The next result shows that this is actually also sufficient when we consider the dual of $\mathcal{K}_r$-PPT bosonic extendibility (note that $(\mathsf{PPTBExt}^{(r-1)}_n)^\circ \subseteq (\mathsf{PPTBExt}^{(\mathcal{K}_r)}_n)^\circ$).

Theorem 8.74. Let $(A, B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}^{\mathrm{sa}}_n(\mathbb{C})$ and let $r \geq 2$. Then $X^{\mathsf{LDUI}}_{A,B} \in (\mathsf{PPTBExt}^{(\mathcal{K}_r)}_n)^\circ$ if and only if

$$A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{K}^{(r-2)}_n.$$

In particular, we have $X^{\mathsf{LDUI}}_{N,M-\mathring{N}} \in (\mathsf{PPTBExt}^{(\mathcal{K}_r)}_n)^\circ$ for any $M \in \mathsf{K}^{(r-2)}_n$ and $N \in \mathcal{M}^{\mathrm{sa}}_n(\mathbb{R})$ such that $\mathrm{d}iag(N) = \mathrm{d}iag(M)$.

Proof. Let us consider a Hermitian polynomial

$$\begin{aligned} h(z) &:= \langle z^{\otimes 2} | X^{\mathsf{LDUI}}_{A,B} | z^{\otimes 2} \rangle \|z\|_2^{2(r-2)} \\ &= \langle z \odot \overline{z} | A + \mathring{B} | z \odot \overline{z} \rangle \|z\|_2^{2(r-2)} \\ &= \frac{1}{2} \langle z \odot \overline{z} | A + A^\top + 2\mathrm{Re}(\mathring{B}) | z \odot \overline{z} \rangle \|z\|_2^{2(r-2)} \end{aligned}$$

for $z \in \mathbb{C}^n$, where the second and third equalities follow from the duality relation Eq. (57) and the observation $z \odot \overline{z} \in \mathbb{R}^n$. If $X^{\mathsf{LDUI}}_{A,B} \in (\mathsf{PPTBExt}^{(\mathcal{K}_r)}_n)^\circ$, then Theorem 8.72 implies that the real polynomial $x \in \mathbb{R}^n \mapsto h(x)$ is a sum of squares, and hence $A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{K}^{(r-2)}_n$.

Conversely, if $A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{K}^{(r-2)}_n$, then Proposition 8.73 implies that $h(z) = p(z \odot \overline{z})$ where $p = \sum_{j=0}^{\lfloor r/2 \rfloor} \sum_\alpha x^\alpha \psi^2_{j,\alpha}$ is written as in Eq. (85). Let us further write

$$\psi_{j,\alpha}(x) = \sum_{\beta \in \mathbb{N}^n_0,\, |\beta| = j} c^{(j,\alpha)}_\beta x^\beta$$

for coefficients $c^{(j,\alpha)}_\beta \in \mathbb{R}$. Now for $0 \leq j \leq \lfloor r/2 \rfloor$ and $\alpha \in \mathbb{N}^n_0$, one has

$$\begin{aligned} (z \odot \overline{z})^\alpha \big(\psi_{j,\alpha}(z \odot \overline{z})\big)^2 &= |z_1|^{2\alpha_1} \cdots |z_n|^{2\alpha_n} \Big(\sum_{|\beta| = j} c^{(j,\alpha)}_\beta |z_1|^{2\beta} \cdots |z_n|^{2\beta_n} \Big)^2 \\ &= \Big| \sum_{|\beta| = j} c^{(j,\alpha)}_\beta z_1^{\alpha_1 + \beta_1} \cdots z_n^{\alpha_n + \beta_n} \overline{z}_1^{\beta_1} \cdots \overline{z}_n^{\beta_n} \Big|^2 \\ &= \big| \langle \varphi_{j,\alpha} | \overline{z}^{\otimes j} z^{\otimes r-j} \rangle \big|^2, \end{aligned}$$

where $|\varphi_{j,\alpha}\rangle := \sum_{|\beta|=j} c_\beta^{(j,\alpha)} \big(|1\rangle^{\otimes\beta_1}\cdots|n\rangle^{\otimes\beta_n} \otimes |1\rangle^{\otimes\alpha_1+\beta_1}\cdots|n\rangle^{\otimes\alpha_n+\beta_n}\big) \in (\mathbb{C}^n)^{\otimes r}$. Consequently, we obtain $h(z) = \sum_{j=0}^{\lfloor r/2\rfloor} \langle \overline{z}^{\otimes j} z^{\otimes r-j} | Z_j | \overline{v}^{\otimes j} z^{\otimes z-j}\rangle$ for positive semidefinite matrices

$$Z_j = \sum_{|\alpha|=r-2j} |\varphi_{j,\alpha}\rangle\langle\varphi_{j,\alpha}| \in \mathsf{PSD}\big(\mathbb{C}^{\otimes r}\big), \quad 0 \leq j \leq \lfloor r/2\rfloor.$$

By comparison with **??**, we conclude that $X_{A,B}^{\mathsf{LDUI}} \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$. ■

We provide further characterizations of the dual cones of separable / PPT bosonic states.

Corollary 8.75. For a pair $(A, B) \in \mathcal{M}_n(\mathbb{R}) \underset{\mathbb{R}^n}{\times} \mathcal{M}_n^{\mathrm{sa}}(\mathbb{C})$,

1. $X_{A,B}^{\mathsf{LDUI}} \in \mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)^\circ$ if and only if $A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{COP}_n$,
2. $X_{A,B}^{\mathsf{LDUI}} \in \mathsf{PPT}(\mathbb{C}^n \vee \mathbb{C}^n)^\circ$ if and only if $A + A^\top + 2\,\mathrm{Re}(\mathring{B}) \in \mathsf{K}_n^{(0)} = \mathsf{SPN}_n$.

In particular, given $M \in \mathsf{COP}_n \setminus \mathsf{SPN}_n$, we can generate an LDUI operator $X_{N,M-\mathring{N}}^{\mathsf{LDUI}}$, where $\mathrm{diag}(N) = \mathrm{diag}(M)$ and $N \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$, as a witness for PPT entanglement of (bipartite) bosonic states.

Proof. Since $\mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n) = conv\{|v^{\otimes 2}\rangle\langle v^{\otimes 2}| : v \in \mathbb{C}^n\}$, $X_{A,B}^{\mathsf{LDUI}} \in \mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)^\circ$ if and only if

$$\begin{aligned}
&\langle z^{\otimes 2}|X_{A,B}^{\mathsf{LDUI}}|z^{\otimes 2}\rangle = \frac{1}{2}\langle z\odot\overline{z}|A + A^\top + 2\mathrm{Re}(\mathring{B})|z\odot\overline{z}\rangle \geq 0 \quad \forall\, z \in \mathbb{C}^n \\
&\iff \langle x^{\odot 2}|A + A^\top + 2\mathrm{Re}(\mathring{B})|x^{\odot 2}\rangle \geq 0 \quad \forall\, x \in \mathbb{R}^n \\
&\iff A + A^\top + 2\mathrm{Re}(\mathring{B}) \in \mathsf{COP}_n,
\end{aligned}$$

showing (1). The assertion (2) simply follows from Theorem 8.74 with $r = 2$. ■

Remark 8.76. The class of bosonic witness introduced in Corollary 8.75 generalize the witnesses considered in [MATS21]. Their "indecomposable bosonic" witness corresponds to setting $(A, B) = (\mathrm{diag}(M), M)$, and $X_{\mathrm{diag}(M),M}^{\mathsf{LDUI}} = \sum_{ij} M_{ij}\,|ij\rangle\langle ji|$. Moreover, our results in Theorem 8.74 show that these witnesses can be generalized using copositive hierarchies to detect **complete** bosonic extendibility of quantum states.

Let us also record the result analogous to Theorem 8.68, which follows directly from Theorem 8.74 and Corollary 8.75.

Corollary 8.77. If $n \geq 6$ and $M \in \mathsf{COP}_n \setminus \bigcup_{r\geq 0} \mathsf{K}_n^{(r)}$, then we have for any $N \in \mathcal{M}_n^{\mathrm{sa}}(\mathbb{R})$,

$$X_{N,M-\mathring{N}}^{\mathsf{LDUI}} \in \mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)^\circ \setminus \bigcup_{r\geq 2} (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ.$$

In particular, $\mathsf{Sep}(\mathbb{C}^n \vee \mathbb{C}^n)^\circ = \overline{\bigcup_{r\geq 2}(\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ} \supsetneq \bigcup_{r\geq 2}(\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$ whenever $n \geq 6$.

Now we shift our focus to the characterization of (complete graph) extendibility of *Dicke states* introduced in Section 8.2.4. First of all, the following proposition is an easy application of [PY24, Proposition 3.2], but we include its proof for completeness.

Proposition 8.78. For $\pi : G \to \mathcal{U}_n$ a unitary representation of a compact group G, consider the $\pi \otimes \pi$-twirling operation

$$\mathcal{T}_{\pi\otimes\pi}(X) := \int_G (\pi(g) \otimes \pi(g)) X (\pi(g) \otimes \pi(g))^* dg, \quad X \in \mathcal{M}_n(\mathbb{C}) \otimes \mathcal{M}_n(\mathbb{C}),$$

where dg denotes the (normalized) Haar measure on G. Then $\mathcal{T}_{\pi\otimes\pi}$ preserves the properties regarding extendibility: if $X \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$ (resp. $(\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$), then $\mathcal{T}_{\pi\otimes\pi}(X) \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$ (resp. $(\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$).

Proof. It is straightforward to check that, if $\tilde{\rho}$ is a $\mathcal{K}_r$-PPT bosonic extension of $\rho \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$, then $\mathcal{T}_{\pi\otimes r}(\tilde{\rho}) = \int \pi(g)^{\otimes r} \tilde{\rho} (\pi(g)^*)^{\otimes r} dg$ is a $\mathcal{K}_r$-PPT bosonic extension of $\mathcal{T}_{\pi\otimes\pi}(\rho)$. On the other hand, if $W \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$, then

$$\mathrm{Tr}(\mathcal{T}_{\pi\otimes\pi}(W)\rho) = \mathrm{Tr}(W\mathcal{T}_{\pi\otimes\pi}(\rho)) \geq 0$$

since $\mathcal{T}_{\pi\otimes\pi}(\rho) \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$. This gives $\mathcal{T}_{\pi\otimes\pi}(W) \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$. ∎

Since $\mathsf{K}_n^{(r)}$ a proper subset of COP_n for all $n \geq 5$ and $r \geq 0$, we obtain the following main result in this section, which provides examples for quantum states in $\mathsf{PPTBExt}_n^{(\mathcal{K}_r)} \setminus \mathsf{Sep}_n$.

Theorem 8.79. The Dicke state $X_{P,P}^{\mathsf{LDUI}}$ is $\mathcal{K}_r$-PPT bosonic extendible ($r \geq 2$) if and only if $P \in (\mathsf{K}_n^{(r-2)})^\circ$. In particular, for $n \geq 5$, any matrix $P \in (\mathsf{K}_n^{(r-2)})^\circ \setminus \mathsf{CP}_n$ gives a $\mathcal{K}_r$-PPT bosonic extendible entangled state $X_{P,P}^{\mathsf{LDUI}}$.

Proof. Suppose $P \in (\mathsf{K}_n^{(r-2)})^\circ$ and let $W \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$. Then by Theorem 8.74 and Proposition 8.78, $X_{A,B}^{\mathsf{LDUI}} := \mathcal{T}_{\mathsf{LDUI}} W \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$ and $(A + \mathring{B}) + (A + \mathring{B})^\top \in \mathsf{K}_n^{(r-2)}$. Therefore, one has

$$\begin{aligned}\langle X_{P,P}^{\mathsf{LDUI}}, W\rangle &= \langle \mathcal{T}_{\mathsf{LDUI}} X_{P,P}^{\mathsf{LDUI}}, W\rangle = \langle X_{A,A}^{\mathsf{LDUI}}, \mathcal{T}_{\mathsf{LDUI}} W\rangle \\ &= \langle X_{P,P}^{\mathsf{LDUI}}, X_{A,B}^{\mathsf{LDUI}}\rangle = \langle P, A + \mathring{B}\rangle \\ &= \frac{1}{2}\langle P, (A + \mathring{B}) + (A + \mathring{B})^\top\rangle \geq 0.\end{aligned}$$

This shows that $X_{P,P}^{\mathsf{LDUI}} \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$. Conversely, suppose $X_{P,P}^{\mathsf{LDUI}} \in \mathsf{PPTBExt}_n^{(\mathcal{K}_r)}$ and let $M \in \mathsf{K}_n^{(r-2)}$. Then Theorem 8.74 again implies that $X_{Y,Y}^{\mathsf{LDUI}} \in (\mathsf{PPTBExt}_n^{(\mathcal{K}_r)})^\circ$ where $Y = \frac{1}{2}(M + diag(M))$. Therefore, we have

$$\langle P, M\rangle = \langle P, Y + \mathring{Y}\rangle = \langle X_{P,P}^{\mathsf{LDUI}}, X_{Y,Y}^{\mathsf{LDUI}}\rangle \geq 0,$$

establishing $P \in (\mathsf{K}_n^{(r-2)})^\circ$. ∎

Remark 8.80. This result gives examples of $\mathcal{K}_r$-PPT bosonic extendible entangled states for arbitrary $r \geq 2$. On the other hand, Theorem 8.79 also implies that the CLDUI state $X_{P,P}^{\mathsf{CLDUI}}$ is $\mathcal{K}_r$-PPT (non-bosonic) extendible for $P \in (\mathsf{K}_n^{(r-2)})^\circ$. The main difference is that $X_{P,P}^{\mathsf{CLDUI}} = (X_{P,P}^{\mathsf{LDUI}})^\Gamma$ is not a bosonic state, but is symmetric in the sense of commuting with the flip operator $F := \sum_{i,j} |ij\rangle\langle ji|$, i.e

$$F X_{P,P}^{\mathsf{CLDUI}} = X_{P,P}^{\mathsf{CLDUI}} F.$$

Corollary 8.81. For $n \geq 5$ and $r \geq 2$, there exists a bosonic state $\tilde{\rho} \in \mathsf{PSD}(\bigvee^r \mathbb{C}^n)$ that is PPT across every bipartition while being genuinely entangled (Remark 8.71). Moreover, such a state also exists within the class of *r-partite diagonal symmetric (or mixture of Dicke) states*, i.e., bosonic states with $\mathcal{DU}_n^{\otimes r}$-symmetry.

Proof. Let $P \in (\mathsf{K}_n^{(r-2)})^\circ \setminus \mathsf{CP}_n$ and let $\tilde{\rho}$ be a $\mathcal{K}_r$-PPT bosonic extension of a bipartite Dicke state $X_{P,P}^{\mathsf{LDUI}}$. We claim that $\tilde{\rho}$ satisfies the advertised property. Indeed, since $(\mathrm{I}_n^{\otimes\{1,2\}} \otimes \mathrm{Tr}^{\otimes[r]\setminus\{1,2\}})(\tilde{\rho}) = X_{P,P}^{\mathsf{LDUI}}$ is entangled, and since partial trace operations are separability preserving, this implies that $\tilde{\rho}$ is not fully separable. Finally, the same property holds if we consider the *$\mathcal{DU}^{\otimes r}$-twirling*

$$\mathcal{T}_{\mathcal{DU}_n^{\otimes r}}(\tilde{\rho}) := \int_{\mathcal{DU}_n} U^{\otimes r} \tilde{\rho} U^{*\otimes r} dU$$

of $\tilde{\rho}$, which is now a diagonal symmetric extension of $X_{P,P}^{\mathsf{LDUI}}$. ■

Remark 8.82. The same conclusion as in Corollary 8.81 was obtained in [RPAR+25]. A careful inspection of the arguments in that paper reveals that the existence of an r-partite PPT Dicke state having a PPT entangled bipartite reduction is assumed without proof. Theorem 8.79 and Corollary 8.81 fills in this gap in a mathematically rigorous way.

We also refer to [ATSL12] for a construction of r-qubit ($r \geq 4$) entangled states that are PPT across all bipartitions. Since we do not have the complete characterization of the hierarchy $\mathsf{PPTBExt}_n^{(r-1)}$, we do not know whether two hierarchies we consider are equivalent for bosonic states, or particularly mixtures of Dicke states. We pose this as the open question.

Question 8.83. For mixtures of Dicke states, are the following two sets equivalent?

$$\mathsf{PPTBExt}_n^{(\mathcal{K}_r)} = \mathsf{PPTBExt}_n^{(r-1)}, \quad r \geq 2$$

The sets are equivalent to if Question 8.70 admits a affirmative solution, in which case the arguments in Theorem 8.79 can be applied analogously to star r-extendibility. We would also like to state the following question regarding the $\mathsf{K}_n^{(r)}$ hierarchy and its potential implications for the theory of entanglement.

Question 8.84. For $n \geq 5$, is the inclusion $\mathsf{K}_n^{(r)} \subseteq \mathsf{K}_n^{(r+1)}$ strict for every $r \geq 1$? The affirmative answer would imply that all the inclusions in Eq. (84) are strict. Furthermore, the same strict inclusions would hold within the class of (mixtures of) Dicke states.

8.9 DISCUSSION AND OPEN PROBLEMS

This work introduces a unified and powerful framework that connects four key areas: the theory of *positive linear maps*, the *optimization theory of copositive matrices*, *algebraic graph theory*, and the rich structure of *quantum entanglement* in mixed states.

The impact of this unification is quite broad. For quantum information theorists, we provide a complete characterization of positivity for a major class of maps and a systematic method for producing new indecomposable maps and highly extendible entangled states. The established "lifting" theorems create a direct bridge from the mature, classical theory of copositive matrices to the quantum world, allowing for the construction of vast families of maps and states having useful properties for entanglement detection. Furthermore, our graph-theoretic construction, which links the properties of maps to fundamental graph parameters, offers a rich and structured source of these crucial examples.

We also believe this work will spur significant new directions of research. The newly introduced families of maps and states invite further investigation, particularly, it would be interesting to have a generalization of the copositive hierarchies to hierarchies for PCOP. The explicit connection between SOS hierarchies and state extendibility opens the door to applying powerful semidefinite programming tools developed in optimization theory to unsolved problems in entanglement theory. The new classes of positive-indecomposable maps might play a role in answering questions around PPT entanglement, particularly the PPT^2 conjecture [Chr12, CMHW19, SN22b] and the Schmidt number of PPT entangled states [HLLMH18, PV19, KG24].

Conflict of interest. The authors declare no competing interests.

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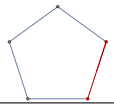
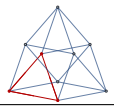
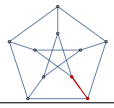
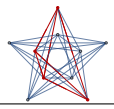
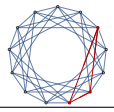
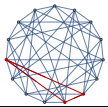
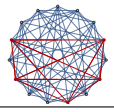
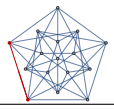
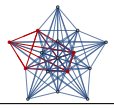
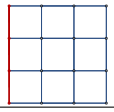
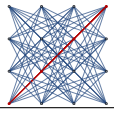
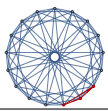
Name	Graph	Parameters	ω	σ	gap
pentagon C_5 = Paley(5)		$(5,2,0,1)$	2	$\frac{5+\sqrt{5}}{4}$	✔
Paley(9)		$(9,4,1,2)$	3	$\frac{3}{2}$	✗
Petersen		$(10,3,0,1)$	2	$\frac{5}{3}$	✔
complement of Petersen		$(10,6,3,4)$	4	$\frac{4}{3}$	✗
Paley(13)		$(13,6,2,3)$	3	$\frac{13+\sqrt{13}}{12}$	✔
GeneralizedQuadrangle(2,2)		$(15,6,1,3)$	3	$\frac{3}{2}$	✗
Triangular(6)		$(15,8,4,4)$	5	$\frac{5}{4}$	✗
Clebsch		$(16,5,0,2)$	2	$\frac{8}{5}$	✔
complement of Clebsch		$(16,10,6,6)$	5	$\frac{6}{5}$	✔
Hamming(2,4)		$(16,6,2,2)$	4	$\frac{4}{3}$	✗
complement of Hamming(2,4)		$(16,9,4,6)$	2	$\frac{4}{3}$	✗
Paley(17)		$(17,8,3,4)$	3	$\frac{17+\sqrt{17}}{16}$	✔

Table 15: Rank 3 strongly regular graphs with ≤ 20 vertices along with their parameters. The last column indicates whether $\sigma(G) < \omega(G)/(\omega(G)-1)$, i.e. whether positive indecomposable maps Φ_t^G exists.

9

Entanglement in the Dicke Subspace

This is the reproduction of the preprint **Entanglement in the Dicke subspace** by Aabhas Gulati, Ion Nechita and Clément Pellegrini. arXiv:2602.15800. [GNP26]

9.1 INTRODUCTION

The characterization of entanglement in mixed quantum states is an important challenge in quantum information theory. Entanglement is a central resource for various tasks in quantum communication [BBC+93], cryptography [Eke91], and even quantum computing [RB01, RBB03]. Although being an important question in quantum information, the separability problem, i.e deciding if bipartite mixed quantum state is entangled or separable has been shown to be NP-hard [Gur03, Gha10]. This implies the efficient algorithmic solution of the problem is out of reach, unless P=NP. Understanding entanglement in multipartite quantum systems is even more difficult, as there exist different notions of entanglement. In this setting, *genuine entanglement* underpins protocols such as secret sharing and multiparty teleportation [HBB99, CZG06].

In general, different criteria for detecting entanglement have been constructed. The most famous of them is the positivity under partial transpose (PPT) criterion: any unentangled (or separable) bipartite state remains positive after transposition is applied to either subsystem [Per96, Hor97]. This criterion is also sufficient in 2×2, or 2×3 systems [HHH96]; entangled states satisfying the PPT condition exist in all other dimensions. These states display some exotic properties; they cannot be distilled into pure entangled states and are central to the irreversibility of entanglement theory [VC01]. Moreover, even finding new constructions of such states has been observed to be highly challenging. Various open problems and conjectures surrounding this class of states remain open, for example, the PPT-squared conjecture [Chr12, CMHW19] and the maximum Schmidt number of PPT entangled states [HLLMH18, PV19, KG24].

The intrinsic indistinguishability of particles is a distinctly quantum mechanical phenomenon. In systems composed of such particles, the principles of quantum mechanics require that the particles be described not by individual quantum states, but rather by a single collective state encompassing the entire system. Moreover, the structure of this collective state depends fundamentally on whether the particles are *bosons* or *fermions*. Specifically, bosonic wavefunctions are symmetric under particle exchange, whereas fermionic wavefunctions are antisymmetric. Importantly, the quantum description of indistinguishable particle systems often involves a substantially reduced number of independent parameters, thereby simplifying the theoretical treatment of many problems in quantum information science.

There has been considerable progress in the understanding of multipartite entanglement in bosonic quantum systems. The bosonic states display the extreme features of multipartite entanglement; as they are either completely separable or genuinely entangled across all systems [ISTY08]. Moreover, even in three qubits, there are no PPT entangled states [ESBL02]. For all $n \geq 4$, n-qubit examples of quantum states satisfying the PPT condition for every bi-partition, and still being entangled, were obtained [ATSL12]. Also, the existence of 2-qutrit PPT entangled bosonic states was shown [TG09]. Surprisingly, in the bosonic subspace, the bipartite entanglement criterion, such as covariance and realignment, coincide with applying the PPT test [TG09].

In this article, we focus on a particular subclass of bosonic states called *mixtures of Dicke states*. It was shown that the theory of bipartite entanglement is connected to well-studied cones in polynomial optimization, the completely positive and copositive matrices [Yu16, TAQ$^+$18]. The NP-hardness of deciding whether a matrix is completely positive implies a corresponding complexity of the separability problem. Moreover, the PPT condition for these states is also in exact correspondence with a well-studied relaxation for completely positive matrices, known as *doubly non-negative matrices* [Yu16, TAQ$^+$18]. The doubly non-negative and completely positive cones coincide if and only if $d \leq 4$, and therefore, no PPT entangled states exist for this regime in the bipartite setting. Construction of PPT entangled states in multipartite states for $d \geq 5$ can be achieved by considering bipartite marginals that are PPT entangled [RPAR$^+$25]. At the same time, it was shown that for any n-qubit state in multipartite *mixtures of Dicke states*, there is no PPT entanglement [Yu16, GNP25b]. The class of mixture of Dicke states also enjoys the local *diagonal unitary symmetry*, recently studied in [SN21]. Recently, a strong conjecture was proposed in a recent work [RPAR$^+$25] that for a multi-partite mixture of Dicke states in $d = 3$ and $d = 4$, all separable states are PPT. Overall, the situation seemed far from understood, and a rigorous and well-understood mathematical framework to explicitly describe PPT and indecomposable maps was lacking. This is a central point for the questions in this paper :

Q_1. What is the appropriate parametrization and tools for the *mixtures of Dicke states* to properly utilise the reduced number of parameters?

Q_2. Can we characterize separability of the class of diagonally symmetric bosonic states using some generalization of completely positive matrices? Can we do something similar for the entanglement witnesses with the same symmetries?

Q_3. Can we characterise the PPT condition for such a given state? Is the PPT criterion also sufficient for separability in $d = 3, 4$ as conjectured in [RPAR+25]? Can we construct new examples of PPT entangled states and indecomposable witnesses?

This article provides a complete answer to all these questions by translating the entanglement properties of these states into well-known objects in tensor analysis and semi-algebraic geometry. The *dramatis personae* of this article are sum of square polynomials and tensors. Deciding whether a polynomial is globally non-negative is a central and computationally difficult problem in optimization theory. A tractable sufficient certificate is *sum-of-squares* (SOS): if $p = \sum_{k=1}^{K} f_k^2$, then $p(x) \geq 0$ for all $x \in \mathbb{R}^d$. Hilbert famously characterized the exceptional cases where non-negativity coincides with SOS [Hil88]; outside these regimes, there exist positive polynomials that are not SOS (e.g., the Motzkin/Robinson examples [Mot67, Rob73]). A canonical example in three variables is

$$p(x, y, z) = x^2y^4 + x^4y^2 + z^6 - 3x^2y^2z^2,$$

which satisfies $p \geq 0$ but is not SOS. To systematically tighten SOS certificates, one can use Positivstellensätze: for instance, test whether $p(x)\|x\|^{2r}$ is SOS for some r. This yields a semidefinite hierarchy for polynomial positivity; by a theorem of Reznick, every positive definite form is detected at some finite level [Rez95].

9.1.1 *Contributions*

We present below, in an informal way, the main ideas and results in this article.

- Tensor-based parametrisation of diagonally symmetric subspace: We introduce a novel way to parameterize the diagonally symmetric subspace in terms of symmetric tensors in Theorem 9.22, and Definition 9.25. This tensor can be understood as an array consisting of the diagonal entries of the state.

- Complete dictionary for entanglement properties: By using the new tensor-based parametrisation, we translate the entanglement properties of diagonally symmetric states into the well-studied properties of tensors. We establish a correspondence

between separability and completely positive tensors (Theorem 9.38), and on the dual side, entanglement witnesses and copositive tensors (Proposition 9.39). We also show the characterization of the PPT property in terms of the flattenings of the even slices of the tensors (Theorem 9.48). Moreover, the dual property of decomposability corresponds to the sum of squares relaxation of copositive tensors (Corollary 9.43). Our findings are summarized in Fig. 36.

- The balanced bipartition gives the strongest PPT criterion: For a mixture of Dicke states on n particles, we show that the PPT property across the most balanced bipartition (the one that transposes the first $\lfloor n/2 \rfloor$ particles, leaving the other $\lceil n/2 \rceil$ unchanged) is the most stringent one, in the sense that it implies the PPT property for all the other bipartitions (Corollary 9.49); this settles in the affirmative [RPAR+25, Conjecture III.1].

- PPT entangled states and indecomposable witnesses: We use some highly celebrated results in polynomial SOS to construct indecomposable witnesses, and to detect examples of PPT entangled states. We show that, except for qubits and bipartite systems with $d \leq 4$, all the other cases contain examples of PPT entangled states (Theorem 9.57). Moreover, these states are PPT across all bi-partitions. This also disproves the conjecture in [RPAR+25], i.e there exist PPT entangled states in 3 qutrits, and beyond.

- Bosonic Extendibility: We introduce the notion of the hypergraph (PPT) extendibility of bosonic states. Due to symmetry properties, it follows that all diagonally symmetric states are extendable if and only if there is a diagonally symmetric extension (Lemma 9.67). Moreover, the marginals of DS states correspond to the marginals of the corresponding symmetric tensor (Theorem 9.27). This shows that the extendibility of such states is equivalent to the classical extendibility problem for exchangeable probability distributions (Theorem 9.68). On the dual side, this implies that the non-negative and sum of squares hierarchy corresponds to the set of extendibility witnesses (Corollary 9.70).

- Dicke subsystems are entangled: We use the tensor parametrisation to compute reduced states of pure Dicke states. We provide a much simpler proof of the NPT property of all marginals (across all bipartitions). We show that all the 2-body marginals of pure entangled Dicke states are entangled (Proposition 9.58). This also reproduces the recently obtained results in [SN25].

Notation	Name	Description	Reference
$\mathsf{Sep}_d^{(n)}$	Bos. separable	$\mathrm{cone}\{\|v\rangle\langle v\|^{\otimes n} \mid v \in \mathbb{C}^d\}$	Eq. (103)
$\mathsf{PPT}_d^{(n)}$	Bos. PPT	$\{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \forall k \in [\lfloor n/2 \rfloor],\ X^{\Gamma_{[k]}} \succeq 0\}$	Definition 9.33
$\mathsf{PSD}_d^{(n)}$	Bos. PSD	$\{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid X \succeq 0\}$	Definition 9.33
$\mathsf{Dec}_d^{(n)}$	Decomposable	$\left\{X = \Pi_d^{(n)} \sum_{k=0}^{\lfloor n/2 \rfloor} P_k^{\Gamma_{[k]}} \Pi_d^{(n)}\right\}$	Corollary 9.37
$\mathsf{EW}_d^{(n)}$	Ent. Witness	$\{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \forall v \in \mathbb{C}^d,\ \langle v^{\otimes n} \| X \| v^{\otimes n}\rangle \geq 0\}$	Proposition 9.31

Table 16: Notation, definition, and main properties for bosonic matrices (Part I).

Notation	Name	Description	Reference
$\mathsf{BExt}_d^{(n,r)}$	Bos. Extendible	$\{\mathrm{Tr}_{[r]}(X) \mid X \in \mathsf{PSD}_d^{(n+r)}\}$	Eq. (110)
$\mathsf{PPTBExt}_d^{(n,r)}$	PPT Bos. Extendible	$\{\mathrm{Tr}_{[r]}(X) \mid X \in \mathsf{PPT}_d^{(n+r)}\}$	Eq. (110)
$\mathsf{ExtW}_d^{(n,r)}$	Extendibility Wit.	$\{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \Pi_d^{(n+r)}(X \otimes I^{\otimes r})\Pi_d^{(n+r)} \succeq 0\}$	Corollary 9.63
$\mathsf{DecExtW}_d^{(n,r)}$	Dec. Extendibility Witness	$\{X \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \Pi_d^{(n+r)}(X \otimes I^{\otimes r})\Pi_d^{(n+r)} \in \mathsf{Dec}_d^{(n+r)}\}$	Theorem 9.62

Table 17: Notation, definition, and main properties for bosonic matrices (Part II).

Notation	Name	Description	Reference
$\mathsf{CP}_d^{(n)}$	Completely Positive	$\mathrm{cone}\{v^{\otimes n} \mid v \in \mathbb{R}_+^d\}$	Definition 9.5
$\mathsf{Mom}_d^{(n)}$	Moment	$\{T \in \vee^n \mathbb{R}^d \mid \forall X \in \mathrm{SF}[T],\ X \succeq 0\}$	Eq. (109)
$\mathsf{NN}_d^{(n)}$	Nonnegative	$\{T \in \vee^n \mathbb{R}^d \mid \forall i \in [d]^n,\ T_i \geq 0\}$	Eq. (90)
$\mathsf{SOS}_d^{(n)}$	Sum-of-Squares	$\{T \in \vee^n \mathbb{R}^d \mid p_T(x \odot x) \in \Sigma_d^{(2n)}\}$	Definition 9.10
$\mathsf{Cop}_d^{(n)}$	Copositive	$\{T \in \vee^n \mathbb{R}^d \mid \forall x \in \mathbb{R}^d,\ p_T(x \odot x) \geq 0\}$	Proposition 9.6
$\mathsf{RSOS}_d^{(n,r)}$	Reznick-SOS	$\{T \in \vee^n \mathbb{R}^d \mid p_T(x \odot x)\|x\|^{2r} \in \Sigma_d^{(2n+2r)}\}$	Eq. (92)
$\mathsf{PNN}_d^{(n,r)}$	Polya-NN	$\{T \in \vee^n \mathbb{R}^d \mid p_T(x \odot x)\|x\|^{2r} \in \chi_d^{(2n+2r)}\}$	Eq. (94)
$\mathsf{MomExt}_d^{(n,r)}$	Moment Extendible	$\{\mathrm{tr}_{[r]}(X) \mid X \in \mathsf{Mom}_d^{(n+r)}\}$	Eq. (112)
$\mathsf{NNExt}_d^{(n,r)}$	Non-Negative Extendible	$\{\mathrm{tr}_{[r]}(X) \mid X \in \mathsf{NN}_d^{(n+r)}\}$	Eq. (113)

Table 18: Notation, definition, and main properties for convex cones of symmetric tensors.

9.1.2 *Organization of the article*

The paper is organized as follows: In Section 9.2, we provide some preliminary material to understand the article. In Section 9.3, we discuss the central object of this article, the diagonally symmetric subspace, and focus on the quantum states in this subspace called

the *mixtures of Dicke states*. We discuss the parametrisation of the diagonally symmetric bosonic subspace in terms of a symmetric tensor. In the Section 9.4, we discuss the entanglement properties of *mixtures of Dicke states* by showing exact correspondence to properties of tensors. In Section 9.4.4, we construct indecomposable entanglement witnesses using positive polynomials that do not have a sum of squares decomposition, like the Motzkin polynomial. We also provide some examples of PPT entangled states in 3 qutrits, and beyond. In the last Section 9.5, we discuss how the bosonic extendibility in the diagonally symmetric subspace, and show connections to non-negative and the sum of squares hierarchy for copositivity.

9.2 PRELIMINARIES AND BACKGROUND

9.2.1 *Notation*

We denote by $\mathbb{R}$ and $\mathbb{C}$ as the fields of real numbers and complex numbers, respectively. We denote by $\mathcal{M}_{d\times d'}(\mathbb{F})$, the set of $d \times d'$ matrices with entries in the field $\mathbb{F}$ which will be either $\mathbb{R}$ or $\mathbb{C}$. If $d = d'$, for ease of notation, we denote the set of matrices as just $\mathcal{M}_d(\mathbb{F}) := \mathcal{M}_{d\times d}(\mathbb{F})$. We use the Dirac bra-ket notation to denote vectors as $|v\rangle \in \mathbb{C}^d$, the dual vectors as $\langle v| \in (\mathbb{C}^d)^*$, and the complex inner product $\langle v, w\rangle := \langle v \mid w\rangle$. We use the indexed vectors $\{|i\rangle\}_{i=1}^d$ for the computational basis. The operator $|v\rangle\langle w| : \mathbb{C}^d \to \mathbb{C}^d$ is a linear operator with the matrix representation vw^* (or $vw^\dagger$ for physicists). By S_n, we denote the group of bijections from $[n] \to [n]$, called the symmetric group. For any finite set X, we use $|X|$ to denote the cardinality of the set. We use $\odot$ to denote the Hadamard product, i.e the entrywise product between vectors, $(v \odot w)_i = v_i w_i$.

9.2.2 *Symmetric subspace and Bosonic states*

Symmetric subspace

In this section, we provide a brief introduction to the symmetric subspace, which, while serving as the description of bosonic particles, also has a fundamental role in various other problems in quantum information. For a much more thorough quantum information-oriented introduction to this topic, the reader should refer to the excellent review [Har13].

For any element π in the symmetric group S_n, we define the following permutation operator $P_\pi : (\mathbb{C}^d)^{\otimes n} \to (\mathbb{C}^d)^{\otimes n}$,

$$P_\pi := \sum_{i_1,i_2\ldots i_n\in[d]} \left|i_{\pi^{-1}(1)} i_{\pi^{-1}(2)} \ldots i_{\pi^{-1}(n)}\right\rangle\!\left\langle i_1 i_2 \ldots i_n\right|.$$

Note that this is also a unitary representation of the group S_n on the space $(\mathbb{C}^d)^{\otimes n}$; in particular, we have $P_{\text{id}} = I^{\otimes n}$ and $(P_\pi)^* = P_{\pi^{-1}}$. We define the symmetric subspace of order n and local dimension d as the linear space of vectors $|\psi\rangle \in (\mathbb{C}^d)^{\otimes n}$ that are invariant under all permutations

$$\vee^n \mathbb{C}^d := \{|\psi\rangle \in (\mathbb{C}^d)^{\otimes n} \mid \forall \pi \in S_n,\ P_\pi |\psi\rangle = |\psi\rangle\}.$$

The symmetric subspace has an equivalent description as the following span [Har13, Theorem 3]:

$$\vee^n \mathbb{C}^d = \text{span}_{\mathbb{C}}\{|\psi\rangle^{\otimes n} \mid |\psi\rangle \in \mathbb{C}^d\}. \tag{86}$$

Moreover, the orthogonal projection into the symmetric subspace $\Pi_d^{(n)} : (\mathbb{C}^d)^{\otimes n} \to \vee^n \mathbb{C}^d$ can be explicitly constructed by the sum of the permutation operators,

$$\Pi_d^{(n)} := \frac{1}{n!} \sum_{\pi \in S_n} P_\pi.$$

Let $\alpha \in \mathbb{N}^d$ be a vector of natural numbers, such that $|\alpha| := \sum_{i \in [d]} \alpha_i = n$. We will denote the set of all such vectors as $\mathbb{N}_d^{(n)}$. We define the counting function, $\gamma : [d]^n \to \mathbb{N}_d^{(n)}$ with the components $\gamma(i)_j := |\{k \in [n] \mid i_k = j\}|$ that count the number of elements of the multi-index that get mapped to the value j. For all occupation vectors $\alpha \in \mathbb{N}_d^{(n)}$, there is a *unique* canonical multi-index (α) in $\gamma^{-1}(\alpha)$ that satisfies the ordering, $(\alpha)_1 \leq (\alpha)_2 \ldots \leq (\alpha)_n$.

We define the following pure quantum states labeled by $\alpha \in \mathbb{N}_d^{(n)}$,

$$|D_\alpha\rangle := \frac{1}{\sqrt{\binom{n}{\alpha}}} \sum_{i \in [d]^n : \gamma(i) = \alpha} |i\rangle \in (\mathbb{C}^d)^{\otimes n},$$

where $\binom{n}{\alpha} = \frac{n!}{\alpha_1! \alpha_2! \ldots \alpha_d!}$ is the multinomial coefficient. These states are known as *qudit Dicke states*, and vector α is called the *occupation vector*.

It is easy to verify that $\Pi_d^{(n)} |D_\alpha\rangle = |D_\alpha\rangle$ for all $\alpha \in \mathbb{N}_d^{(n)}$, hence the Dicke states are symmetric. These states are an orthonormal basis for the symmetric subspace $\vee^n \mathbb{C}^d$ [Har13, Theorem 3]. Therefore, the cardinality of the set $\mathbb{N}_d^{(n)}$ is equal to the dimension of the symmetric subspace. Hence we have,

$$d_{\text{sym}} = \dim(\vee^n \mathbb{C}^d) = |\mathbb{N}_d^{(n)}| = \binom{d+n-1}{d-1} = \binom{d+n-1}{n}.$$

For $n = 1$, the Dicke states are just equal to the computational basis:

$$|D_{(0,\ldots,1_i,\ldots,0)}\rangle = |i\rangle\,.$$

For the first non-trivial case, $n = 2$, we have the following possible occupation vectors

$$\begin{aligned} \forall i \neq j \quad & (0, \dots 1_i, \dots 1_j, \dots 0), \\ \forall i \quad & (0, \dots 2_i, \dots 0). \end{aligned}$$

These correspond to the following states in the computational basis:

$$\begin{aligned} |D_{(0,\dots 1_i,\dots 1_j,\dots 0)}\rangle &= \frac{|ij\rangle + |ji\rangle}{\sqrt{2}} \\ |D_{(0,\dots 2_i,\dots 0)}\rangle &= |ii\rangle \,. \end{aligned}$$

Multipartite bosonic states

We will now discuss the extension of the bosonic symmetry to linear operators. We have the following definition.

Definition 9.1. A matrix $X \in \mathcal{M}_d^{\otimes n}$ is called bosonic if any of the following equivalent statements are true.

(1) $X = \Pi_d^{(n)} X \Pi_d^{(n)}$.

(2) $\mathrm{ran}(X), \mathrm{ran}(X^*) \subseteq \vee^n \mathbb{C}^d$.

(3) $\forall \sigma \in S_n, \quad X = P_\sigma X = X P_\sigma$.

Proof. We show that all the above definitions are equivalent.

(1) $\implies$ (2). We observe that, $\mathrm{ran}(\Pi_d^{(n)} X \Pi_d^{(n)}) \subseteq \mathrm{ran}(\Pi_d^{(n)}) = \vee^n \mathbb{C}^d$, and the same for the adjoint.

(2) $\implies$ (3). Let $|\psi\rangle \in \mathbb{C}^d$. We have, $X|\psi\rangle \in \vee^n \mathbb{C}^d$ as $\mathrm{ran}(X) \in \vee^n \mathbb{C}^d$. This shows,

$$\forall \sigma, |\psi\rangle \in \mathbb{C}^d, \quad P_\sigma X |\psi\rangle = X |\psi\rangle \,.$$

Also, by a similar argument, we have,

$$\forall \sigma, |\psi\rangle \in \mathbb{C}^d, \quad P_\sigma X^* |\psi\rangle = X^* |\psi\rangle \implies (X P_\sigma)^* = X^* \implies X P_\sigma = X.$$

(3) $\implies$ (1). $X = P_\sigma X \implies X = \frac{1}{n!} \sum_{\sigma \in S_n} P_\sigma X = \Pi_d^{(n)} X$. Similarly, we have, $X = X \Pi_d^{(n)}$. This completes the proof.

■

We denote the linear space of bosonic matrices as

$$\mathcal{M}[\vee^n \mathbb{C}^d] := \{X \in \mathcal{M}_d^{\otimes n} \mid X = \Pi_d^{(n)} X \Pi_d^{(n)}\}$$

and the real linear space of hermitian bosonic matrices as

$$\mathrm{Herm}[\vee^n \mathbb{C}^d] := \{X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid X = \Pi_d^{(n)} X \Pi_d^{(n)}\}.$$

From [Har13, Section 1.1], we also have the following descriptions of these spaces.

$$\mathcal{M}[\vee^n \mathbb{C}^d] = \mathrm{span}_{\mathbb{C}} \left\{ |\psi\rangle\langle\psi|^{\otimes n} \;\middle|\; |\psi\rangle \in \mathbb{C}^d \right\}, \tag{87}$$

$$\mathrm{Herm}[\vee^n \mathbb{C}^d] = \mathrm{span}_{\mathbb{R}} \left\{ |\psi\rangle\langle\psi|^{\otimes n} \;\middle|\; |\psi\rangle \in \mathbb{C}^d \right\}. \tag{88}$$

We finally present a useful proposition about linear operators, which connects the restriction of the operator to the symmetric subspace to product forms.

Proposition 9.2. The following statements are equivalent for $X \in \mathcal{M}_d^{\otimes n}$,

(1) $\forall\, |v\rangle \in \mathbb{C}^d, \quad \langle v^{\otimes n}| X |v^{\otimes n}\rangle = 0.$

(2) $\Pi_d^{(n)} X \Pi_d^{(n)} = 0.$

Proof. The reverse direction is trivial. For the forward direction, from Eq. (87) note the following equivalence:

$$\forall\, |v\rangle \in \mathbb{C}^d, \quad \langle v^{\otimes n}| X |v^{\otimes n}\rangle = 0 \iff \forall W \in \mathcal{M}[\vee^n \mathbb{C}^d], \quad \mathrm{Tr}(XW) = 0.$$

Moreover, this is equivalent to the statement

$$\forall \tilde{W} \in \mathcal{M}_d^{\otimes n}, \quad \mathrm{Tr}(X \Pi_d^{(n)} \tilde{W} \Pi_d^{(n)}) = \mathrm{Tr}(\Pi_d^{(n)} X \Pi_d^{(n)} \tilde{W}) = 0.$$

This shows the claim. ∎

Remark 9.3. Note that the bosonic matrices are a strict subset of the class of permutation symmetric matrices, $\{X \in \mathcal{M}_d^{\otimes n} \mid \forall \sigma \in S_n, P_\sigma X = X P_\sigma\}$. To see this, note that the matrix $\mathbb{I}_{d^n} = \mathbb{I}_d^{\otimes n}$ is permutation symmetric, but not bosonic, as $\mathrm{ran}(\mathbb{I}_{d^n}) = (\mathbb{C}^d)^{\otimes n} \supsetneq \vee^n \mathbb{C}^d$.

Since the Dicke states form a basis of the symmetric subspace of n qudits, they can also be used to describe a basis for the vector space of operators acting on the symmetric subspace.

Proposition 9.4. Any bosonic matrix $X \in \mathcal{M}[\vee^n \mathbb{C}^d]$ can be expanded in terms of Dicke states.

$$X = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} \langle D_\alpha | X | D_\beta \rangle \left| D_\alpha \middle\rangle\middle\langle D_\beta \right|.$$

All the sets of bosonic matrices that we shall discuss in this work are presented in **??**, which can be used as a reference for the acronyms and the main results about each set.

9.2.3 *Tensors and Polynomials*

One of the main conceptual contributions of this work is a correspondence between Dicke states and real symmetric tensors. In this section, we shall describe the main properties of tensors that are relevant for us. We refer the reader to Table 18 for a quick reference on the main sets of tensors and their properties used in this paper.

Notations and diagrams for tensors

For any multi-index $i \in [d]^n$, we denote the components of the tensor $T \in (\mathbb{R}^d)^{\otimes n}$ as $T_{i_1 i_2 \dots i_n}$ in the canonical basis $e_i := e_{i_1} \otimes e_{i_2} \dots e_{i_n}$. This will be shortened to T_i whenever appropriate. We use the notation $i \sqcup j \in [d]^{n+m}$ to show the join of the multi-indices $i \in [d]^n$ and $j \in [d]^m$. For two tensors $Q \in (\mathbb{R}^d)^{\otimes n}$ and $T \in (\mathbb{R}^d)^{\otimes m}$, we have the tensor $(Q \otimes T) \in (\mathbb{R}^d)^{\otimes (n+m)}$ defined component-wise as,

$$\forall i \in [d]^n, j \in [d]^m, \quad (Q \otimes T)_{i \sqcup j} := Q_i T_j.$$

For any multi-index $i \in [d]^n$ and $\sigma \in S_n$, we denote by $\sigma \cdot i := (i_{\sigma(1)}, i_{\sigma(2)} \dots i_{\sigma(n)})$.

We also use the diagrammatic notation for tensors wherever it is useful. A tensor with n indices is represented with a spider with n legs as in Fig. 32. The tensor product $Q \otimes T$ will be denoted by placing two tensors together. A contraction of a tensor is represented by joining two wires as Fig. 33, and represents the following operation,

$$(T')_{i_1 i_2 \dots i_{n-2}} = \sum_{j=1}^{d} T_{jj i_1 i_2 i_3 \dots i_{n-2}}.$$

A tensor with one index is a vector. A matrix can be interpreted as a tensor with 2 indices. The matrix multiplication of two matrices M and K can be represented as a tensor contraction.

$$\sum_{i_2=1}^{d} (M \otimes K)_{i_1 i_2 i_2 j_3} = \sum_{i_2=1}^{d} M_{i_1 i_2} K_{i_2 i_3}.$$

Moreover, the Euclidean inner product of two tensors can also be represented as a tensor contraction.

$$\langle Q, T\rangle := \sum_{i\in[d]^n} T_i Q_i = \sum_{i\in[d]^n} (T\otimes Q)_{i\sqcup i}.$$

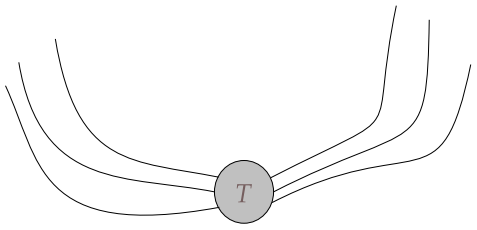


Figure 32: The tensor spider T with 6 legs.

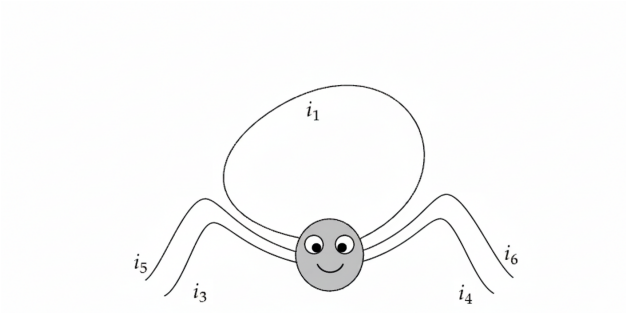


Figure 33: A tensor contraction: the contracted tensor has now 4 legs i_3, i_4, i_5, i_6. The other two legs are equal $i_1 = i_2$ and summed over.

Symmetric tensors and polynomials

In this article, we will work primarily with *real* tensors with permutation symmetry. Formally, any tensor $T \in (\mathbb{R}^d)^{\otimes n}$ is *symmetric tensor* if it stays invariant under the permutation of its indices, i.e,

$$\forall\sigma \in S_n, \forall i \in [d]^n, \quad T_i = T_{\sigma\cdot i}.$$

Note that in the case of the 2 indices, by interpreting the indices to be rows and column indices of a matrix, these tensors correspond exactly to real symmetric matrices. The linear space of such tensors will be denoted by $\vee^n\mathbb{R}^d$. We can define the following projection map, $\Pi_d^{(n,\mathbb{R})} : \mathbb{R}^{\otimes n} \to \vee^n\mathbb{R}^d$ such that,

$$\forall i \in [d]^n, \quad \Pi_d^{(n,\mathbb{R})}[T]_i := \frac{1}{n!}\sum_{\sigma\in S_n} T_{\sigma\cdot i}.$$

For $\alpha \in \mathbb{N}^d, x \in \mathbb{R}^d$, we define the expression x^α to denote the monomial $x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}$. Note that the degree of such a monomial is $\sum_i \alpha_i := |\alpha|$. Let us denote by $[x]_d^n$ the vector of homogeneous monomials of degree n and in d variables, by ordering the monomials using the lexicographic ordering. This is done by imposing the ordering $x^\alpha > x^\beta$ if in $\alpha - \beta$, the first non-zero entry from the left is positive. An example of such an ordering in the case of monomials of degree 2 and 2 variables is, $[x]_2^2 := (x_1^2, x_1 x_2, x_2^2)$.

It is well-known that the symmetric tensors have a linear bijection to the set of homogeneous polynomials of degree d and n variables, which we denote as $\mathbb{H}[x]_{d,n}$. This bijection is the following map $T \mapsto p_T$:

$$p_T(x) := \langle T, x^{\otimes n} \rangle = \sum_{i \in [d]^n} T_i x_{i_1} x_{i_2} \dots x_{i_n} = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \binom{n}{\alpha} T_{(\alpha)} x^\alpha. \tag{89}$$

Moreover, note the following characterization of *real* symmetric tensors [CGLM08], which is analogous to that of complex tensors in Eq. (86):

$$\vee^n \mathbb{R}^d = \mathrm{span}_{\mathbb{R}} \{ v^{\otimes n} \mid v \in \mathbb{R}^d \}.$$

Convex duality

Let V be a real vector space and $\mathcal{C}$ be a convex cone. The *conic dual* of a convex cone $\mathcal{C} \subseteq V$ is defined by the following set.

$$\mathcal{C}^\circ := \{ X \in V^* \mid \forall Y \in \mathcal{C},\ X(Y) \geq 0 \}.$$

If for two convex cones, $\mathcal{C}, \mathcal{K}$, we have $\mathcal{C} \subseteq \mathcal{K}$, it implies that $\mathcal{K}^\circ \subseteq \mathcal{C}^\circ$. A cone is called self-dual if $\mathcal{C}^\circ \cong \mathcal{C}$. If the vector space V has an inner product $\langle ., . \rangle$, then all the linear functionals are of the form,

$$X(Y) = \langle L_X, Y \rangle,$$

for a unique $L_X \in V$. This provides a natural isomorphism between V and V^*. In this article, we consider tensor cones $C \subseteq \vee^n \mathbb{R}^d$ with the Euclidean inner product. Then, the entrywise non-negative is an example of a self-dual convex cone.

$$\mathsf{NN}_d^{(n)} := \{ Q \in \vee^n \mathbb{R}^d \mid \forall i \in [d]^n,\ Q_i \geq 0 \}. \tag{90}$$

Completely Positive (CP) and Copositive (Cop) tensors

We first introduce the notion of completely positive tensors. This notion generalizes that of completely positive matrices, which have been investigated since the 1960s [HJN63]. These are symmetric matrices that can be written as a sum of rank-1 projectors, i.e

$$X = |v_1\rangle\langle v_1| + |v_2\rangle\langle v_2| \dots + |v_K\rangle\langle v_K|$$

where $|v_q\rangle \in \mathbb{R}^d_+$ is a vector with non-negative entries. We recommend the excellent book by A. Berman and N. Shaked-Monderer [SMB21] as a comprehensive reference on this topic. This cone of completely positive matrices is quite well-studied due to its importance in the theory of optimization, and also recently found a connection to entanglement theory for bosonic states [Yu16, TAQ+18]. Let us now define the general notion for tensors,

Definition 9.5. A symmetric tensor $Q \in \vee^n(\mathbb{R}^d)$ is called *completely positive* if there exists a finite set of entry-wise non-negative vectors $\{v_q\}_{q=1}^K \in \mathbb{R}^d_+$ such that

$$Q = v_1^{\otimes n} + v_2^{\otimes n} + \ldots + v_K^{\otimes n}.$$

The set of completely positive tensors is a convex, pointed, and closed cone with a non-empty interior [PVZ15, Proposition 1] in the real vector space of symmetric tensors $\vee^n\mathbb{R}^d$. We denote this convex cone as $\mathsf{CP}_d^{(n)}$ where n denotes the number of legs (indices) and d is the local dimension. Clearly, any completely positive tensor is entrywise non-negative, as all the components of v_q are non-negative. We refer the reader to [QXX14, LQ15, NTYZ22] for the recent work on this class of tensors. The membership problem for even completely positive matrices is known to be NP-hard [MK87]. Despite the hardness of general characterization, some results have been obtained in this direction by different approaches; looking at structured tensors [LQ16], in low dimensions [NYZ18], or solving a growing sequence of semi-definite programs [FZ14, FZ17, NTYZ22]. Similarly to the matrix case, some classes of polynomial optimization problems can be reformulated in terms of the completely positive tensors [PVZ15]. Surprisingly, it has been shown that for $d = 2$, deciding complete positivity is equivalent to checking positivity of two Hankel matrices [FNZ19].

We introduce the *conic dual* of the completely positive tensors, called *copositive tensors* [Qi13]:

$$\mathsf{Cop}_d^{(n)} := (\mathsf{CP}_d^{(n)})^\circ.$$

Recall that for all symmetric tensors $Q \in \vee^n\mathbb{R}^d$, there is an associated homogeneous polynomial $p_Q(x) = \langle Q, x^{\otimes n}\rangle$; $p_Q(x)$ is a homogeneous polynomial of degree n in d variables with real coefficients. The following proposition provides another characterization of copositivity.

Proposition 9.6. A symmetric tensor $Q \in \vee^n\mathbb{R}^d$ is copositive if and only if

$$\forall x \in \mathbb{R}^d_+ \qquad p_Q(x) \geq 0.$$

Note that in the previous definition, we only need the polynomial to be positive for all non-negative vectors x, but in general, the polynomial $p_Q(x)$ can take negative values. This generalizes the notion of copositive matrices, which correspond to the second-order copositive tensors [Dia62, HJN63, Dür10, BDDK+00]. The membership problem for copositive matrices is known to be co-NP-hard [MK87]. Like the completely positive cone, this convex cone is well-studied due to its importance in the theory of optimization as copositivity offers a unified convex way to reformulate non-convex mixed quadratic programs into convex programs [Dür10]. For a comprehensive review of copositive matrices, we again refer the reader to the detailed book by Berman and Shaked-Monderer [SMB21].

Sum-of-squares

We review in this section some basic but important facts about multivariate polynomials that can be written as sums of squares. Such polynomials play a central role in semi-algebraic geometry, see [BPT12].

Definition 9.7. Let $p \in \mathbb{H}[x]_{d,2n}$ be a homogeneous polynomial in d variables $(x_1 \dots x_d) =: x$ and degree $2n$. Such a polynomial p is said to be a *sum of squares* polynomial (or in short a SOS polynomial) if there exist a finite number of homogeneous polynomials $f_k(x)_{k=1}^K \in \mathbb{H}[x]_{d,n}$ having degree n, such that,

$$p(x) = \sum_{k=1}^{K} f_k^2(x).$$

We denote the set of sum of squares polynomials in even degree $2n$ and d variables as $\Sigma_d^{2n}[x] \subseteq \mathbb{H}[x]_{d,2n}$. The polynomials that can be written as a sum of squares are clearly globally nonnegative (as $\forall f \in \mathbb{R}[x], f(x)^2 \geq 0$). But the converse of the statement is false, which is the content of Hilbert's celebrated results [Hil88]. This means that there exist globally positive homogeneous polynomials that are not SOS. The following Table 19 summarizes Hilbert's theorem for the case of homogeneous polynomials. Note that the same result holds true also for *symmetric* homogeneous polynomials [GKR17], i.e polynomials that satisfy,

$$\forall \sigma \in S_d \quad p(x_1, x_2 \dots x_n) = p(x_{\sigma(1)}, x_{\sigma(2)} \dots x_{\sigma(d)}).$$

Next, we show a reformulation of the sum of squares condition of the polynomial in terms of positive semidefinite matrices. Similar results are well-known in the literature, see [PW98, Lau08] under the name of the *Gram-Matrix Method*. This formulation also

	$2n = 2$	$2n = 4$	$2n \geq 6$
$d = 2$	Yes	Yes	Yes
$d = 3$	Yes	Yes	No
$d \geq 4$	Yes	No	No

Table 19: Can any homogeneous or symmetric homogeneous polynomial of degree $2n$ in d variables be represented as a sum of squares?

provides an efficient way to check the sum of squares property of polynomials, by recasting it as a semi-definite program (SDP) [BV04, Las09, BPT12].

Theorem 9.8. A homogeneous polynomial $p \in \mathbb{H}[x]_{d,2n}$ of degree $2n$ is a sum of squares (SOS) if and only if there exists a PSD matrix, $P \in \mathrm{Herm}[\mathcal{M}_d(\mathbb{R})^{\otimes n}]$ such that

$$p(x) = \langle x^{\otimes n}|P|x^{\otimes n}\rangle\,.$$

Proof. ($\Longleftarrow$) Assume that there exists a PSD matrix P such that $p(x) = \langle x^{\otimes n}|P|x^{\otimes n}\rangle$. Since it is PSD, P can be written as $X^\top X$, where $X \in \mathcal{M}_d(\mathbb{R})^{\otimes n}$. Therefore,

$$p(x) = \langle x^{\otimes n}|P|x^{\otimes n}\rangle = \langle x^{\otimes n}|X^\top X|x^{\otimes n}\rangle = \sum_{i\in[d]^n} f_i^2(x)$$

where $\forall i \in [d]^n$, $f_i(x) = \sum_{j\in[d]^n} X_{i,j}x_{j_1}x_{j_2}\ldots x_{j_n}$. This implies that $p(x)$ is a sum of squares polynomial.

($\Longrightarrow$) For the reverse implication, assume that the polynomial $p(x)$ is a sum of squares, i.e, of the form

$$p(x) = \sum_{k=1}^{K} f_k^2(x).$$

For all k, expand $f_k(x) = \sum_\alpha \mu_{k,\alpha}x^\alpha$ as a sum of monomials. Note that, we can also expand $f_k(x) = \langle\tilde{\mu}_k, x^{\otimes n}\rangle$ where $\forall i \in [d]^n$, $(\tilde{\mu}_k)_i = \binom{n}{\gamma(i)}^{-1}\mu_{k,\gamma(i)}$, see Eq. (89). Then, we have:

$$p(x) = \sum_{k=1}^{K}\langle\tilde{\mu}_k, x^{\otimes n}\rangle^2 = \sum_{k=1}^{K}\langle x^{\otimes n}, \tilde{\mu}_k\rangle\langle\tilde{\mu}_k, x^{\otimes n}\rangle = \langle x^{\otimes n}|\sum_{k=1}^{K}|\tilde{\mu}_k\rangle\langle\tilde{\mu}_k|\,|x^{\otimes n}\rangle\,.$$

By choosing $P := \sum_{k=1}^{K}|\tilde{\mu}_k\rangle\langle\tilde{\mu}_k|$, we conclude the proof. ∎

Remark 9.9. It is easy to show with a slight modification of the above proof that the polynomial is SOS if and only if there is a PSD matrix P such that $p(x) = ([x]_d^n)^\top P[x]_d^n$ where $[x]_d^n$ is the vector of monomials of degree n in d variables. The matrix P in this case is known as the *Gram*-Matrix [PW98, Lau08].

Recall that there is a homogenous polynomial of d variables and degree n associated to the tensor $Q \in \vee^n \mathbb{R}^d$,

$$p_Q(x) := \sum_{i \in [d]^n} Q_{i_1 i_2 \ldots i_n} x_{i_1} x_{i_2} \ldots x_{i_n}.$$

From Proposition 9.6, it is clear that Q is a copositive tensor if and only if $p_Q(x \odot x) \geq 0$ for all $x \in \mathbb{R}^d$. This motivates the definition of sum-of-squares (SOS) tensors.

Definition 9.10 (SOS Tensors)**.** A symmetric tensor T will be called a sum-of-squares tensor, or in short, an SOS Tensor, if the polynomial, $p_T(x \odot x)$ is a sum of squares. We denote the cone of these tensors using the notation,

$$\mathsf{SOS}_d^{(n)} := \{T \in \vee^n \mathbb{R}^d \mid p_T(x \odot x) \in \Sigma_d^{(2n)}\}.$$

It follows from the definition that all SOS tensors are copositive (as all SOS polynomials are positive). The SOS tensors form a pointed convex cone. Note that in Definition 9.10, we do not demand that the tensor polynomial p_T is a sum of squares polynomial, but a weaker condition that $p_T(x \odot x)$ is an SOS polynomial. For example, consider the two-variable polynomial $p_1(x_1, x_2) = x_1 x_2$. This polynomial is not positive for all x, hence also not a sum of squares. But the polynomial $p_1(x_1^2, x_2^2) = x_1^2 x_2^2$ is an SOS polynomial. The homogenous polynomials of this form were studied in [ZVP06], and the form of these polynomials was completely characterized. We rephrase the result in the next theorem.

Theorem 9.11 ([ZVP06, Proposition 9])**.** Let $p(x) \in \mathbb{H}[x]_{d,n}$ be a real homogeneous polynomial in $x \in \mathbb{R}^d$ of degree n such that $p(x \odot x)$ is a sum of squares: $p(x \odot x) \in \Sigma_d^{(2n)}$. Then the polynomial p admits a decomposition of the form

$$p(x) = \sum_{j=0}^{\lfloor n/2 \rfloor} \sum_{\alpha \in \mathbb{N}_d^{(n-2j)}} x^\alpha \psi_{j,\alpha}(x) \tag{91}$$

where $|\alpha| := \alpha_1 + \cdots + \alpha_d$, $x^\alpha := x_1^{\alpha_1} \cdots x_d^{\alpha_d}$, and each $\psi_{j,\alpha}$ is a homogeneous SOS polynomial of degree $2j$: $\psi_{j,\alpha}(x) \in \Sigma_d^{(2j)}$.

Let us consider the SOS tensors for $n = 2$. In this case, by definition, $Q \in \mathsf{SOS}_d^{(n)}$, if the polynomial $p_Q(x \odot x) = \sum_{i,j} Q_{ij} x_i^2 x_j^2 \in \Sigma_d^{(4)}$. We apply Theorem 9.11 to obtain the following decomposition:

$$\begin{aligned} p_Q(x) = \sum_{i,j\in[d]} Q_{ij} x_i x_j &= \sum_{|\alpha|=2} x^\alpha \psi_{0,\alpha}(x) + \sum_{|\alpha|=0} x^\alpha \psi_{1,\alpha}(x) \\ &= \sum_{i,j\in[d]} x_i x_j \lambda_{ij} + 1 \cdot \langle x|A|x\rangle \,. \end{aligned}$$

We obtain for the first term with $|\alpha| = 2$, all the monomials $x_i x_j$ and the degree 0 SOS polynomial $\lambda_{ij} := \psi_{0,\alpha}(x) \in \mathbb{R}_+$. For the second term, we have $x^\alpha = 1$ and the degree 2 SOS polynomial, $\psi_{1,\alpha}(x) = \langle x|A|x\rangle$ for some $A \in \mathsf{PSD}_d$. Therefore this shows that $Q_{ij} = \lambda_{ij} + A_{ij}$. If we interpret the indices of Q as a matrix, we get, $Q = \{\lambda_{ij} + A_{ij}\}_{i,j=1}^d \in \mathsf{NN}_d + \mathsf{PSD}_d$. The reverse is also true. If $Q \in \mathsf{NN}_d + \mathsf{PSD}_d$, this implies that $p_Q(x \odot x) \in \Sigma_d^{(4)}$. This fully characterizes the SOS cone in $n = 2$.

Remark 9.12. The previous characterization also shows that the convex cone of SOS tensors is closed (since sum of square polynomials of degree n and d variables is closed). Moreover, there exists an $\varepsilon > 0$ such that the open ball $B(\varepsilon, |e\rangle^{\otimes n}) \subseteq \mathsf{SOS}_d^{(n)}$ implying that the cone has a non-empty interior where $|e\rangle := \sum_i e_i$

Remark 9.13. The convex cone of $\mathsf{NN} + \mathsf{PSD}$ is well-studied, usually denoted as SPN in the literature. It is the inner approximation to the set of copositive matrices, and is dual to the cone of *doubly non-negative matrices*, that are the positive-semidefinite matrices with non-negative entries, $\mathsf{DNN} := \mathsf{NN} \cap \mathsf{PSD}$. For results about these matrix cones, we refer the reader to [SMB21]. The sum of squares tensors can be considered a generalisation of SPN matrix cone.

We also present here the characterization of the duals of sum of square polynomials. For polynomials, we define the duals without any reference to any inner product, and instead, we look at the linear functionals that are positive on all SOS polynomials.

$$(\Sigma_d^{(2n)})^\circ := \{f : \mathbb{H}[x]_{d,2n} \to \mathbb{R} \mid \forall\, p \in \Sigma_d^{(2n)},\ f(p) \geq 0\}.$$

Recall that the monomials of a degree n in d variables, $[x]_d^n$ are labeled by the vectors $\alpha \in \mathbb{N}^d$ such that $|\alpha| = n$. The set of these monomials is of size $\binom{n+d-1}{d-1}$. Then, we have the following definition.

Definition 9.14 (Moment Matrix [Lau08])**.** Let $(y_\alpha)_{|\alpha|=2n}$ be a sequence labelled by the monomial vectors, $\alpha \in \mathbb{N}^d$ such that $|\alpha| = 2n$. Then, define the following $\binom{n+d-1}{d-1} \times \binom{n+d-1}{d-1}$ matrix with rows and columns indexed using the monomial vectors,

$$\mathcal{M}_n(y)_{\alpha\beta} := y_{\alpha+\beta}.$$

This matrix is called the moment matrix associated with the sequence y_α.

Let f be a linear functional on homogeneous polynomials. Then, we associate a moment matrix with the linear functional f by choosing the sequence $y_\alpha := f(x^\alpha)$ where $\alpha \in \mathbb{N}^d, |\alpha| = 2n$. We then have the following result about the dual of SOS polynomials.

Theorem 9.15. The dual cone of SOS polynomials,

$$(\Sigma_d^{(2n)})^\circ = \{f : \mathbb{H}[x]_{d,2n} \to \mathbb{R} \mid \mathcal{M}_n(y) \succeq 0 \text{ where } y_\alpha := f(x^\alpha)\}.$$

Proof. Recall that a polynomial is an SOS polynomial, i.e $p \in \Sigma_d^{(2n)}$ if and only if there exists a positive semidefinite matrix P such that $p(x) = ([x]_d^n)^\top P [x]_d^n$. Expanding this, we get,

$$p(x) = ([x]_d^n)^\top P [x]_d^n = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} P_{\alpha\beta}\, x^{\alpha+\beta},$$

where we recall that $\mathbb{N}_d^{(n)}$ denotes the set of d-tuples of non-negative integers that sum up to n. Applying the linear functional f to this expression while having $f(x^\alpha) = y_\alpha$, we obtain,

$$f(p) = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} P_{\alpha\beta}\, y_{\alpha+\beta} = \operatorname{Tr}\big(P\, \mathcal{M}_n(y)\big).$$

Moreover, this is positive for all PSD matrices P, if and only if $\mathcal{M}_n(y) \succeq 0$. ∎

The last result, Theorem 9.15, completely characterizes the dual cone of the SOS polynomials; a linear functional is in the dual cone if and only if the corresponding moment matrix is positive-semidefinite. We refer the reader to the excellent notes by Laurent

[Lau08, Section 4.4] for more details on moment matrices, particularly for the connection to the moment problem.

SOS and Non-Negative Hierarchy

In [Par00], an inner approximation of copositive matrices was introduced based on the SOS hierarchy that approximates positive polynomials. It consists of the following convex cones.

$$\mathsf{RSOS}_d^{(r)} := \{Q \in \vee^2 \mathbb{R}^d \,|\, p_Q(x \odot x)||x||^{2r} \in \Sigma_d^{(2r)}\} \tag{92}$$

Each of the sets $\mathsf{RSOS}_d^{(r)}$ involves checking the sum of squares property of the polynomial $p_Q(x \odot x) = \sum_{i,j\in[d]} Q_{ij} x_i^2 x_j^2$, after multiplying it with another polynomial, $||x||^{2r}$, that is SOS by definition. We then have the following inclusions,

$$\mathsf{PSD}_d + \mathsf{NN}_d = \mathsf{RSOS}_d^{(0)} \subseteq \mathsf{RSOS}_d^{(1)} \subseteq \mathsf{RSOS}_d^{(2)} \subseteq \mathsf{RSOS}_d^{(3)} \ldots \subseteq \mathsf{RSOS}_d^{(r)} \subseteq \mathsf{Cop}_d.$$

The following are well-known results about this hierarchy.

- $\mathsf{RSOS}_n^{(0)} = \mathsf{SPN}_d = \mathsf{NN}_d + \mathsf{PSD}_d$. In particular we have, $\mathsf{Cop}_d = \mathsf{RSOS}_d^{(0)}$ for $d \leq 4$.
- [Par00, DDGH13] If $d \geq 5$, $\mathsf{RSOS}_d^{(0)} \subsetneq \mathsf{RSOS}_d^{(1)} \subseteq \cdots \subseteq \mathsf{RSOS}_d^{(r)} \subsetneq \mathsf{Cop}_d$.
- [LV23, SV24] $\bigcup_{r\geq 0} \mathsf{RSOS}_5^{(r)} = \mathsf{Cop}_5$ and $\mathrm{int}(\mathsf{Cop}_n) \subsetneq \bigcup_{r\geq 0} \mathsf{RSOS}_d^{(r)} \subsetneq \mathrm{cl}\left(\bigcup_{r\geq 0} \mathsf{RSOS}_d^{(r)}\right) = \mathsf{Cop}_d$ for $d \geq 6$.

A similar approach of constructing the sum of squares (SOS) hierarchy is also possible for tensors.

$$\mathsf{RSOS}_d^{(m,r)} := \{Q \in \vee^m \mathbb{R}^d \,|\, p_Q(x \odot x)||x||^{2r} \in \Sigma_d^{2(m+r)}\}.$$

These sets satisfy similar inclusions for each m.

$$\mathsf{RSOS}_d^{(m,0)} \subseteq \mathsf{RSOS}_d^{(m,1)} \subseteq \mathsf{RSOS}_d^{(m,2)} \subseteq \mathsf{RSOS}_d^{(m,3)} \ldots \subseteq \mathsf{RSOS}_d^{(m,r)} \subseteq \mathsf{Cop}_d^{(m)}.$$

- For $d = 2$, $\mathsf{RSOS}_2^{(m,0)} = \mathsf{Cop}_2^{(m)}$. This follows from the fact that all homogenous polynomials in 2 variables are SOS [Hil88].
- $\mathrm{int}(\mathsf{Cop}_d^{(m)}) \subseteq \bigcup_{r\geq 0} \mathsf{RSOS}_d^{(m,r)} \subseteq \mathrm{cl}\left(\bigcup_{r\geq 0} \mathsf{RSOS}_d^{(m,r)}\right) = \mathsf{Cop}_d^{(m)}$ by Reznick's Positivstellensätze [Rez95].

Let $e := \sum_{i=1}^{d} e_i$ be the all-ones vector. Then, we can rewrite,

$$p_Q(x \odot x)||x||^{2r} = \langle Q \otimes e^{\otimes r}, (x \odot x)^{\otimes(m+r)} \rangle = \langle \Pi_d^{(m+r,\mathbb{R})}[Q \otimes e^{\otimes r}], (x \odot x)^{\otimes(m+r)} \rangle .$$

This implies that the hierarchy can be rephrased purely in terms of tensors.

$$\mathsf{RSOS}_d^{(m,r)} = \{Q \in \vee^m \mathbb{R}^d \mid \Pi_d^{(m+r,\mathbb{R})}[Q \otimes e^{\otimes r}] \in \mathsf{SOS}_d^{(m+r)}\}. \tag{93}$$

Let $\chi_d^{(n)} \subseteq \mathbb{H}[x]_{d,n}$ be the cone of polynomials with non-negative coefficients. It is easy to see that if a tensor polynomial $p_T \in \chi_d^{(n)}$ it implies that $p_T(x \odot x) \in \Sigma_d^{(2n)}$. We consider the following hierarchy of convex sets considered in [DKP02], which also provides an inner approximation of copositive matrices.

$$\mathsf{PNN}_d^{(r)} := \Big\{ Q \in \vee^2 \mathbb{R}^d \;\Big|\; \Big(\sum_{i,j \in [d]} Q_{ij}\, x_i x_j \Big) \Big(\sum_{l=1}^{d} x_l \Big)^r \in \chi_d^{(r+2)} \Big\}. \tag{94}$$

For all r, we have the inclusion $\mathsf{PNN}_d^{(r)} \subseteq \mathsf{RSOS}_d^{(r)}$, i.e, this hierarchy acts as a weaker approximation than the SOS one. This hierarchy satisfies the following properties.

- $\mathsf{PNN}_d = \mathsf{C}_d^{(0)}$
- $\forall d \geq 2, \quad \mathsf{PNN}_d^{(0)} \subseteq \mathsf{PNN}_d^{(1)} \subseteq \mathsf{PNN}_d^{(2)} \subseteq \mathsf{PNN}_d^{(3)} \ldots \subseteq \mathsf{PNN}_d^{(r)} \subseteq \mathsf{Cop}_d.$
- $\mathrm{int}(\mathsf{Cop}_d) \subseteq \bigcup_{r \geq 0} \mathsf{PNN}_d^{(r)} \subsetneq \mathrm{cl}\left(\bigcup_{r \geq 0} \mathsf{PNN}_d^{(r)} \right) = \mathsf{Cop}_d$ follows from Polya's Positivstellensätze [Pól11, DKP02].

A similar approach of constructing the non-negative (NN) hierarchy is also possible for tensors.

$$\begin{aligned} \mathsf{PNN}_d^{(m,r)} &:= \{Q \in \vee^m \mathbb{R}^d \,|\, p_Q(x)(\sum_{l=1}^{d} x_l)^r \in \chi_d^{(m+r)}\} \\ &= \{Q \in \vee^m \mathbb{R}^d \,|\, p_Q(x \odot x)\|x\|^{2r} \in \chi_d^{2(m+r)}\}. \end{aligned}$$

These sets satisfy similar inclusions for each m.

$$\mathsf{PNN}_d^{(m,0)} \subseteq \mathsf{PNN}_d^{(m,1)} \subseteq \mathsf{PNN}_d^{(m,2)} \subseteq \mathsf{PNN}_d^{(m,3)} \ldots \subseteq \mathsf{PNN}_d^{(m,r)} \subseteq \mathsf{Cop}_d^{(m)}.$$

This hierarchy can also be rephrased purely in terms of tensors.

$$\mathsf{PNN}_d^{(m,r)} = \{Q \in \vee^m \mathbb{R}^d \mid \Pi_d^{(m+r,\mathbb{R})}[Q \otimes e^{\otimes r}] \in \mathsf{NN}_d^{(m+r)}\}. \tag{95}$$

9.3 DIAGONALLY SYMMETRIC SUBSPACE

In this section, we introduce the class of multipartite bosonic quantum states called *mixtures of Dicke states* or *Diagonally Symmetric States*. These states have been studied in the case of bipartite systems [TAQ+18, SN21, GNS25] and, recently, the multipartite extension has been considered in [RPAR+25]. We begin by discussing the basic structural properties of these states, along with their symmetries. Recall that any n-partite bosonic matrix $X \in (\mathcal{M}_d(\mathbb{C}))^{\otimes n}$ has an expansion into the orthonormal Dicke basis

$$X = \sum_{\alpha,\beta \in \mathbb{N}_d^{(n)}} \lambda(X)_{\alpha,\beta} |D_\alpha\rangle\langle D_\beta|,$$

where $\lambda(X)_{\alpha,\beta} := \langle D_\alpha | X | D_\beta \rangle$.

Let us begin by introducing the diagonally symmetric subspace. We denote by $\mathcal{DU}_d$ the abelian group of diagonal unitary matrices. These are exactly the diagonal matrices with complex phases on the diagonal

$$\mathcal{DU}_d := \{U_\theta \mid U_\theta := \mathrm{diag}(e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_d}),\ \theta \in [0, 2\pi)^d\}.$$

Definition 9.16 (Diagonally Symmetric Subspace)**.** A matrix $X \in (\mathcal{M}_d)^{\otimes n}$, will be called diagonally symmetric if it satisfies the following two symmetry conditions:

1. Bosonic symmetry,
$$\Pi_d^{(n)} X \Pi_d^{(n)} = X$$
2. Diagonal unitary invariance,
$$\forall U \in \mathcal{DU}_d \quad [U^{\otimes n}, X] = 0.$$

We will denote the vector space of diagonally symmetric (DS) matrices in $(\mathcal{M}_d)^{\otimes n}$ as $\mathsf{DS}_d^{(n)}$, and the *real* vector space of self-adjoint diagonally symmetric (DS) matrices as $\mathrm{Herm}[\mathsf{DS}_d^{(n)}]$. In the next Proposition 9.17, we show that this space consists of matrices that are diagonal in the Dicke basis.

Proposition 9.17. Let $d, n \in \mathbb{N}$. We have:

(1) $\mathsf{DS}_d^{(n)} = \mathrm{span}_{\mathbb{C}}\left\{ |D_\alpha\rangle\langle D_\alpha| \;\middle|\; \alpha \in \mathbb{N}_d^{(n)} \right\}$,

(2) $\mathrm{Herm}[\mathsf{DS}_d^{(n)}] = \mathrm{span}_{\mathbb{R}}\left\{ |D_\alpha\rangle\langle D_\alpha| \;\middle|\; \alpha \in \mathbb{N}_d^{(n)} \right\}$.

Therefore, the matrices $\{|D_\alpha\rangle\langle D_\alpha|\}_{\alpha\in\mathbb{N}_d^{(n)}}$ form an ONB (orthonormal basis) of the DS subspace.

Proof. Consider an operator $X \in \mathsf{DS}_d^{(n)}$. By Definition 9.16, it satisfies the two symmetries.

$$\Pi_d^{(n)} X \Pi_d^{(n)} = X,$$

$$[U^{\otimes n}, X] = 0 \text{ for all } U \in \mathcal{DU}_d.$$

Since $\Pi_d^{(n)} X \Pi_d^{(n)} = X$, then by Proposition 9.4, $X \in \mathcal{M}_d^{\otimes n}$ admits an expansion in the Dicke basis:

$$X = \sum_{\alpha,\beta\in\mathbb{N}_d^{(n)}} \lambda(X)_{\alpha,\beta}\, |D_\alpha\rangle\langle D_\beta|$$

for some complex coefficients, $\lambda(X)_{\alpha,\beta}$. Let $U_\theta := \mathrm{diag}(e^{i\theta_1}, \ldots, e^{i\theta_d}) \in \mathcal{DU}_d$ be an arbitrary diagonal unitary matrix. The action of the unitary matrix $U_\theta^{\otimes n}$ on Dicke states is:

$$U_\theta^{\otimes n} |D_\alpha\rangle = \frac{1}{\binom{n}{\alpha}} \sum_{j\,:\,\gamma(j)=\alpha} U_\theta^{\otimes n} |j\rangle = \frac{1}{\binom{n}{\alpha}} \sum_{j\,:\,\gamma(j)=\alpha} e^{i\alpha\cdot\theta} |j\rangle = e^{i\alpha\cdot\theta} |D_\alpha\rangle\,,$$

where $\alpha \cdot \theta$ is the Euclidean dot product of vectors. Hence, we have

$$\forall \alpha, \beta \in \mathbb{N}_d^{(n)}, \quad U_\theta^{\otimes n} |D_\alpha\rangle\langle D_\beta| \, (U_\theta^{\otimes n})^* = e^{i(\alpha-\beta)\cdot\theta} |D_\alpha\rangle\langle D_\beta|\,.$$

By using the diagonal unitary invariance of X,

$$X = U_\theta^{\otimes n} X (U_\theta^{\otimes n})^* = \sum_{\alpha,\beta\in\mathbb{N}_d^{(n)}} \lambda(X)_{\alpha,\beta}\, e^{i(\alpha-\beta)\cdot\theta}\, |D_\alpha\rangle\langle D_\beta| \qquad \text{for all } \theta \in [0, 2\pi)^d.$$

Since the Dicke basis is orthonormal, we must have, for all $\alpha, \beta \in \mathbb{N}_d^{(n)}$ and for all θ in $[0, 2\pi)^d$ that,

$$\lambda(X)_{\alpha,\beta} = e^{i(\alpha-\beta)\cdot\theta} \lambda(X)_{\alpha,\beta}.$$

This implies either $\lambda(X)_{\alpha,\beta} = 0$ or $\forall \theta \in [0, 2\pi]$, $e^{i(\alpha-\beta)\cdot\theta} = 1$. The latter condition holds if and only if $\alpha = \beta$ implying $\lambda(X)_{\alpha,\beta} = 0$ whenever $\alpha \neq \beta$. Therefore,

$$X = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \lambda(X)_{\alpha,\alpha}\, |D_\alpha\rangle\langle D_\alpha| \in \mathrm{span}_{\mathbb{C}}\{|D_\alpha\rangle\langle D_\alpha|\}_{\alpha\in\mathbb{N}_d^{(n)}}.$$

We can thus conclude:

$$\mathsf{DS}_d^{(n)} \subseteq \mathrm{span}_{\mathbb{C}}\{|D_\alpha\rangle\langle D_\alpha|\}. \tag{96}$$

Conversely, assume any operator of the form,

$$X = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda_\alpha \, |D_\alpha\rangle\langle D_\alpha|$$

is clearly supported on the symmetric subspace, so $\Pi_d^{(n)} X \Pi_d^{(n)} = X$, and is invariant under all $U_\theta^{\otimes n}$, since $U_\theta^{\otimes n} \, |D_\alpha\rangle\langle D_\alpha| \, (U_\theta^{\otimes n})^* = |D_\alpha\rangle\langle D_\alpha|$. Thus, we have the inclusion,

$$\mathrm{span}_{\mathbb{C}}\{|D_\alpha\rangle\langle D_\alpha|\} \subseteq \mathsf{DS}_d^{(n)}. \tag{97}$$

By combining Eq. (96) and Eq. (97), we complete the proof of the first assertion. For the second assertion, note that any state of the form,

$$\sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda_\alpha \, |D_\alpha\rangle\langle D_\alpha|$$

is self-adjoint if and only if $\lambda_\alpha \in \mathbb{R}$. The rest of the proof is analogous to the complex case. ■

Note that the diagonal symmetry property of Dicke states was first noted in the papers [Yu16, WY14]. By a slight abuse of notation, we write $\lambda(X)_\alpha := \lambda(X)_{\alpha,\alpha}$. In this paper, we are interested in studying the quantum states in this subspace, i.e, PSD matrices (with trace 1). Then, these properties can be captured by imposing positivity conditions and normalization constraints on the coefficients $\lambda(X)_\alpha$.

Proposition 9.18. Let $X \in \mathsf{DS}_d^{(n)}$, such that

$$X = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda(X)_\alpha \, |D_\alpha\rangle \, \langle D_\alpha| \, .$$

Then, the following equivalences hold,

1. $X \in \mathsf{Herm}_d^{(n)} \iff \forall \alpha \in \mathbb{N}_d^{(n)}, \quad \lambda(X)_\alpha \in \mathbb{R}$,
2. $X \in \mathsf{PSD}_d^{(n)} \iff \forall \alpha \in \mathbb{N}_d^{(n)}, \quad \lambda(X)_\alpha \in \mathbb{R}_+$.

Moreover, we have for the trace of X

$$\mathrm{Tr}(X) = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda(X)_\alpha,$$

and the rank of X

$$\mathrm{rk}(X) = |\{\alpha \in \mathbb{N}_d^{(n)} \mid \lambda(X)_\alpha \neq 0\}|.$$

Proof. The proof follows from the orthogonality of the Dicke states; the spectrum of the normal matrix X is the set $\{\lambda(X)_\alpha\}_{\alpha\in\mathbb{N}_d^{(n)}}$. ∎

It follows from Proposition 9.18 that X is a quantum state if and only if $\lambda(X)$ is a finite probability distribution over the set $\mathbb{N}_d^{(n)}$, and these quantum states are called *mixtures of Dicke states*. These are the states introduced and studied for qubits in [WY14, Yu16], for bipartite qudit systems [Yu16, TAQ+18], and for multi-partite qudit systems in the recent paper [RPAR+25]. Note that for the parametrisation in terms of the vectors $\lambda(X)_\alpha$, we get the inner product between two states X, Y in the diagonally symmetric subspace as

$$\mathrm{Tr}(X^*Y) = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \overline{\lambda(X)}_\alpha \lambda(Y)_\alpha.$$

9.3.1 *Permutation symmetry on local bases*

Besides the bosonic symmetry (the action of S_n on tensor legs) and diagonal unitary invariance, it is sometimes natural to impose an additional invariance under permutations of the *local basis labels* $[d]$.

Definition 9.19 (S_d-invariant DS states)**.** For $\tau \in S_d$, let $V_\tau \in \mathcal{M}_d$ be the permutation unitary defined by

$$V_\tau |j\rangle := |\tau(j)\rangle \qquad \forall j \in [d].$$

We say that a DS matrix $X \in \mathsf{DS}_d^{(n)}$ is S_d-*invariant* if

$$\forall \tau \in S_d, \qquad V_\tau^{\otimes n} X \left(V_\tau^{\otimes n}\right)^* = X.$$

We denote by $\mathsf{DS}_d^{(n),S_d} \subseteq \mathsf{DS}_d^{(n)}$ the subspace of S_d-invariant DS matrices.

The action of S_d permutes the components of occupation vectors. For $\alpha \in \mathbb{N}_d^{(n)}$ and $\tau \in S_d$, define $(\tau \cdot \alpha) \in \mathbb{N}_d^{(n)}$ by

$$(\tau \cdot \alpha)_j := \alpha_{\tau^{-1}(j)} \qquad \forall j \in [d].$$

Then, for a DS matrix

$$X = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \lambda(X)_\alpha |D_\alpha\rangle \langle D_\alpha|,$$

the condition in Definition 9.19 is equivalent to

$$\forall \tau \in S_d,\ \forall \alpha \in \mathbb{N}_d^{(n)}, \qquad \lambda(X)_\alpha = \lambda(X)_{\tau\cdot\alpha}. \tag{98}$$

In other words, the vector $\lambda(X)$ is constant on S_d-orbits, so the resulting family of matrices has fewer parameters than the whole DS space.

Let

$$\mathsf{Par}_d(n) := \{\mu \in \mathbb{N}_d^{(n)} \mid \mu_1 \geq \mu_2 \geq \cdots \geq \mu_d\}$$

be the set of integer partitions of n with (at most) d parts. For $\alpha \in \mathbb{N}_d^{(n)}$, denote by $\mathrm{sort}(\alpha) \in \mathsf{Par}_d(n)$ the non-increasing rearrangement of the entries of α, and by

$$\mathrm{Orb}(\alpha) := \{\tau \cdot \alpha \mid \tau \in S_d\}$$

its orbit. Then $\mathrm{sort}(\alpha)$ is an orbit representative, so the orbits in $\mathbb{N}_d^{(n)}$ are in bijection with $\mathsf{Par}_d(n)$.

Proposition 9.20 (Extremal points of the S_d-invariant DS simplex)**.** Let

$$\mathcal{S}_d^{(n),S_d} := \{\rho \in \mathrm{Herm}[\mathsf{DS}_d^{(n),S_d}] \mid \rho \in \mathsf{PSD}_d^{(n)},\ \mathrm{Tr}(\rho) = 1\}$$

be the convex set of S_d-invariant mixtures of Dicke states. Then $\mathcal{S}_d^{(n),S_d}$ is a simplex whose extreme points are indexed by $\mathsf{Par}_d(n)$. Concretely, for $\mu \in \mathsf{Par}_d(n)$ define

$$\rho_\mu := \frac{1}{|\,\mathrm{Orb}(\mu)|} \sum_{\alpha \in \mathrm{Orb}(\mu)} |D_\alpha\rangle\langle D_\alpha|\,.$$

Then $\{\rho_\mu\}_{\mu\in\mathsf{Par}_d(n)}$ are exactly the extreme points of $\mathcal{S}_d^{(n),S_d}$, and every $\rho \in \mathcal{S}_d^{(n),S_d}$ admits a unique convex decomposition

$$\rho = \sum_{\mu\in\mathsf{Par}_d(n)} p_\mu\, \rho_\mu \qquad \text{with } p_\mu \geq 0,\ \sum_\mu p_\mu = 1.$$

In particular, $\mathcal{S}_d^{(n),S_d}$ is parameterized by $|\mathsf{Par}_d(n)| - 1$ real parameters.

Proof. Any DS quantum state is determined by a probability distribution λ on $\mathbb{N}_d^{(n)}$ via $\rho = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \lambda_\alpha |D_\alpha\rangle\langle D_\alpha|$. By Eq. (98), ρ is S_d-invariant if and only if λ is constant on each orbit $\mathrm{Orb}(\alpha)$. Thus specifying $\rho \in \mathcal{S}_d^{(n),S_d}$ is equivalent to specifying a probability distribution $(p_\mu)_{\mu\in\mathsf{Par}_d(n)}$ on the set of orbits, by setting $\lambda_\alpha := p_{\mathrm{sort}(\alpha)}/|\,\mathrm{Orb}(\mathrm{sort}(\alpha))|$. This identifies $\mathcal{S}_d^{(n),S_d}$ affinely with the standard simplex over $\mathsf{Par}_d(n)$, whose vertices

correspond to placing all mass on a single orbit. The corresponding DS states are precisely the orbit-averages ρ_μ. ■

Example 9.21 (Small-n examples)**.** We give explicit descriptions of $\mathsf{Par}_d(n)$ and the corresponding extreme points ρ_μ from Proposition 9.20, noting that some partitions only exist when d is large enough.

(i) $n = 1$. For any $d \geq 1$, we have $\mathsf{Par}_d(1) = \{(1, 0, \ldots, 0)\}$, so $\mathcal{S}_d^{(1),S_d}$ consists of a single state:

$$\rho_{(1,0,\ldots,0)} = \frac{1}{d}\sum_{j=1}^{d} |j\rangle\langle j| = \frac{I_d}{d}.$$

(ii) $n = 2$. If $d = 1$, then $\mathsf{Par}_1(2) = \{(2)\}$. If $d \geq 2$, then

$$\mathsf{Par}_d(2) = \{(2, 0, \ldots, 0),\ (1, 1, 0, \ldots, 0)\},$$

and $\mathcal{S}_d^{(2),S_d}$ is a 1-simplex with vertices

$$\rho_{(2,0,\ldots,0)} = \frac{1}{d}\sum_{j=1}^{d} |jj\rangle\langle jj|,$$

$$\rho_{(1,1,0,\ldots,0)} = \frac{1}{\binom{d}{2}}\sum_{1\leq i<j\leq d} |D_{ij}\rangle\langle D_{ij}|, \qquad |D_{ij}\rangle := \frac{|ij\rangle + |ji\rangle}{\sqrt{2}}.$$

(iii) $n = 3$. If $d = 1$, then $\mathsf{Par}_1(3) = \{(3)\}$. If $d = 2$, then $\mathsf{Par}_2(3) = \{(3, 0),\ (2, 1)\}$. If $d \geq 3$, then

$$\mathsf{Par}_d(3) = \{(3, 0, \ldots, 0),\ (2, 1, 0, \ldots, 0),\ (1, 1, 1, 0, \ldots, 0)\},$$

so $\mathcal{S}_d^{(3),S_d}$ is a 2-simplex with vertices

$$\rho_{(3,0,\ldots,0)} = \frac{1}{d}\sum_{j=1}^{d} |jjj\rangle\langle jjj|,$$

$$\rho_{(2,1,0,\ldots,0)} = \frac{1}{d(d-1)}\sum_{\substack{i,j\in[d]\\ i\neq j}} |D_{iij}\rangle\langle D_{iij}|, \qquad |D_{iij}\rangle := \frac{|iij\rangle + |iji\rangle + |jii\rangle}{\sqrt{3}},$$

$$\rho_{(1,1,1,0,\ldots,0)} = \frac{1}{\binom{d}{3}}\sum_{1\leq i<j<k\leq d} |D_{ijk}\rangle\langle D_{ijk}|, \qquad |D_{ijk}\rangle := \frac{1}{\sqrt{6}}\sum_{\pi\in S_3} |\pi\cdot(ijk)\rangle.$$

In particular, the vertex $\rho_{(1,1,1,0,\ldots,0)}$ only exists when $d \geq 3$.

9.3.2 *Tensor-based parametrisation*

As we saw in the last section, *mixtures of Dicke states* X can be completely parameterized by the d_{sym} positive real numbers ($d_{\mathsf{sym}} - 1$ if we include normalization), the parameters $\lambda(X)_k$. In this section, we complement this with another useful parametrisation of the diagonally symmetric subspace in terms of a symmetric tensor. Recall that we have the occupation counting function, $\gamma : [d]^n \to \mathbb{N}_d^{(n)}$ defined component-wise as,

$$\big(\gamma(i)\big)_j := |\{k \in [n] \mid i_k = j\}|.$$

Note that γ is not an invertible map: for example, it is symmetric under permutations

$$\forall \sigma \in S_n,\, i \in [d]^n,\ \gamma(\sigma \cdot i) = \gamma(i).$$

This is reflected in the fact that the input and output spaces have different cardinalities, $d_{\mathsf{sym}} = \binom{n+d-1}{d-1} \neq d^n$. Nonetheless, for all occupation vectors $k \in \mathbb{N}_d^{(n)}$, there is a ***unique*** canonical multi-index (k) in $\gamma^{-1}(k)$ that satisfies the ordering, $(k)_1 \leq (k)_2 \cdots \leq (k)_n$. Recall that for a multi-index $i \in [d]^n$, the stabilizer subgroup of S_n, $\mathrm{stab}(i) := \{\pi \mid P_\pi |i\rangle = |i\rangle\}$ is the set of permutations that leave the multi-index i invariant. In the next theorem, we introduce a new parametrisation of the $\mathsf{DS}_d^{(n)}$ subspace, and prove some of its useful properties.

Theorem 9.22. Let X be a n-partite matrix in $\mathsf{DS}_d^{(n)}$. Then, we define the tensor $Q[X] \in (\mathbb{C}^d)^{\otimes n}$ component-wise as,

$$\forall i \in [d]^n, \quad Q[X]_i := \langle i|X|i\rangle\,.$$

Then, we have the following results,

(1) $Q[X]$ is a symmetric tensor, i.e, $Q[X] \in \vee^n \mathbb{C}^d$. Moreover, if $X \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$, if and only if $Q[X] \in \vee^n \mathbb{R}^d$, i.e $Q[X]$ is a real symmetric tensor. Moreover, $X \in \mathsf{PSD}_d^{(n)} \iff Q[X] \in \mathsf{NN}_d^{(n)}$.

(2) Since $X \in \mathsf{DS}_d^{(n)}$, we have an expansion in the Dicke basis,

$$X = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda(X)_\alpha\, |D_\alpha\rangle\, \langle D_\alpha|\,.$$

Then, we have the following connection between the vectors $\lambda(X)$ and the tensor $Q[X]$,

$$\forall i \in [d]^n \quad \binom{n}{\gamma(i)} Q[X]_i = \lambda(X)_{\gamma(i)}.$$

Equivalently, for all $\alpha \in \mathbb{N}_d^{(n)}$ and all $i \in \gamma^{-1}(\alpha)$, we have

$$\binom{n}{\alpha} Q[X]_i = \lambda(X)_\alpha. \tag{99}$$

(3) X has the following expansion,

$$X = \sum_{i \in [d]^n} \sum_{\pi \in S_n} \frac{\binom{n}{\gamma(i)}}{n!} Q[X]_i P_\pi \left|i\right\rangle \left\langle i\right|.$$

(4) The trace of the matrix X,

$$\mathrm{Tr}(X) = \sum_{i \in [d]^n} Q[X]_i = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda(X)_\alpha.$$

Proof. Let $X \in \mathsf{DS}_d^{(n)}$, and $Q[X] \in \mathbb{C}_d^{\otimes n}$ is defined component-wise by,

$$\forall i \in [d]^n, \qquad Q[X]_i := \langle i|X|i\rangle.$$

(1) Let $\pi \in S_n$ be any permutation and let P_π denote the corresponding permutation operator on $(\mathbb{C}^d)^{\otimes n}$. Since $X \in \mathsf{DS}_d^{(n)}$, by Definition 9.16, we have $P_\pi X = X P_\pi = X$ for every π. For any multi-index $i \in [d]^n$ and some $\pi \in S_n$,

$$Q[X]_{\pi \cdot i} = \langle \pi \cdot i|X|\pi \cdot i\rangle = \langle i|P_{\pi^{-1}} X P_\pi|i\rangle = \langle i|X|i\rangle = Q[X]_i.$$

Therefore, $Q[X]$ is invariant under the action of S_n and hence is a symmetric tensor, $Q[X] \in \vee^n \mathbb{C}^d$. If additionally, X is Hermitian then each diagonal matrix element is real $\langle i|X|i\rangle \in \mathbb{R}$, hence $Q[X] \in \vee^n \mathbb{R}^d$.

(2) Let $X \in \mathsf{DS}_d^{(n)}$ have the decomposition in the Dicke basis:

$$X = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \lambda(X)_\alpha \left|D_\alpha\right\rangle\!\left\langle D_\alpha\right|,$$

For any computational basis vector $|i\rangle$,

$$\langle i|D_\alpha\rangle = \frac{1}{\sqrt{\binom{n}{\alpha}}} \mathbb{1}_{\gamma(i)=\alpha}$$

Hence,

$$Q[X]_i = \langle i|X|i\rangle = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \lambda(X)_\alpha \, |\langle i|D_\alpha\rangle|^2 = \lambda(X)_{\gamma(i)} \, \frac{1}{\binom{n}{\gamma(i)}}.$$

Rearranging gives the claimed identity

$$\binom{n}{\gamma(i)} Q[X]_i = \lambda(X)_{\gamma(i)}, \tag{100}$$

which shows that the Dicke-basis coefficients $\lambda(X)_\alpha$ are constant on each orbit $\gamma^{-1}(\alpha)$.

(3) Since $X \in \mathsf{DS}_d^{(n)}$, it has the expansion in the Dicke basis.

$$X = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \lambda(X)_\alpha \, |D_\alpha\rangle\langle D_\alpha|.$$

Then, by using Eq. (99), and by expanding the Dicke state, $|D_\alpha\rangle = \frac{1}{\binom{n}{\alpha}} \sum_{\substack{i\in[d]^n \\ \gamma(i)=\alpha}} |i\rangle$, we get

$$X = \sum_{\alpha\in\mathbb{N}_d^{(n)}} Q[X]_{(\alpha)} \sum_{\substack{i,j\in[d]^n \\ \gamma(i)=\alpha,\, \gamma(j)=\alpha}} |i\rangle\langle j|$$

By re-labeling the indices $l := (\alpha)$, we have the following equation,

$$X = \sum_{\substack{l\in[d]^n \\ l_1\le\cdots\le l_n}} Q[X]_l \sum_{\substack{i,j\in[d]^n \\ \gamma(i)=\gamma(l),\, \gamma(j)=\gamma(l)}} |i\rangle\langle j|$$

Now $\gamma(i) = \gamma(l) \iff \exists\pi \in S_n,\ i = \pi\cdot l$. Therefore, our expression reduces to,

$$\sum_{\substack{l\in[d]^n \\ l_1\le\cdots\le l_n}} Q[X]_l \, \frac{\binom{n}{\gamma(l)}^2}{n!^2} \sum_{\pi,\sigma\in S_n} |\pi\cdot l\rangle\langle\sigma\cdot l|$$

where we divide by $|\operatorname{stab}(l)|^2 = \frac{n!^2}{\binom{n}{\gamma(l)}^2}$ to avoid overcounting. By replacing ordered indices, $l_1 \le \cdots \le l_n$ by all indices $l \in [d]^n$, we divide by $\frac{\binom{n}{\gamma(l)}}{n!}$,

$$\sum_{l\in[d]^n} Q[X]_l \, \frac{\binom{n}{\gamma(l)}}{n!^2} \sum_{\pi,\sigma\in S_n} |\pi\cdot l\rangle\langle\sigma\cdot l|$$

Finally, by relabeling permutations, we have,

$$\sum_{l\in[d]^n} Q[X]_l \, \frac{\binom{n}{\gamma(l)}}{n!} \sum_{\pi'\in S_n} |\pi'\cdot l\rangle\langle l|\,.$$

which is the claimed expression.

(4) By definition of $Q[X]$,

$$\mathrm{Tr}(X) = \sum_{j\in[d]^n} \langle j|X|j\rangle = \sum_{j\in[d]^n} Q[X]_j.$$

Recall that from Proposition 9.18, $\mathrm{Tr}(X) = \sum_{\alpha\in\mathbb{N}_d^{(n)}} \lambda(X)_\alpha$. This concludes the proof.

■

Note that in the previous Theorem 9.22, we establish a new tensor parametrisation of the diagonally symmetric subspace. In particular, it shows that the relevant parameters for a diagonally symmetric matrix X are just entries on the diagonal of the state, which can be arranged as a symmetric tensor $Q[X]$. This parametrisation will be quite useful for studying the entanglement properties in the remaining sections. We end this section by characterizing the HS inner product between two diagonally symmetric matrices in terms of the tensor parametrisation.

Remark 9.23 (S_d-symmetry in the tensor parametrisation)**.** Let $X \in \mathsf{DS}_d^{(n),S_d}$ and define $Q[X]$ as in Theorem 9.22. For $\tau \in S_d$ and $i = (i_1, \ldots, i_n) \in [d]^n$, write $\tau(i) := (\tau(i_1), \ldots, \tau(i_n))$. Then

$$\forall \tau \in S_d,\ \forall i \in [d]^n, \qquad Q[X]_{\tau(i)} = Q[X]_i.$$

Equivalently, $Q[X]_i$ depends only on $\mathrm{sort}(\gamma(i)) \in \mathsf{Par}_d(n)$, so an S_d-invariant DS tensor has $|\mathsf{Par}_d(n)|$ independent diagonal values (and $|\mathsf{Par}_d(n)| - 1$ after normalization to a state). Note that the action of S_d on indices i defined above is different that the action of S_n on the same set, which ensures that the tensor $Q[X]$ is symmetric.

Proposition 9.24. The Hilbert-Schmidt Inner product between the two DS matrices X and Y satisfies,

$$\mathrm{Tr}(X^*Y) = \sum_{\substack{i\in[d]^n \\ i_1\le i_2\ldots\le i_n}} \overline{Q[X]}_i Q[Y]_i \binom{n}{\gamma(i)}^2 = \sum_{i\in[d]^n} \overline{Q[X]}_i Q[Y]_i \binom{n}{\gamma(i)}. \quad (101)$$

Proof. Recall that for two DS matrices,

$$\mathrm{Tr}(X^*Y) = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \overline{\lambda(X)}_\alpha \lambda(Y)_\alpha.$$

Using Theorem 9.22, it follows that $\lambda(X)_\alpha = Q_{(\alpha)}\binom{n}{\alpha}$ hence the previous expression can be reduced to

$$\mathrm{Tr}(X^*Y) = \sum_{\alpha \in \mathbb{N}_d^{(n)}} \overline{Q[X]}_{(\alpha)} Q[Y]_{(\alpha)} \binom{n}{\alpha}^2 = \sum_{\substack{i \in [d]^n \\ i_1 \leq i_2 \ldots \leq i_n}} \overline{Q[X]}_i Q[Y]_i \binom{n}{\gamma(i)}^2.$$

By replacing the ordered indices with unordered indices, we get

$$\mathrm{Tr}(X^*Y) = \sum_{i \in [d]^n} \overline{Q[X]}_i Q[Y]_i \binom{n}{\gamma(i)}.$$

■

Note that Proposition 9.24 shows that the inner product of two matrices parametrized using the diagonal tensor $X \leftrightarrow Q[X]$ is *not* equal to the Euclidean inner product between two tensors corresponding to the matrices, i.e, $\mathrm{Tr}(XY) \neq \langle Q[X], Q[Y] \rangle$. This leads to a inconsistency while looking at duals, as in entanglement theory, the duals are usually considered with respect to the Hilbert-Schmidt inner product, while for tensors, the Euclidean product is standard. To solve this, we introduce another related parametrisation of the DS subspace.

Definition 9.25. Let $X \in \mathsf{DS}_d^{(n)}$. Then, define the symmetric tensor,

$$W[X]_i := Q[X]_i \binom{n}{\gamma(i)} = \langle i|X|i\rangle \binom{n}{\gamma(i)}.$$

Let us consider the following map, $\mathrm{diag} : \vee^n \mathbb{R}^d \mapsto \mathcal{M}(\vee^n \mathbb{C}^d)$, defined as,

$$\mathrm{diag}[Q] := \sum_{i \in [d]^n} Q_i \left|i\right\rangle \left\langle i\right|.$$

This maps a symmetric real tensor to a diagonal matrix in $\mathcal{M}_d(\mathbb{C})^{\otimes n}$. Note that this matrix is not bosonic, i.e, it is not supported only on the symmetric subspace (if all the entries of the tensor Q are non-zero, then $\mathrm{diag}[Q]$ is supported on the whole tensor space).

Proposition 9.26. Let $X \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$. Then, we have the following equality:

$$X = \Pi_d^{(n)} \operatorname{diag}[W[X]]\Pi_d^{(n)}$$

Proof. By using Theorem 9.22, we have

$$X = \sum_{i\in[d]^n} \sum_{\pi\in S_n} P_\pi \frac{\binom{n}{\gamma(i)}}{n!} Q[X]_i \left|i\right\rangle \left\langle i\right| .$$

Hence, we have

$$X = \sum_{i\in[d]^n} \sum_{\pi\in S_n} \frac{1}{n!} P_\pi W[X]_i \left|i\right\rangle \left\langle i\right| = \Pi_d^{(n)} \sum_{i\in[d]^n} W[X]_i \left|i\right\rangle \left\langle i\right| = \Pi_d^{(n)} \operatorname{diag}[W[X]]$$
$$= \Pi_d^{(n)} \operatorname{diag}[W[X]]\Pi_d^{(n)}$$

where the last equality follows from the self-adjointness of X. ∎

In the remaining sections, we use these parametrisations for the set of diagonally symmetric states, as well as diagonally symmetric entanglement witnesses. Note that by Proposition 9.24, we now have

$$\langle X, Y\rangle_{\mathcal{B}(\vee^n\mathbb{C}^d)} = \langle Q[X], W[Y]\rangle_{\vee^n\mathbb{C}^d} . \tag{102}$$

Hence, the Hilbert-Schmidt product now corresponds exactly to the Euclidean product of tensors in the Q and W parametrisations. The fact that the Hilbert-Schmidt product is the same as the Euclidean product in the Q and W parametrisations will be used in later section to relate the duality of bosonic matrices with diagonal symmetry to that of the corresponding Q and W parametrisations.

9.3.3 *Reduced states and marginals*

From the previous section, we know that the diagonally symmetric matrices X are parameterized with a symmetric tensor $Q[X]$. The next theorem shows that the quantum marginals (reduced density matrices) of these states have a direct correspondence with the "classical" marginals of this tensor. First, recall that the marginal of a symmetric tensor $T \in \vee^n\mathbb{R}^d$, with respect to a set of indices $A \subseteq [n]$ is given by

$$\forall j \in [d]^{n-|A|} \qquad [\mathrm{tr}_A(T)]_j := \sum_{i\in[d]^{|A|}} T_{i\sqcup j}.$$

Note that, for symmetric tensors, the marginal depends only on the cardinality of the set A.

Theorem 9.27. Let $X \in \mathsf{DS}_d^{(n)}$ be a diagonally symmetric matrix. For any $A \subseteq [n]$, let $\mathrm{Tr}_A(X)$ denote the marginal of the state over the tensor factors in A. We have then

- $\mathrm{Tr}_A(X) \in \mathsf{DS}_d^{(n-|A|)}$;
- $Q[\mathrm{Tr}_A(X)] = \mathrm{tr}_A(Q[X])$.

Proof. To prove the first assertion, we show that the reduced states also lie in the diagonally symmetric subspace. Firstly, we can show that any reduced bosonic state satisfies

$$\forall \sigma \in S_m, \quad P_\sigma \,\mathrm{Tr}_A(X) = \mathrm{Tr}_A\left((P_\sigma \otimes \mathbb{I}_{|A|})(X)\right) = \mathrm{Tr}_A(X),$$

where the last equality follows from the fact that X is bosonic. Moreover, we have,

$$\forall U \in \mathcal{DU}_d \quad U^{\otimes(n-|A|)}\,\mathrm{Tr}_A(X)(U^{\otimes(n-|A|)})^* = \mathrm{Tr}_A(U^{\otimes n} X (U^{\otimes n})^*) = \mathrm{Tr}_A(X),$$

where the first equality follows from the cyclicity of the trace and the second follows from the diagonal invariance of the matrix X. The second assertion follows from the direct computation:

$$\begin{aligned}
\forall i \in [d]^{n-|A|}, \quad Q[\mathrm{Tr}_A(X)]_i &= \langle i|[\mathrm{Tr}_A(X)|i\rangle = \mathrm{Tr}(X\,|i\rangle\langle i| \otimes \mathbb{I}_A) \\
&= \sum_{j \in [d]^A} \mathrm{Tr}(X\,|i,j\rangle\langle i,j|) \\
&= \sum_{j \in [d]^A} Q[X]_{i \sqcup j} = (\mathrm{tr}_A\, Q[X])_i.
\end{aligned}$$

Above, we use the notation $i \sqcup j$ to denote the vector

$$(i_1, \ldots, i_{n-|A|}, j_1, \ldots, j_{|A|}) \in [d]^n.$$

■

We use the previous result to compute the marginals of the pure Dicke states $|D_\alpha\rangle$. By Theorem 9.27, the marginals lie in the DS subspace. We compute the marginals for two reasons: firstly, it shows that the approach of tensors in terms of the tensor parametrisation is highly convenient, and secondly, the entanglement properties of these marginals have been of independent interest [SN25]. Let $|D_\alpha\rangle$ be a pure Dicke state, defined as

$$|D_\alpha\rangle = \frac{1}{\binom{n}{\alpha}^{1/2}} \sum_{i\,:\,\gamma(i)=k} |i\rangle\,.$$

The tensor parametrisation of this state is as follows:

$$\forall i \in [d]^n \quad Q[|D_\alpha\rangle\langle D_\alpha|]_i = |\langle i|D_\alpha\rangle|^2 = \frac{1}{\binom{n}{\gamma(i)}} \mathbb{1}_{\gamma(i)=\alpha}.$$

We compute next the marginal of the pure Dicke state using the marginal of the tensor, by using Theorem 9.27.

Proposition 9.28. For an arbitrary Dicke state $|D_\alpha\rangle$ and a marginal set $A \subseteq [n]$, we have:

$$\forall j \in [d]^{n-|A|}, \qquad Q[\mathrm{Tr}_A(|D_\alpha\rangle\langle D_\alpha|)]_j = \mathrm{tr}_A[Q(|D_\alpha\rangle\langle D_\alpha|)]_j = \frac{\binom{|A|}{\alpha-\gamma(j)}}{\binom{n}{\alpha}} \mathbb{1}_{\gamma(j)\leq\alpha}.$$

Proof. For the marginal of the tensor, we have:

$$\begin{aligned}
[\mathrm{tr}_A(Q[|D_\alpha\rangle\langle D_\alpha|])]_j &= \sum_{i\in[d]^{|A|}} (Q[|D_\alpha\rangle\langle D_\alpha|])_{i\sqcup j} = \sum_{i\in[d]^{|A|}} \frac{1}{\binom{n}{\alpha}} \mathbb{1}_{\gamma(i\sqcup j)=\alpha} \\
&= \frac{1}{\binom{n}{\alpha}} \sum_{i\in d^{|A|}} \mathbb{1}_{\gamma(i)+\gamma(j)=\alpha} \\
&= \frac{\binom{|A|}{\alpha-\gamma(j)}}{\binom{n}{\alpha}} \mathbb{1}_{\gamma(j)\leq\alpha}.
\end{aligned}$$

■

9.4 ENTANGLEMENT AND PPT PROPERTY

In this section, we show an exact correspondence between the entanglement properties of mixtures of Dicke states to some well-known positivity property of symmetric tensors; our findings are summarized in Fig. 36. We then completely characterize for which local Hilbert space dimension and number of particles there exist PPT entangled DS states. Finally, we show in the last subsection that all marginals of entangled pure Dicke states have negative partial transpose across all bipartitions, recovering a recent result of [SN25] in a simpler, more conceptual way. By establishing these results, we have a comprehensive framework for entanglement in mixtures of Dicke states, which we use to study PPT entanglement and bosonic extendibility in the later sections using well-known ideas and results about positive polynomials and tensors.

9.4.1 *Bose-symmetry and entanglement*

We begin this section with a brief review of multipartite entanglement in mixed states, with the focus on the particular results about bosonic states. Note the following two examples of entangled states in 3 qubits.

$$(|00\rangle + |11\rangle) \otimes |1\rangle \qquad |000\rangle + |111\rangle$$

Although both states are entangled, there is a difference between the structure of entanglement. The first state is entangled in a bipartite fashion, while for the GHZ state, no such decomposition into the bipartite entanglement exists. This motivates the following definition.

Definition 9.29 ([ISTY08, MMRRP+25]). Let $\mathcal{H} = \bigotimes_{i=1}^{n} \mathcal{H}_i$ be the Hilbert space of an n-partite quantum system. A pure state $|\psi\rangle \in \mathcal{H}$ is called *k-producible* if there exists a partition of $[n]$ into disjoint subsets $S_1, \ldots, S_m$ such that $|S_j| \leq k$ for all j and

$$|\psi\rangle = \bigotimes_{j=1}^{m} |\varphi_j\rangle,$$

where $|\varphi_j\rangle$ is a pure state on the subsystems indexed by S_j. A mixed state $X \in \mathcal{M}_d^{\otimes n}$ is called *k-producible* if,

$$X \in \operatorname{cone}\{|\psi\rangle\langle\psi| \mid |\psi\rangle \text{ is } k\text{-producible}\}.$$

The entanglement depth of a state ρ is the smallest k such that ρ is k-producible. A state is *genuinely $(k+1)$-partite entangled* if it is $(k+1)$-producible but not k-producible.

It is clear from the previous definition that bipartite quantum states are either separable (i.e. have entanglement depth 1) or 2-partite entangled. In comparison to bipartite systems, entanglement theory in the multipartite case is much more complicated. Surprisingly, for *multipartite* bosonic states, a stronger result holds.

Theorem 9.30 ([ISTY08, Theorem 1]). Let $X \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$. Then, the state has entanglement depth 1 or n. Particularly, if it has entanglement depth 1, there exist $\{|v_k\rangle\}_{k=1}^K$ such that,

$$X = \sum_{k=1}^{K} |v_k\rangle\langle v_k|^{\otimes n}.$$

We denote all separable bosonic states (entanglement depth = 1) as

$$\mathsf{Sep}_d^{(n)} := \mathrm{cone}\{|v_k\rangle\langle v_k|^{\otimes n} \mid |v_k\rangle \in \mathbb{C}^d\}, \tag{103}$$

which forms a proper convex cone. We define the set of bosonic entanglement witnesses as the conic dual of the separable cone

$$\mathsf{EW}_d^{(n)} := \left(\mathsf{Sep}_d^{(n)}\right)^\circ.$$

From the form of the extremal rays of the cone $\mathsf{Sep}_d^{(n)}$, we obtain the following characterization of entanglement witnesses in the DS subspace.

Proposition 9.31. Let $O \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$. Then, $O \in \mathsf{EW}_d^{(n)}$ if and only if

$$\forall\, |v\rangle \in \mathbb{C}^d \quad \langle v^{\otimes n}|O|v^{\otimes n}\rangle \geq 0.$$

Recall that all *bipartite* separable states satisfy the PPT (Positivity under Partial Transposition) property, i.e, PPT is a necessary condition for separability. The separable bosonic states (ref. Theorem 9.30) are separable across any bipartitions; hence, they also satisfy the PPT property across *each* such partition. In general, a bosonic state might only satisfy the PPT property across some bipartitions, and not all. Let I be a subset of $[n]$. We use Γ_I to denote the partial transpose of the systems indexed by I. We can use bosonic symmetry to show that the PPT property only depends on the size of the bipartition we consider while applying the partial transpose, and not on the particular systems that are transposed.

Proposition 9.32. Let $\rho \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$ be a bosonic matrix. Let I and J be arbitrary subsets of $[n]$ such that $|I| = |J|$. Then,

$$\rho^{\Gamma_I} \geq 0 \iff \rho^{\Gamma_J} \geq 0.$$

Proof. For a bosonic state, we have,

$$\forall \pi \in S_n \; P_\pi \rho P_{\pi^{-1}} = \rho.$$

Let π be a permutation that maps the elements of the set I to J. Then,

$$\rho^{\Gamma_I} = (P_\pi \rho P_{\pi^{-1}})^{\Gamma_I} = (P_\pi \rho^{\Gamma_J} P_{\pi^{-1}}).$$

■

Therefore, following the previous Proposition 9.32, consider the following convex cones.

Definition 9.33. Let $0 \leq k \leq \lfloor n/2 \rfloor$. We define the following convex cones,

$$\mathsf{PPT}_d^{(n,0)} := \{\rho \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \rho \geq 0\}$$

$$\mathsf{PPT}_d^{(n,k)} := \{\rho \in \mathrm{Herm}[\vee^n \mathbb{C}^d] \mid \rho^{\Gamma_{[k]}} \geq 0\}.$$

Note that $\mathsf{PPT}^{(n,0)}$ is the bosonic PSD matrices, and $\mathsf{PPT}^{(n,k)}$ is the set of bosonic matrices having the PPT property across the bipartition $[k] : [n]\backslash[k]$. Clearly, all the separable states (see Eq. (103), Theorem 9.30) satisfy the following inclusion.

$$\mathsf{Sep}_d^{(n)} \subseteq \bigcap_{k=0}^{\lfloor n/2 \rfloor} \mathsf{PPT}_d^{(n,k)} =: \mathsf{PPT}_d^{(n)}. \tag{104}$$

This means that the separable states satisfy the PPT property across all the bipartitions.

Remark 9.34. The set inclusion in Eq. (104) is strict except for the case $d = 2, n = 2, 3$. This has been shown by explicit construction of PPT entangled states for $n \geq 4$ qubits. [TAH+12, ATSL12].

We now introduce the conic dual of the PPT sets. Note that we will consider the conic dual in the ambient space of $\mathrm{Herm}[\vee^n \mathbb{C}^d] \subseteq \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$. We define the following convex cone of decomposable bosonic matrices,

$$\mathsf{Dec}_d^{(n,k)} := \left(\mathsf{PPT}_d^{(n,k)}\right)^\circ.$$

We also have the following characterization of the $\mathsf{Dec}_d^{(n,k)}$.

Theorem 9.35. $O \in \mathsf{Dec}_d^{(n,k)}$ if and only if there exist positive semi-definite operators, $P \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$ such that,

$$O \;=\; \Pi_d^{(n)}(P^{\Gamma_{[k]}})\Pi_d^{(n)}. \tag{105}$$

Proof. We will show the proof in two steps. ($\Longleftarrow$) Consider that there exist positive-semidefinite matrix $P \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$ such that,

$$O \;=\; \Pi_d^{(n)}(P^{\Gamma_{[k]}})\Pi_d^{(n)}.$$

Then for all $\rho \in \mathsf{PPT}_d^{(n,k)}$, we have,

$$\begin{aligned}\mathrm{Tr}(O\rho) = \mathrm{Tr}\Big(\Pi^{(n)}\big(P^{\Gamma_{[k]}}\big)\Pi_d^{(n)}\rho\Big) &= \mathrm{Tr}\Big(\big(P^{\Gamma_{[k]}}\big)\Pi_d^{(n)}\rho\Pi_d^{(n)}\Big)\\ &= \mathrm{Tr}\big(P^{\Gamma_{[k]}}\rho\big)\\ &= \mathrm{Tr}\big(P\,\rho^{\Gamma_{[k]}}\big) \geq 0\,.\end{aligned}$$

This shows that $O \in (\mathsf{PPT}_d^{(n,k)})^\circ = \mathsf{Dec}_d^{(n,k)}$.

($\Longrightarrow$) To show the reverse direction, assume that $O \in \mathsf{Dec}_d^{(n,k)}$. Then, note that,

$$\mathsf{PPT}_d^{(n,k)} = \{\rho \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid \rho^{\Gamma_{[k]}} \geq 0\} \cap \{\rho \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid \Pi_d^{(n)}\rho\Pi_d^{(n)} = \rho\}. \tag{106}$$

Consider the convex cone $(\mathsf{PPT}_d^{(n,k)})^\circ$ as dual in the larger ambient space $\mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$. Therefore, by the properties of the dual, we get (for closed cones),

$$(\mathsf{PPT}_d^{(n,k)})^\circ = \mathrm{cl}\left(\{X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid X^{\Gamma_{[k]}} \geq 0\} + \{X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid \Pi_d^{(n)} X \Pi_d^{(n)} = X\}^\perp\right).$$

This equality is because in Eq. (106), the first cone is self-dual, while the second cone is a subspace; moreover, the conic dual of an intersection is the closure of the sum. Also note that if $O \in (\mathsf{PPT}_d^{(n,k)})^\circ$ where dual is considered in $\mathrm{Herm}[\vee^n \mathbb{C}^d]$, then, it is an element of the dual with respect to $\mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$. Using this, we have the sequence of operators $\{P_l\}_{l\geq 1}, \{Q_l\}_{l\geq 1}$,

$$O = \lim_{l\to\infty} \tilde{P}_l + Q_l$$

where $\forall l, \quad \tilde{P}_l^{\Gamma_{[k]}} \geq 0$ and $\Pi_d^{(n)} Q_l \Pi_d^{(n)} = 0$. Denote $P_l := \tilde{P}_l^{\Gamma_{[k]}}$. Therefore,

$$\begin{aligned} O &= \Pi_d^{(n)} O \Pi_d^{(n)} \\ &= \Pi_d^{(n)} \left(\lim_{l\to\infty} \left(P_l^{\Gamma_{[k]}} + Q_l \right) \right) \Pi_d^{(n)} \\ &= \Pi_d^{(n)} \left(\lim_{l\to\infty} P_l^{\Gamma_{[k]}} \right) \Pi_d^{(n)} \\ &= \Pi_d^{(n)} P^{\Gamma_{[k]}} \Pi_d^{(n)}. \end{aligned}$$

where $P := \lim_{l\to\infty} P_l$. Also $P \geq 0$ as the cone of PSD matrices is closed. ■

Remark 9.36. By the previous result in Proposition 9.2, we can also show easily,

$$\forall z \in \mathbb{C}^d \qquad \langle z^{\otimes n}|O|z^{\otimes n}\rangle = \langle z^{\otimes n}|P^{\Gamma_{[k]}}|z^{\otimes n}\rangle = \langle \bar{z}^{\otimes k} \otimes z^{\otimes n-k}|P|\bar{z}^{\otimes k} \otimes z^{\otimes n-k}\rangle \geq 0.$$

This also shows easily that $\mathsf{Dec}_d^{(n,k)} \subseteq \mathsf{EW}_d^{(n)}$.

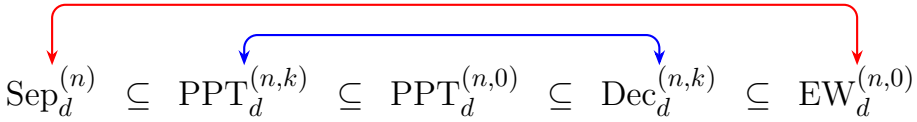
Corollary 9.37. We have the following conic-duality:

$$\left(\bigcap_{k=0}^{\lfloor n/2 \rfloor} \mathsf{PPT}_d^{(n,k)} \right)^\circ = \mathrm{cl}\left(\sum_{k=0}^{\lfloor n/2 \rfloor} \mathsf{Dec}_d^{(n,k)} \right) =: \mathsf{Dec}_d^{(n)},$$

where the latter set can be described explicitly as

$$\mathsf{Dec}_d^{(n)} = \left\{ O \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}] \mid \exists \{P_k \succeq 0\}_{k=0}^{\lfloor n/2 \rfloor},\ O = \Pi_d^{(n)} \left(\sum_{k=0}^{\lfloor n/2 \rfloor} P_k^{\Gamma_{[k]}} \right) \Pi_d^{(n)} \right\}.$$

We have the following inclusions and dualities of convex cones in the bosonic subspace.



Having established the basics of bosonic entanglement, we move on to studying entanglement in the diagonally symmetric (DS) subspace. By using the tensor parametrisation (ref. Theorem 9.22) of this subspace, we establish an exact correspondence of the entanglement properties in the DS subspace with those of tensors.

9.4.2 *Separability and Entanglement Witnesses*

In this section, we establish an exact correspondence between the separability of the diagonally symmetric state $X \in \mathsf{DS}_d^{(n)}$ and the convex properties of the tensor $Q[X]$. We accomplish this by extending the known results about the bipartite separability problem in mixtures of Dicke states. We now state and prove the main result of this section: the separability of a bosonic diagonally symmetric matrix X is equivalent to the complete positivity of the associated tensor $Q[X]$.

Theorem 9.38. Let $X \in \mathsf{DS}_d^{(n)}$ be a diagonally symmetric matrix. Then:

$$X \in \mathsf{Sep}_d^{(n)} \iff Q[X] \in \mathsf{CP}_d^{(n)}.$$

Proof. ($\implies$) To show the first implication, we assume the state X is separable, i.e, there exist vectors $\{|x_q\rangle \in \mathbb{C}\}_{q=1}^K$, such that,

$$X = \sum_{q=1}^{K} |x_q\rangle\langle x_q|^{\otimes n}.$$

By Theorem 9.22, we have $\forall i \in [d]^n$, $Q[X]_i := \langle i|X|i\rangle$. Hence, we have, by the separable decomposition of X,

$$\forall i \in [d]^n \quad Q[X]_i = \langle i|X|i\rangle = \sum_{q=1}^{K} |(x_q)_{i_1}|^2 |(x_q)_{i_2}|^2 \dots |(x_q)_{i_n}|^2. \tag{107}$$

By defining $v_q := x_q \odot \overline{x_q}$, it is clear that $\forall q,\ v_q \geq 0$. With this notation, the previous equation reads

$$Q[X] = \sum_{q=1}^{K} v_q^{\otimes n}.$$

This implies that $Q[X] \in \mathsf{CP}_d^{(n)}$.

($\impliedby$) To show the reverse implication, we assume that $Q[X] \in \mathsf{CP}_d^{(n)}$. This implies that there exists a finite number of entrywise positive vectors $\{v_q \in \mathbb{R}_+^d\}_{q=1}^K$ such that

$$Q[X] = \sum_{q=1}^{K} v_q^{\otimes n}.$$

Consider the vectors, $\{x_q\}_{q=1}^K$ defined as $\forall q,\ (x_q)_i := \sqrt{(v_q)_i}$. By this definition, it immediately follows that $\forall q \in [K],\ x_q \odot x_q = v_q$. Consider the following separable quantum state $\sigma \in \mathsf{Sep}_d^{(n)}$, defined as

$$\sigma := \sum_{q=1}^{K} |x_q\rangle\langle x_q|^{\otimes n}.$$

Note that, $\Pi\sigma\Pi = \sigma$. i.e σ is a bosonic state. We have the twirled quantum state,

$$\mathcal{T}_{\mathcal{DU}}(\sigma) = \int_{\mathcal{DU}_d} U^{\otimes n} \sum_{q=1}^{K} |x_q^{\otimes n}\rangle \langle x_q^{\otimes n}| \, (U^{\otimes n})^* \, \mathrm{d}U = \sum_{q=1}^{K} \int_{\mathcal{DU}_d} U^{\otimes n} \, |x_q^{\otimes n}\rangle \langle x_q^{\otimes n}| \, (U^{\otimes n})^* \, \mathrm{d}U \tag{108}$$

Firstly note that, $\Pi_d^{(n)} \mathcal{T}_{\mathcal{DU}}(\sigma) \Pi_d^{(n)} = \mathcal{T}_{\mathcal{DU}}(\sigma)$ and due to twirling $\forall U \in \mathcal{DU}_d$, $[\mathcal{T}_{\mathcal{DU}}(\sigma), U^{\otimes n}] = 0$, therefore by Proposition 9.17, the state $\mathcal{T}_{\mathcal{DU}}(\sigma) \in \mathsf{DS}_d^{(n)}$. Secondly, since twirling is an LOCC operation, $\mathcal{T}_{\mathcal{DU}}(\sigma) \in \mathsf{Sep}_d^{(n)}$. Finally note that

$$\begin{aligned} Q[\mathcal{T}_{\mathcal{DU}}(\sigma)]_i &= \langle i|\mathcal{T}_{\mathcal{DU}}(\sigma)|i\rangle = \langle i| \int_{\mathcal{DU}_d} U^{\otimes n} \sum_{q=1}^{K} |x_q^{\otimes n}\rangle \langle x_q^{\otimes n}| \, (U^{\otimes n})^* \, \mathrm{d}U \, |i\rangle \\ &= \sum_{q=1}^{K} \int_{\mathcal{DU}_d} \langle i|x_q^{\otimes n}\rangle \langle x_q^{\otimes n}|i\rangle \, \mathrm{d}U = Q[\sigma]_i, \end{aligned}$$

showing that $Q[\mathcal{T}_{\mathcal{DU}}(\sigma)] = Q[X]$; above we have use that $U^{\otimes n} |i\rangle$ is equal to $|i\rangle$ up to a phase for all diagonal unitary matrix $U \in \mathcal{DU}_d$. Hence, by Theorem 9.22, we conclude $\mathcal{T}_{\mathcal{DU}}(\sigma) = X$, finishing the proof. ∎

The proof strategy we employed above is very similar to that presented in [Yu16] for the bipartite case. Theorem 9.38 characterizes the separability properties of mixtures of Dicke states. Recall that checking for complete positivity is known to be NP-hard.

We now use the duality relation from Eq. (102) to characterize entanglement witnesses in the diagonally symmetric subspace in terms of the copositive tensors.

Proposition 9.39. The following equivalence holds for a matrix $O \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$.

$$O \in \mathsf{EW}_d^{(n)} \iff W[O] \in \mathsf{Cop}_d^{(n)}.$$

Proof. This follows from the duality of separable states and entanglement witnesses, read at the level of Q and W parametrizations. More explicitly, by the result in Proposition 9.26, we have

$$\forall\, |v\rangle \in \mathbb{C}^d \quad \langle v^{\otimes n}|O|v^{\otimes n}\rangle = \langle v^{\otimes n}|\Pi_d^{(n)} \, \mathrm{diag}[W[O]]\Pi_d^{(n)}|v^{\otimes n}\rangle = \langle W[O], (\bar{v} \odot v)^{\otimes n}\rangle \geq 0.$$

∎

Remark 9.40. The connection between entanglement witnesses and copositive *matrices* has already been noted in [MATS21] for the bipartite case. More precisely,

it is shown in [MATS21] that, at $n = 2$, for the witness parametrized by a matrix $C \in \mathrm{Herm}[\mathcal{M}_d]$ in the way $X_C = \sum_{i,j} C_{ij} \, |ij\rangle\langle ji|$,

$$X_C \in \mathsf{EW}_d^{(2)} \iff C \in \mathsf{Cop}_d^{(2)}.$$

This is slightly different from our parametrization, but has the same inner product, i.e for all $Y \in \mathrm{Herm}[\mathsf{DS}_d^{(2)}]$ we have,

$$\mathrm{Tr}(X_C Y) = \langle C, Q[Y] \rangle \, .$$

Example 9.41 (Projective entanglement witnesses)**.** We show some examples of bosonic diagonally symmetric entanglement witnesses.

$$R_\alpha(\mu) := \Pi_d^{(n)} - \mu \, |D_\alpha\rangle\langle D_\alpha| \, .$$

Then, by computing the tensor parametrization of the witness, we obtain,

$$\begin{aligned} \forall i \in [d]^n, \, W[R_\alpha]_i = \binom{n}{\gamma(i)} \langle i | \Pi_d^{(n)} - \mu \, |D_\alpha\rangle\langle D_\alpha| \, |i\rangle &= 1 - \mu \frac{\binom{n}{\gamma(i)}}{\binom{n}{\alpha}} \mathbb{1}_{\gamma(i)=\alpha} \\ &= 1 - \mu \mathbb{1}_{\gamma(i)=\alpha} \end{aligned}$$

Consider the polynomial,

$$\langle W[R_\alpha], x^{\otimes n} \rangle = \Big(\sum_{i=1}^d x_i \Big)^n - \mu \binom{n}{\alpha} x^\alpha.$$

By applying the AM-GM weighted inequality, we obtain for all $x \in \mathbb{R}_+^d$,

$$\frac{1}{n} \Big(\sum_{i=1}^d x_i \Big) = \frac{1}{n} \Big(\sum_{i=1}^d \alpha_i \frac{x_i}{\alpha_i} \Big) \geq \prod_{i=1}^d \Big(\frac{x_i}{\alpha_i} \Big)^{\frac{\alpha_i}{n}} \iff \Big(\sum_{i=1}^d x_i \Big)^n \geq \frac{n^n}{\prod_{i=1}^d \alpha_i^{\alpha_i}} x^\alpha$$

Using Proposition 9.39, we have that for all

$$-\infty \leq \mu \leq \frac{1}{\binom{n}{\alpha} \prod_{i=1}^d \big(\frac{\alpha_i}{n} \big)^{\alpha_i}},$$

$R_\alpha(\mu)$ is a bosonic entanglement witness. In the case of n qubits, the Dicke state with occupation numbers $(n/2, n/2)$ yields the entanglement witness

$$\Pi_2^{(n)} - \mu_* \left| D_{(n/2,n/2)} \right\rangle\!\left\langle D_{(n/2,n/2)} \right|$$

with $\mu_* = \frac{2^n}{\binom{n}{n/2}} \sim \sqrt{\frac{\pi n}{2}}$ as $n \to \infty$. Similar computations with entanglement witnesses constructed from Dicke states were considered in [Tót07, BG13].

9.4.3 *Decomposability and PPT*

In the preceding section, we demonstrated that the separability of the states in the diagonally symmetric subspace is equivalent to the complete positivity of the tensor $Q[X]$. The convex cones $\mathsf{PPT}_d^{(n,k)}$ are outer tractable approximation of the separable states. The pertinent question is how to describe the PPT property in terms of the tensor $Q[X]$. The analytical computation of PPT conditions in the diagonally symmetric subspace was obtained in [RPAR+25, Lemma III.4 and Lemma III.5] by block diagonalization of the matrix X^Γ. These conditions appear highly non-trivial to describe. This motivates us to focus on the dual objects, the sets of decomposable witnesses, $\mathsf{Dec}_d^{(n,k)}$. Surprisingly, these sets can be shown to have a correspondence with the sum of squares property of tensors.

We now state and prove the main result of this section. Briefly, this result provides a correspondence between decomposable witnesses O and the properties of the polynomial $p_{W[O]}$ in the diagonally symmetric subspace. For the rather long and technical proof of this theorem, see Section 9.8.

Theorem 9.42. The following results hold for $O \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$.

1. $O \in \mathsf{Dec}_d^{(n,l)} \implies p_{W[O]}(x) \in \mathrm{cone}\{x^\alpha \psi \mid |\alpha| \in \{n, n-2, n-4 \ldots n-2l\}, \psi \in \Sigma_d^{(n-|\alpha|)}\}$.
2. Let $k \leq \lfloor n/2 \rfloor$ such that $\alpha \in \mathbb{N}_d^{(n-2k)}$ and $\psi \in \mathbb{H}[x]_{d,k}$. Then,

$$p_{W[O]}(x) = x^\alpha \psi^2 \implies O \in \mathsf{Dec}_d^{(n,l)}$$

for all $l \in [k, n-k]$.

In particular, we have the equivalence,

$$O \in \mathsf{Dec}_d^{(n,l)} \iff p_{W[O]}(x) \in \mathrm{cone}\{x^\alpha \psi \mid |\alpha| \in \{n, n-2, n-4 \ldots n-2l\}, \psi \in \Sigma_d^{(n-|\alpha|)}\}.$$

and hence the following inclusions between the decomposable sets.

$$\forall l \in [\lfloor n/2 \rfloor - 1], \quad \mathsf{Dec}_d^{(n,l)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}] \subseteq \mathsf{Dec}_d^{(n,l+1)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}].$$

To make the notation less clunkier, we define the increasing series of sets,

$$\mathsf{SOS}_d^{(n,l)} := \{T \mid p_T(x) \in \mathrm{cone}\{x^\alpha \psi \mid |\alpha| \in \{n, n-2, n-4 \ldots n-2l\}, \psi \in \Sigma_d^{(n-|\alpha|)}\}\}.$$

Recall that an n-th order symmetric tensor is called a sum-of-squares (represented as $\mathsf{SOS}_d^{(n)} = \mathsf{SOS}_d^{(n,\lfloor n/2 \rfloor)}$ by Theorem 9.11) tensor if its associated polynomial is a sum of squares polynomial in "x^2",

$$p_T(x \odot x) \in \Sigma_d^{(2n)}.$$

Corollary 9.43. For any $O \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$, we have

$$W[O] \in \mathsf{SOS}_d^{(n)} \iff O \in \mathsf{Dec}_d^{(n,\lfloor n/2 \rfloor)} = \sum_{l=0}^{\lfloor n/2 \rfloor} \mathsf{Dec}_d^{(n,l)}.$$

Let us summarise what we have shown in the previous result. For a diagonally symmetric (DS) operator O, the $\lfloor n/2 \rfloor$- decomposability property is equivalent to the symmetric tensor $W[O]$ being SOS. Surprisingly, we also find that $\lfloor n/2 \rfloor$- decomposability implies decomposability of the DS operator for all $l \leq \lfloor n/2 \rfloor$. Recall that for $X, Y \in \mathsf{DS}_d^{(n)}$, we have,

$$\langle X, Y \rangle = \langle Q[X], W[Y] \rangle .$$

We use this fact to characterize the property of PPT in the diagonally symmetric subspace, culminating with Theorem 9.48, in which we show that the PPT condition with respect to the most balanced bipartion implies the PPT conditions with respect to all other bipartitions. To accomplish this, we characterise the dual of SOS tensors.

Moment Tensors. Let $f : \mathbb{H}[x]_{d,n} \to \mathbb{R}$. For all $\alpha \in \mathbb{N}^d$ such that $|\alpha| = n - 2j$, we define the following matrices, with the columns and rows labelled by β, β' such that $|\beta| = |\beta'| = j$.

$$(\mathcal{M}^{(\alpha,j)}[f])_{\beta,\beta'} := f(x^{\alpha+\beta+\beta'}).$$

This defines a finite family of *moment matrices* labeled by the monomial vector α and j.

Define the linear functional over the homogeneous polynomials.

$$\mathcal{L}_T : \mathbb{H}[x]_{d,n} \to \mathbb{R}, \qquad \mathcal{L}_T(x^\mu) := T_{(\mu)} \quad (|\mu| = n),$$

and extend it by linearity. Then $\mathcal{L}_T(p_Q) = \langle T, Q \rangle$ for every symmetric tensor Q, and the moment-matrix entries are

$$\left(\mathcal{M}^{(\alpha,j)}[\mathcal{L}_T]\right)_{\beta,\beta'} := \mathcal{L}_T\left(x^{\alpha+\beta+\beta'}\right), \qquad |\alpha| = n - 2j,\ |\beta| = |\beta'| = j.$$

We can show the following result.

Theorem 9.44. The following statements are equivalent and characterise the SOS tensors.

(1) $T \in (\mathsf{SOS}_d^{(n,k)})^\circ$

(2) $\forall j = 0, \dots, k, |\alpha| = n - 2j, \quad \mathcal{M}^{(\alpha,j)}[\mathcal{L}_T] \succeq 0.$

Proof. We denote by $\Delta_d^{(n)} := \{p \in \mathbb{H}[x]_{d,n} \mid p(x \odot x) \in \Sigma_d^{(2n)}\}$. By Theorem 9.11, we have the general characterization of polynomials $p(x)$ such that $p(x \odot x)$ is SOS. Note that such polynomials belong to the following convex cone.

$$p(x) \in \mathrm{cone}\{x^\alpha \varphi^2(x) | \, |\alpha| + 2\deg(\varphi) = n\}.$$

Therefore $T \in (\mathsf{SOS}_d^{(n,k)})^\circ \iff \mathcal{L}_T \in (\Delta_d^{(n)})^\circ \iff \forall |\alpha| + 2\deg(\varphi) = n$ we have $\mathcal{L}_T(x^\alpha \varphi^2(x)) \geq 0$. Let $\varphi(x) = \sum_{|\beta| = \frac{\deg(\varphi)}{2}} c_\beta x^\beta$. Then, by plugging this into the functional,

$$\mathcal{L}_T\Big(\sum_{\beta\beta'} c_\beta c_{\beta'} x^{\alpha+\beta+\beta'}\Big) = \sum_{\beta\beta'} c_\beta c_{\beta'} \mathcal{M}^{\alpha,j}[\mathcal{L}_T]_{\beta,\beta'} \geq 0.$$

Since this is true for all $c_\beta \in \mathbb{R}^{|\beta|}$, $\mathcal{M}^{\alpha,j}[\mathcal{L}_T] \succeq 0$. ∎

In the remainder of this section, we want to interpret this family of moment matrices in the language of tensors rather than linear functionals. We do this by showing that the conditions in Theorem 9.44 can be exactly obtained by the combination of the following two operations on tensors.

- Tensor flattenings: Let $T \in \vee^{2n}\mathbb{R}^d$ be a symmetric tensor of even order $2n$ and dimension d. Then, such a tensor can be associated to a matrix of size $d^n \times d^n$ by dividing the indices equally to arrange it as a matrix,

  $$M_{\alpha\beta} := T_{\alpha_1\alpha_2\dots\alpha_n\beta_1\beta_2\dots\beta_n}.$$

  This is called a tensor flattening (represented diagrammatically in Fig. 34). Note that we consider only the flattenings that are *balanced*, i.e, we consider an equal number of indices to create a matrix.

- Tensor slices: Let $T \in \vee^n\mathbb{R}^d$ be a symmetric tensor of even order n and dimension d. For a subset of indices $I \subset [n]$, we define the tensor $S \in \vee^{(n-|I|)}\mathbb{R}^d$ by fixing the indices of the tensor T belonging to I, i.e $\forall k \in I$, $i_k = a_k \in \mathbb{N}$:

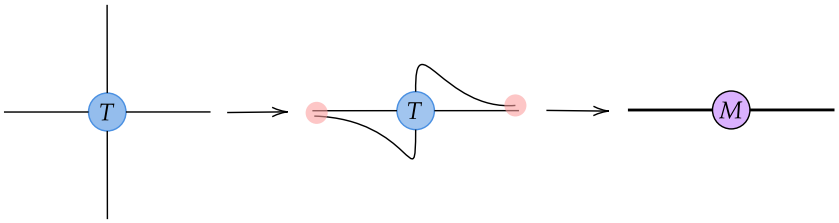


Figure 34: The figure represents a balanced flattening of a tensor $T \in \vee^4 \mathbb{R}^d$.

$$S_{j_1 \ldots j_{n-|I|}} := T_{a_1 \ldots a_{|I|} j_1 \ldots j_{n-|I|}}$$

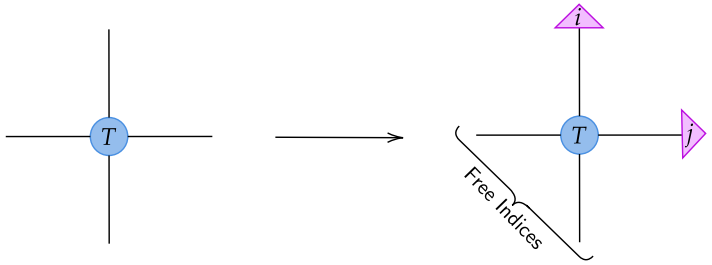


Figure 35: The figure represents a slice of a tensor $T \in \vee^4 \mathbb{R}^d$. by fixing two indices to be i, j.

This is represented diagrammatically in Fig. 35.

In what follows, we shall consider all the even-order slices of a given tensor. For tensors of even order $2n$, we have even slices of order $2n, 2n-2, 2n-4, \ldots, 2, 0$, and for tensors of odd order $2n-1$, we have even slices of order $2n-2, 2n-4, \ldots, 2, 0$. We consider the family of *flattenings* of all the *even* slices of the tensor, and we call this family of square matrices, the *slice flattenings* associated with a tensor T, denoted $\mathrm{SF}[T]$. We also use $\mathrm{SF}^{(k)}[T]$ to denote the flattenings of even slices of size $\leq 2k$ (even order tensors) and $\leq 2k+1$ (odd order tensors).

Proposition 9.45. Let Q be a completely positive tensor.

(1) Any slice of the tensor is completely positive tensor.

(2) Any balanced flattening of the tensor is a completely positive matrix.

(3) All the slice flattenings are completely positive matrices.

Proof. Let Q have the completely positive decomposition, $Q = \sum_{q=1}^{N} v_q^{\otimes n}$.

(1) Let S be the slice of the tensor over the indices I, by fixing indices $\forall k \in I, i_k = a_k$. Then, we have

$$S = \sum_{q=1}^{N} \prod_{k \in I} (v_q)_{a_k} v_q^{\otimes n-|I|} \in \mathsf{CP}_d^{(n-|I|)}$$

as $\prod_{k\in I}(v_q)_{a_k} \geq 0$.

(2) For n odd there is no balanced flattening. Hence, we assume $n = 2m$ is even. Then, we have that the balanced flattening of the tensor

$$F = \sum_{q=1}^{N} \left| v_q^{\otimes m} \right\rangle\!\!\left\langle v_q^{\otimes m} \right|.$$

(3) The proof follows from combining the result in Item (1) and Item (2).

■

We define the following convex cones of moment tensors:

$$\mathsf{Mom}_d^{(n,k)} := \{T \in \vee^n \mathbb{R}^d \mid \forall X \in \mathrm{SF}^{(k)}[T],\ X \succeq 0\},$$

and for $k = \lfloor n/2 \rfloor$ we denote the set of *all slice flattenings* positive semidefinite by

$$\mathsf{Mom}_d^{(n)} := \mathsf{Mom}_d^{(n,\lfloor n/2 \rfloor)}. \tag{109}$$

By Proposition 9.45, this is outer relaxation of completely positive tensors. Moreover, we have the following equivalence that establishes that moment tensors are conic duals to SOS tensors.

Theorem 9.46. We have the following conic duality:

$$\forall k \in [\lfloor n/2 \rfloor], \quad (\mathsf{Mom}_d^{(n,k)})^\circ = \mathsf{SOS}_d^{(n,k)}$$

Proof. Recall that we have the following equivalence

$$T \in (\mathsf{SOS}_d^{(n,k)})^\circ \quad \iff \quad \forall\, j = 0, \ldots, k\ |\alpha| = n - 2j,\ \mathcal{M}^{(\alpha,j)}[\mathcal{L}_T] \succeq 0.$$

We now explain how the moment matrices $\mathcal{M}^{(\alpha,j)}[\mathcal{L}_T]$ are obtained from slice–flattenings of T. Recall the entries of this matrix

$$\left(\mathcal{M}^{(\alpha,j)}[\mathcal{L}_T]\right)_{\beta,\beta'} = \mathcal{L}_T\left(x^{\alpha+\beta+\beta'}\right), \qquad |\alpha| = n - 2j,\ |\beta| = |\beta'| = j.$$

Fix $\alpha \in \mathbb{N}_d^{(n-2j)}$. Consider the even slice $S^{(\alpha)} \in \vee^{2j}\mathbb{R}^d$ of T obtained by fixing the first $n-2j$ indices to the canonical multi-index (α):

$$S^{(\alpha)}_{u\cup v} := T_{(\alpha)\cup u\cup v}, \qquad u, v \in [d]^j.$$

Its balanced flattening is the $d^j \times d^j$ matrix

$$F^{(\alpha)}_{u,v} := S^{(\alpha)}_{u\cup v} = T_{(\alpha)\cup u\cup v}.$$

Because T is symmetric, the entries $F^{(\alpha)}_{u,v}$ only depend on the occupation vectors $\beta := \gamma(u)$ and $\beta' := \gamma(v)$. Consequently, $F^{(\alpha)}$ has repeated rows/columns whenever two multi-indices have the same occupation pattern.

Let D be the $\{0,1\}$-matrix that duplicates rows/columns according to occupation vectors (one column per $\beta \in \mathbb{N}_d^{(j)}$, one row per $u \in [d]^j$, with $D_{u,\beta} = 1$ iff $\gamma(u) = \beta$). Then one checks that

$$F^{(\alpha)} = D\, \mathcal{M}^{(\alpha,j)}[\mathcal{L}_T]\, D^\top,$$

so $\mathcal{M}^{(\alpha,j)}[\mathcal{L}_T]$ is exactly the *effective* flattening obtained from $F^{(\alpha)}$ by deleting repeated rows and columns. In particular, positive semidefiniteness is preserved (and reflected) by this deletion/duplication: since D has full column rank, we have $F^{(\alpha)} \succeq 0 \iff \mathcal{M}^{(\alpha,j)}[\mathcal{L}_T] \succeq 0$.

■

> **Remark 9.47.** The size of the tensor flattenings of the general tensor of $2n$ legs is $d^n \times d^n$. But due to symmetry in the tensor, this leads to repeated multiple rows and columns in the matrix, leading to the size of the largest *effective* flattening (after deletion of the repeated rows and columns) being $\binom{n+d-1}{d-1} \times \binom{n+d-1}{d-1}$. For $d = 2$, we get the largest effective flattening of size $(n+1) \times (n+1)$.

We end this section by showing the exact PPT conditions for the quantum states in the diagonally symmetric subspace. We present these conditions in terms of the slice flattening of the tensor $Q[X]$. Note that the same conditions for PPT have been obtained in [RPAR+25], in which they also pose the conjecture whether in the diagonally symmetric subspace, the PPT just across the *largest* bipartition of the n-partite state implies PPT across all bipartitions (and also positivity of the state). The next result discusses the PPT conditions and the positive resolution of this conjecture.

Theorem 9.48. Let $X \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$. Then, we have the following equivalence:

$$X \in \mathsf{PPT}_d^{(n,k)} \iff Q[X] \in \mathsf{Mom}_d^{(n,k)}.$$

In particular, we have for the PPT sets:

$$\forall l \in [\lfloor n/2 \rfloor - 1], \quad \mathsf{PPT}_d^{(n,l+1)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}] \subseteq \mathsf{PPT}_d^{(n,l)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}].$$

Proof. Firstly, note the following equality between the sets.

$$\mathsf{Dec}_d^{(n,k)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}] = \{\mathcal{T}_{\mathcal{DU}}(O) \mid O \in \mathsf{Dec}_d^{(n,k)}\}.$$

$$\mathsf{PPT}_d^{(n,k)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}] = \{\mathcal{T}_{\mathcal{DU}}(X) \mid X \in \mathsf{PPT}_d^{(n,k)}\}.$$

Moreover, we have for all $W \in \mathrm{Herm}[\vee^n \mathbb{C}^d]$ and $X \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$, the following trace relation.

$$\mathrm{Tr}(XO) = \mathrm{Tr}(\mathcal{T}_{\mathcal{DU}}(X)O) = \mathrm{Tr}(X\mathcal{T}_{\mathcal{DU}}(O)).$$

Then, we have the following equivalences for $X \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$:

$$\begin{aligned}
X \in \mathsf{PPT}_d^{(n,k)} &\iff \forall O \in \mathsf{Dec}_d^{(n,k)},\ \mathrm{Tr}(XO) \geq 0 \\
&\iff \forall O \in \mathsf{Dec}_d^{(n,k)},\ \mathrm{Tr}\big(X\,\mathcal{T}_{\mathcal{DU}}(O)\big) \geq 0 \\
&\iff \forall O \in \mathsf{Dec}_d^{(n,k)} \cap \mathrm{Herm}\big[\mathsf{DS}_d^{(n)}\big],\ \mathrm{Tr}(XO) \geq 0 \\
&\iff \forall O \in \mathsf{Dec}_d^{(n,k)} \cap \mathrm{Herm}\big[\mathsf{DS}_d^{(n)}\big],\ \langle Q[X], W[O]\rangle \geq 0 \\
&\iff \forall W[O] \in \mathsf{SOS}_d^{(n,k)},\ \langle Q[X], W[O]\rangle \geq 0 \\
&\iff Q[X] \in \mathsf{Mom}_d^{(n,k)}.
\end{aligned}$$

■

The following direct corollary of the theorem above settles in the affirmative the Conjecture III.1 in [RPAR+25].

Corollary 9.49. Let $X \in \mathrm{Herm}[\mathsf{DS}_d^{(n)}]$ be a mixture of Dicke states on n particles with local dimension d. If X is PPT with respect to the most balanced bipartition $n = \lfloor n/2 \rfloor + \lceil n/2 \rceil$, then X is PPT with respect to all other bipartitions:

$$\forall l \in [\lfloor n/2 \rfloor], \quad \mathsf{PPT}_d^{(n,\lfloor n/2 \rfloor)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}] \subseteq \mathsf{PPT}_d^{(n,l)} \cap \mathrm{Herm}[\mathsf{DS}_d^{(n)}].$$

In other words, in the case of mixture of Dicke states, the PPT criterion with respect to the most balanced bipartion is stronger than the PPT criterion with respect to all other bipartitions.

The previous theorem implies that if we desire PPT of a partition of size k, this means that flattenings of all even slices of size $\geq n - 2k$ are positive-semidefinite. For $k = 0$, the PPT condition reduces to the positivity of the matrix $X \in \mathsf{DS}_d^{(n)}$, which is equivalent to the entrywise positivity of the tensor $Q[X]$. We present the PPT conditions for the case of $n = 2$ and $n = 3$ in the following tables.

Property	**Condition on $Q[\cdot]$**
$X \in \mathsf{PPT}_d^{(2,0)}$	$\forall i, j \in [d],\ Q[X]_{ij} \geq 0$
$X \in \mathsf{PPT}_d^{(2,1)}$	$\forall i, j \in [d],\ Q[X]_{ij} \geq 0$ and $\{Q[X]_{ij}\}_{i,j=1}^{d} \succeq 0$
$X \in \mathsf{Sep}_d^{(2)}$	$Q[X] \in \mathsf{CP}_d^{(2)}$

Table 20: PPT and separability conditions for $n = 2$.

Property	**Condition on $Q[\cdot]$**
$X \in \mathsf{PPT}^{(3,0)}$	$\forall i, j, k \in [d],\ Q[X]_{ijk} \geq 0$
$X \in \mathsf{PPT}_d^{(3,1)}$	$\forall i, j, k \in [d],\ Q[X]_{ijk} \geq 0$ and $\forall k,\ \{Q[X]_{ijk}\}_{i,j=1}^{d} \succeq 0$
$X \in \mathsf{Sep}_d^{(3)}$	$Q[X] \in \mathsf{CP}_d^{(3)}$

Table 21: PPT and separability conditions for $n = 3$.

We summarize the main connections between the entanglement properties in the diagonally symmetric subspace and the corresponding tensor properties in Fig. 36.

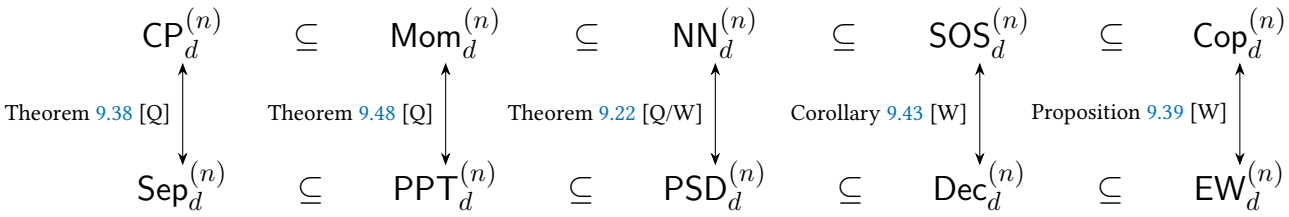


Figure 36: The different notions of positivity for Hermitian matrices in the DS subspace (bottom row) and the corresponding class of real symmetric tensors (top row). References for the proof of the correspondence are given, along with the parametrization (Q and/or W) realizing the correspondance.

9.4.4 *Existence of PPT entangled states*

In the last section, we established a complete dictionary of entanglement properties in the diagonally symmetric subspace. We now proceed to do a systematic study of PPT entanglement by using the correspondences. Recall that a mixture of Dicke states, $X \in \mathsf{DS}_d^{(n)}$, is PPT for bipartitions if and only if $Q[X] \in \mathsf{Mom}_d^{(n)}$. On the dual side, we have that a witness $O \in \mathsf{DS}_d^{(n)}$ is decomposable if and only if $W[O] \in \mathsf{SOS}_d^{(n)}$. The PPT entangled states correspond exactly to the moment tensors, $\mathsf{Mom}_d^{(n)}$ that are not in $\mathsf{CP}_d^{(n)}$, and on the dual side, the witnesses correspond to $\mathsf{Cop}_d^{(n)}$ which are not $\mathsf{SOS}_d^{(n)}$.

In the remainder of this section, we analyze the three different regimes: multipartite qubit systems, bipartite systems, and the rest. The first two have already been scrutinized in [Yu16, TAQ+18].

Qubit systems. We begin by recalling the following standard fact [Hil88] about homogeneous polynomials of 2 variables (see also Table 19): non-negative homogeneous polynomials in two variables of even degree are sums-of-squares; equivalently, every non-negative polynomial in one real variable is a sum of (two) squares. This directly implies the following result in [Yu16, Theorem 2].

Theorem 9.50 ([Yu16]). Let $X \in \mathsf{DS}_2^{(n)}$. Then, X is separable if and only if it is PPT across all bipartitions.

Proof. By Hilbert's result [Hil88] it follows that $\mathsf{Cop}_2^{(n)} = \mathsf{SOS}_2^{(n)}$. Therefore, on the dual side it follows that $\mathsf{CP}_2^{(n)} = \mathsf{Mom}_2^{(n)}$ showing the result. ∎

We also explicitly show the conditions for PPT and hence, the necessary and sufficient conditions for separability in the Section 9.9. Moreover, note that the PPT across all bipartitions is implied by just the PPT of the most balanced bipartition.

Bipartite qudit systems. For the bipartite mixtures of Dicke states, this problem reduces to the matrix case. Recall the results about homogeneous polynomials of degree 4 [Hil88], as presented in Table 22. The table implies that for $d = 3$, $\mathsf{SOS}_3^{(2)} = \mathsf{Cop}_3^{(2)}$ and similarly, on the dual side, $\mathsf{CP}_3^{(2)} = \mathsf{Mom}_3^{(2)}$. Surprisingly, this equivalence also holds for $d = 4$, as stated in the next theorem.

d	$2n = 4$
2	Yes
3	Yes
≥ 4	No

Table 22: Can any homogeneous polynomial of degree $2n$ in d variables be represented as a sum of squares?

Theorem 9.51 ([SMB21, TAQ+18, Yu16])**.** For $d \leq 4$, $\mathsf{CP}_d^{(2)} = \mathsf{Mom}_d^{(2)}$. Therefore, for $d \leq 4$, a bipartite mixture of Dicke states is separable if and only if it is PPT.

Recall that $\mathsf{Mom}_d^{(2)} = \mathsf{NN}_d \cap \mathsf{PSD}_d := \mathsf{DNN}_d$. For the $d = 5$, the following matrix is an element of doubly non-negative (DNN_d) but not CP_d as shown in [GNS25].

$$A = \begin{pmatrix} 2\cos\frac{\pi}{5} & 1 & 0 & 0 & 1 \\ 1 & 2\cos\frac{\pi}{5} & 1 & 0 & 0 \\ 0 & 1 & 2\cos\frac{\pi}{5} & 1 & 0 \\ 0 & 0 & 1 & 2\cos\frac{\pi}{5} & 1 \\ 1 & 0 & 0 & 1 & 2\cos\frac{\pi}{5} \end{pmatrix}.$$

Remark 9.52. The polynomial $f(x, y, z, w) = x^2y^2 + y^2z^2 + z^2x^2 + w^4 - 4xyzw$ is a positive polynomial which is not SOS, in line with Table 22. But the previous theorem implies that there doesn't exist any "square root" of this polynomial, i.e $f(x, y, z, w) \neq p(x^2, y^2, z^2, w^2)$ for any polynomial p.

Three qutrits. It was conjectured in [RPAR+25] that for local dimensions $d = 3, 4$, there is no PPT entanglement in the class of mixtures of Dicke states for *any* number of systems, analogous to the bipartite case. We will show that this conjecture is false by constructing explicit examples of PPT entangled states in three qutrits. This also implies (Theorem 9.57) that there exist PPT entangled states in all the remaining cases, $d \geq 3$ and $n \geq 3$.

Let us first focus on the construction of witnesses for PPT entanglement, i.e, finding explicit copositive tensors that are not SOS. This is also equivalent to finding homogeneous polynomials p such that $p(x \odot x)$ is globally non-negative but not a sum of squares. Surprisingly, a lot of these examples already exist in the literature. Let us present a few of them.

Motzkin Polynomial [Mot67]

$$p_{\text{mot}}(x, y, z) = x^2y + y^2x + z^3 - 3xyz$$

Robinson Polynomial [Rob73]

$$p_{\text{rob}}(x, y, z) = x^6 + y^6 + z^6 + 3x^2y^2z^2 - \left(x^2y^4 + x^4y^2 + x^2z^4 + x^4z^2 + y^2z^4 + y^4z^2\right)$$

The exact conditions for positivity and sum of squares for symmetric polynomials (symmetric under the exchange of any variables) have been considered in [CLR87], which is a rich source of examples of positive polynomials that are not SOS. The exact conditions for positivity of such polynomials, along with the SOS conditions, are outlined in [CLR87].

Example 9.53 ([CLR87, Theorems 3.7 and 4.25])**.** Consider $M_r = \sum_{i=1}^{d} x_i^r$ and the following polynomial.

$$p_{a,b,c}(x) = aM_3 + bM_1M_2 + cM_1^3.$$

This polynomial is a homogeneous polynomial of degree 3 in d variables. Define the polynomial $p^*_{a,b,c}(t) = a + bt + ct^2$. Then, we have the following equivalences:

- $\forall x \geq 0, \quad p_{a,b,c}(x) \geq 0 \iff \forall k \in [d], \quad p^*_{a,b,c}(k) \geq 0.$
- $p_{a,b,c}(x \odot x) \in \Sigma_d^{(6)} \iff \forall t \in \{1\} \cup [2, d], \quad p^*_{a,b,c}(t) \geq 0.$

In particular, Robinson's polynomial R is given by $a = 3, b = -5/2, c = 1/2$. The corresponding R^* polynomial can be factorized as, $R^*(t) = \frac{1}{2}(6 - 5t + t^2) = \frac{1}{2}(2 - t)(3 - t)$. This implies that:

$$R^*(t) < 0 \iff 2 < t < 3$$

that violates the SOS condition. Surprisingly, in these constructions, the positivity and SOS conditions are independent of the number of variables d. Therefore, for the same parameter values, this provides examples of tensors in $\mathsf{Cop}_d^{(3)}$ that are not in $\mathsf{SOS}_d^{(3)}$ for all d.

Let us discuss the case of Motzkin's polynomial in detail, which, in fact, was the first explicit positive polynomial that was not a sum of squares. Firstly, it is easy to check that this polynomial is positive for all $x \geq 0$ by the AM-GM inequality.

$$p_{\text{mot}}(x, y, z) = x^2y + y^2x + z^3 - 3xyz = 3(\frac{x^2y + y^2x + z^3}{3} - xyz) \geq 0.$$

We now show that the Motzkin polynomial is not SOS. This proof strategy is well-known in the literature.

Theorem 9.54. The Motzkin polynomial "entrywise squared" is not a sum of squares.

$$p_{\text{mot}}(x \odot x) \notin \Sigma_d^{(2n)}.$$

Proof. We recall that the Newton polytope of a general polynomial expanded in the polynomial basis is given by

$$\mathcal{N}(p) = \text{conv}\{\alpha \in \mathbb{N}^d \mid p(x) = \sum_{\alpha \in \mathbb{N}^d} \lambda_\alpha x^\alpha,\ \lambda_\alpha \neq 0\}$$

Then, we have the following property, $\mathcal{N}(pq) = \mathcal{N}(p) + \mathcal{N}(q)$ and hence $\mathcal{N}(p^2) = 2\mathcal{N}(p)$. Moreover, we have $\mathcal{N}(p + q) = \text{conv}\{\mathcal{N}(p) \cup \mathcal{N}(q)\}$. Now, for any polynomial that is a sum of squares, i.e, $p_{\text{mot}}(x \odot x) = \sum_k f_k^2(x)$, we have,

$$\mathcal{N}(p_{\text{mot}}(x \odot x)) = 2\,\text{conv}\{\bigcup_k \mathcal{N}(f_k\}$$

Let us assume to the contrary that the Motzkin polynomial is a sum of squares. The Newton polytope of the Motzkin polynomial is given by

$$\mathcal{N}(p_{\text{mot}}(x \odot x)) = \text{conv}\{(4, 2, 0), (2, 4, 0), (0, 0, 6), (2, 2, 2)\}$$

and thus

$$1/2 \cdot \mathcal{N}(p_{\text{mot}}(x \odot x)) = \text{conv}\{(2,1,0),(1,2,0),(0,0,3),(1,1,1)\}.$$

Note that $\mathcal{N}(f_k) \subseteq 1/2 \cdot \mathcal{N}(p_{\text{mot}}(x \odot x))$. Therefore, we can assume that $f_k = (a_k x_1 x_2^2 + b_k x_1^2 x_2 + c_k x_1 x_2 x_3 + d_k x_3^3)$ and hence the coefficient of $x_1^2 x_2^2 x_3^2$ is $\sum_k c_k^2 \geq 0$, which is a contradiction with the value -3 in $p_{\text{mot}}(x \odot x)$. Therefore, the Motzkin polynomial cannot be a sum of squares. ■

The proof of the previous theorem actually works for all polynomials of the form,

$$p(x_1, x_2, x_3) = x_1^4 x_2^2 + x_2^4 x_1^2 + x_3^6 - \alpha x_1^2 x_2^2 x_3^2$$

which is a positive, not SOS polynomial for $\alpha \in (0, 3]$. For a historical perspective on the problem of positive polynomials and sum of squares, we recommend the book [Pow21, Chapter 2].

Therefore, since we showed that there exist copositive tensors in $\vee^3 \mathbb{R}^3$ that are not SOS tensors, by duality, there are PPT entangled diagonally symmetric states for 3 qutrits. For any polynomial p, we can define the inequality on completely positive tensors by using the tensor-polynomial correspondence. The strategy is as follows: Select a polynomial $f(x)$ such that $\forall x \geq 0, f(x) \geq 0$. Then, we use the correspondence to construct a copositive tensor T such that $p_T = f$. Then, for all $Q \in \mathsf{CP}_d^{(n)}$ we have,

$$\langle Q, T \rangle \geq 0.$$

Moreover, if $f(x \odot x)$ is not a sum of squares, the tensor $T \notin \mathsf{SOS}_d^{(n)}$ acts as an indecomposable witness. Let us now present an explicit example of a PPT entangled state in 3 qutrits.

Example 9.55. Let $Q \in \vee^3 \mathbb{R}^3$ have entries

$$Q_{ijk} = \begin{cases} p, & \text{if } i = j = k, \\ r, & \text{if } i, j, k \text{ are all distinct}, \\ q, & \text{otherwise.} \end{cases}$$

For each i, define the slice matrix $S^{(i)} \in \mathbb{R}^{3 \times 3}$ by

$$S^{(i)}_{jk} := Q_{ijk}.$$

All slices are proportional to

$$S^{(i)} \sim \begin{bmatrix} p & q & q \\ q & q & r \\ q & r & q \end{bmatrix}.$$

The PPT conditions (see Section 9.4.3) imply that for all $i \in \{1,2,3\}$ we must have $S^{(i)} \succeq 0$. This matrix is PSD if and only if

$$p \geq q \geq r \geq 0, \qquad p(q+r) \geq 2q^2.$$

Using Robinson's polynomial defined previously, we obtain the inequality

$$\forall Q \in \mathsf{CP}_d^{(3)} \quad Q_{111}+Q_{222}+Q_{333}+3Q_{123}-Q_{112}-Q_{122}-Q_{113}-Q_{133}-Q_{223}-Q_{233} \geq 0.$$

Under the present parametrization, this becomes

$$3p+3r-6q \;\geq\; 0.$$

Hence, we obtain the optimization problem.

$$\begin{aligned} \eta^\star = \text{minimize} \quad & 3p+3r-6q \\ \text{subject to} \quad & p \geq q \geq r \geq 0, \\ & p(q+r) \geq 2q^2, \\ & 3p+18q+6r = 1. \end{aligned}$$

The last constraint comes from the normalization of the state. A numerical computation yields an optimal value $\eta^\star \approx -0.02 < 0$. In particular, there exists a feasible triple (p,q,r) with $3p+3r-6q<0$, showing that the tensor is not CP even though all slices are PSD. This tensor corresponds to a PPT entangled 3 qutrit mixture of Dicke states.

Remark 9.56. Note that the PPT entangled state that we construct has no bipartite reduction that is entangled. This is because the marginals of diagonally symmetric bosonic states are in the same class (ref. Theorem 9.27), and in $3 \vee 3$ systems, the states in the DS subspace have no PPT entanglement (ref. Theorem 9.51). In terms

of the permutation symmetric mixtures of Dicke states from Section 9.3.1, the tensor Q in the example above corresponds to the matrix

$$3\alpha\rho_{(3,0,\ldots,0)} + 6\beta\rho_{(2,1,0\ldots,0)} + \gamma\rho_{(1,1,1,0\ldots,0)}.$$

The values discussed in the example above allow us to construct a matrix with S_d symmetry which is PPT entangled in the case of 3 qutrits ($n = d = 3$).
This is because the witness we consider based on the Robinson's polynomials is symmetric under variable permutation; such polynomials correspond dually to the sub-family of mixtures of Dicke states that have local basis permutation symmetry (Section 9.3.1).

We conclude the section by showing that such positive non-SOS polynomials can be constructed for all $d > 3$ and $n > 3$. This conclusively settles the question of the existence of PPT entangled states in the diagonally symmetric subspace.

Theorem 9.57 (PPT entanglement in $d \geq 3, n \geq 3$)**.** There exist entangled states that are PPT across all bipartitions for all $d \geq 3, n \geq 3$ in the DS subspace.

Proof. We will exhibit homogeneous polynomials $p \in \mathbb{H}[x]_{d,n}$ in d variables and degree n such that $p(x \odot x) \geq 0$ but $p(x \odot x)$ is not a sum of squares. Note that for $d = 3, n = 3$, the Motzkin/Robinson polynomials are of this type. Moreover, Example 9.53 includes such polynomials for all $d \geq 3, n = 3$. We show that for each d, examples for each n can be obtained by induction.

Let p be a homogeneous polynomial of degree k such that $p(x \odot x)$ is not a sum of squares. Then, $\tilde{p} = x_1 \cdot p$ is a homogeneous polynomial of degree $k + 1$. It is easy to verify that the polynomial $\tilde{p}(x \odot x)$ is positive as $\tilde{p}(x \odot x) = x_1^2 p(x \odot x) \geq 0$. Assume that it has an SOS decomposition.

$$\tilde{p}(x \odot x) = \sum_i h_i^2(x)$$

Moreover, if $x_1 = 0$, it implies that $\tilde{p}(x \odot x) = 0$ and hence $h_i(x) = 0$. This implies that $h_i = x_1 z_i$ for some homogenous polynomials $z_i \in \mathbb{H}[x]_{d,k}$. Therefore, $x_1^2 p(x \odot x) = \tilde{p}(x \odot x) = \sum_i h_i^2(x) = x_1^2 z_i^2$. This implies $p(x \odot x)$ is a sum of squares. Therefore, by contradiction, $\tilde{p}(x \odot x)$ is not a SOS polynomial. By starting this induction from the case $n = 3$, we prove the theorem. ∎

Let us summarise our results in the table 23.

	$n = 2$	$n = 3$	$n \geq 4$
$d = 2$	No	No	No
$d = 3$	No	Yes	Yes
$d = 4$	No	Yes	Yes
$d \geq 5$	Yes	Yes	Yes

[TAQ+18, Yu16]
This article
[RPAR+25, GNP25b]

Table 23: Is there PPT entanglement in mixtures of Dicke states of n parties and local dimension d?

9.4.5 *Marginals of entangled Dicke states are NPT*

In [SN25], it was shown that for any marginal of a pure Dicke state $|D_\alpha\rangle$, such that $\mathrm{supp}(\alpha) > 1$, is NPT (Negative Partial Transpose) across all bipartitions. If $\mathrm{supp}(\alpha) = 1$, then the state $|D_\alpha\rangle$ is separable. We recover the results slightly differently; we show that all the 2-body marginals are entangled as they have negative partial transpose. Our proof is relatively straightforward, thanks to the characterization of marginals of Dicke mixtures from Theorem 9.27.

Proposition 9.58. Consider an entangled Dicke state $|D_\alpha\rangle$ with $\alpha \in \mathbb{N}_d^{(n)}$ such that $\mathrm{supp}(\alpha) > 1$. Then, all the 2-body marginals of $|D_\alpha\rangle$ have negative partial transpose (i.e. they are NPT).

Proof. Consider $l \neq m \in \mathrm{supp}(\alpha)$, and let Q be the Q parametrization of the marginal of the Dicke state corresponding to indices $l, m \in [d]$. By Proposition 9.28 we have

$$Q_{lm} = \frac{\binom{n-2}{\alpha-\gamma(lm)}}{\binom{n}{\alpha}} \mathbb{1}_{\gamma(lm)\leq\alpha},$$

where $\gamma(lm)$ is the vector having 1's in positions l and m and 0's elsewhere. We now claim that $Q_{ll}Q_{mm} < Q_{lm}^2$. To see this, we expand the two expressions:

$$\begin{aligned} Q_{ll}Q_{mm} &= \frac{\binom{n-2}{\alpha-\gamma(ll)}}{\binom{n}{\alpha}} \mathbb{1}_{\{\gamma(ll)\leq\alpha\}} \frac{\binom{n-2}{\alpha-\gamma(mm)}}{\binom{n}{\alpha}} \mathbb{1}_{\{\gamma(mm)\leq\alpha\}} \\ &= \frac{1}{\binom{n}{\alpha}^2} \frac{(n-2)!^2}{\prod\limits_{i\neq l,m} (\alpha_i!)^2 \, (\alpha_l-2)!\,\alpha_l! \, (\alpha_m-2)!\,\alpha_m!} \mathbb{1}_{\{\gamma(ll),\gamma(mm)\leq\alpha\}} \\ &< \frac{1}{\binom{n}{\alpha}^2} \frac{(n-2)!^2}{\prod\limits_{i\neq l,m} (\alpha_i!)^2 \, (\alpha_l-1)!^2 \, (\alpha_m-1)!^2} \mathbb{1}_{\{\gamma(lm)\leq\alpha\}} = Q_{lm}^2. \end{aligned}$$

where the strict inequality follows from noting that $\mathbb{1}_{\{\gamma(lm)\leq\alpha\}} = 1$ and

$$(\alpha_l-2)!\,\alpha_l!\,(\alpha_m-2)!\,\alpha_m! > (\alpha_l-1)!^2(\alpha_m-1)!^2.$$

This shows that the matrix Q is not PSD, and hence the 2-body marginal state X is NPT. ■

Corollary 9.59 ([SN25]). Let $\alpha \in \mathbb{N}_d^{(n)}$ such that $\mathrm{supp}(\alpha) > 1$. Then, all the marginals of the entangled pure Dicke state $|D_\alpha\rangle$ are NPT across all bipartitions.

Proof. Let $X = \mathrm{Tr}_{[r]}(|D_\alpha\rangle\langle D_\alpha|)$ for $1 \leq r < n$. Then, we claim that $X^{\Gamma_{[k]}} \not\geq 0$ for all $1 \leq k < r$. This can be shown by noting that

$$\mathrm{Tr}_{[r]\setminus\{1,k+1\}}(X^{\Gamma_{[k]}}) = \left(\mathrm{Tr}_{[r]\setminus\{1,k+1\}}(X)\right)^\Gamma = \left(\mathrm{Tr}_{[n]\setminus\{1,k+1\}}(|D_\alpha\rangle\langle D_\alpha|)\right)^\Gamma$$

By Proposition 9.58, $\left(\mathrm{Tr}_{[n]\setminus\{1,k+1\}}(|D_\alpha\rangle\langle D_\alpha|)\right)^\Gamma \not\geq 0$ implying $X^{\Gamma_{[k]}} \not\geq 0$. ■

9.5 BOSONIC EXTENDIBILITY

In the final section of this article, we shift our focus to another important entanglement-theoretic property of quantum states known as *extendibility* [DPS04, Ter04, CKMR07]. This property is concerned with the existence of an extension, i.e, a state supported on a larger number of systems, such that some chosen reductions of such a state are equal to the original quantum state. There exist various notions of the extendibility of quantum states, see [DPS04, NOP09, ACG+26, SJZ24, GNP25b]. In this article, we study the one that is well-suited to bosonic states, which we call the *hypergraph extendibility*, generalizing the complete graph extendibility from [ACG+26]. Let us begin by defining this notion.

Definition 9.60. Let $r, n \in \mathbb{N}$ be non-negative integers. A matrix $\tilde{X} \in \mathrm{Herm}[\vee^{n+r}\mathbb{C}^d]$ is called a (n,r)-*hypergraph bosonic extension* of a matrix $X \in \mathrm{Herm}[\vee^{n}\mathbb{C}^d]$ if both of the following conditions hold:

(1) $\tilde{X} \succeq 0$

(2) $\forall\big(A \subseteq [n+r],\, |A| = r\big) \quad \mathrm{Tr}_A(\tilde{X}) = X.$

We call such an extension a (n,r)-*hypergraph PPT bosonic extension* if the extension $\tilde{X}$ is also PPT across all bipartitions. Note that, thanks to the symmetry property, one could have replace the "$\forall$" in the second point above by an "$\exists$".

If X, Y have a (n,r)-hypergraph (PPT) bosonic extension $\tilde{X}, \tilde{Y}$ (resp.), then $\tilde{X}+\tilde{Y}$ is the (n,r)-hypergraph (PPT) bosonic extension of $X+Y$. Similarly, $\tilde{X}$ is a (n,r)-hypergraph (PPT) bosonic extension of X , then, $\lambda\tilde{X}$ is the (n,r)-hypergraph (PPT) bosonic extension of λX. We denote these cones of (n,r)-hypergraph bosonic extendable states as $\mathsf{BExt}_d^{(n,r)}$ and (n,r)-hypergraph PPT bosonic extendable states as $\mathsf{PPTBExt}_d^{(n,r)}$, where $r \geq 0$:

$$\mathsf{BExt}_d^{(n,r)} := \{X \in \mathrm{Herm}[\vee^n\mathbb{C}^d] \mid \exists \tilde{X} \in \mathsf{PSD}_d^{(n+r)} \text{ s.t. } \mathrm{Tr}_{[r]}\,\tilde{X} = X\} \tag{110}$$

$$\mathsf{PPTBExt}_d^{(n,r)} := \{X \in \mathrm{Herm}[\vee^n\mathbb{C}^d] \mid \exists \tilde{X} \in \mathsf{PPT}_d^{(n+r)} \text{ s.t. } \mathrm{Tr}_{[r]}\,\tilde{X} = X\}. \tag{111}$$

Remark 9.61. Note that for $r = 0$, $\mathsf{BExt}_d^{(n,0)}$ reduces to the set of all n-partite bosonic states, while $\mathsf{PPTBExt}_d^{(n,0)}$ reduces to the set of n-partite bosonic states with all bipartitions PPT:

$$\mathsf{BExt}_d^{(n,0)} = \mathsf{PSD}_d^{(n)}$$
$$\mathsf{PPTBExt}_d^{(n,0)} = \mathsf{PPT}_d^{(n)}.$$

Recall that any separable state in the bosonic subspace, $X \in \mathrm{Herm}[\vee^n\mathbb{C}^d]$ is of the form

$$X = \sum_{k=1}^{K} |v_k\rangle\langle v_k|^{\otimes n} \text{ for } |v_k\rangle \in \mathbb{C}^d.$$

Consider, for any $r \geq 0$, the following operator $\tilde{X} \in \mathrm{Herm}[\mathcal{M}_d^{\otimes(n+r)}]$:

$$\tilde{X} := \sum_{k=1}^{K} \frac{1}{||v_k||^{2r}} |v_k\rangle\langle v_k|^{\otimes(n+r)}.$$

It is easy to verify that $\tilde{X}$ is an (n,r)-hypergraph bosonic extension of X. Moreover, this extension is also PPT across all bipartitions. Hence, we have the following inclusions, showing that the newly introduced sets form a decreasing hierarchy of outer approximations of the separable set:

$$\begin{array}{ccccccccccc}
\mathsf{Sep}_d^{(n)} & \subseteq \cdots \subseteq & \mathsf{BExt}_d^{(n,r)} & \subseteq \cdots \subseteq & \mathsf{BExt}_d^{(n,1)} & \subseteq & \mathsf{BExt}_d^{(n,0)} & = & \mathsf{PSD}_d^{(n)} \\
\| & \cdots & \cup\mid & \cdots & \cup\mid & & \cup\mid & & \cup\mid \\
\mathsf{Sep}_d^{(n)} & \subseteq \cdots \subseteq & \mathsf{PPTBExt}_d^{(n,r)} & \subseteq \cdots \subseteq & \mathsf{PPTBExt}_d^{(n,1)} & \subseteq & \mathsf{PPTBExt}_d^{(n,0)} & = & \mathsf{PPT}_d^{(n)}
\end{array}$$

We now provide a formal characterization of the dual sets, i.e, the set of *extendibility witnesses*. Such a characterization has already been obtained in [GNP25b, Theorem 8.9] and [BL25, Theorem 4.1] for the bipartite case $n = 2$. The essential argument can be easily extended to the case of $n > 2$; we provide the proof for the sake of completeness.

Theorem 9.62 (PPT Extendibility Witness)**.** The following statements are equivalent,

(1) $X \in (\mathsf{PPTBExt}_d^{(n,r)})^\circ := (\mathsf{DecExtW}_d^{(n,r)})$

(2) $\Pi_d^{(n+r)}(X \otimes I_d^{\otimes r})\Pi_d^{(n+r)} \in \sum_{k=0}^{\lfloor (n+r)/2 \rfloor} \mathsf{Dec}_d^{(n+r,k)}$, i.e. there exist PSD matrices $W_k \in \mathrm{Herm}[\mathcal{M}_d^{\otimes(n+r)}]$ for $k = 0, \ldots, \lfloor (n+r)/2 \rfloor$ such that

$$\Pi_d^{(n+r)}\big(X \otimes I_d^{\otimes r}\big)\Pi_d^{(n+r)} = \Pi_d^{(n+r)}\left(W_0 + \sum_{k=1}^{\lfloor (n+r)/2 \rfloor} W_k^{\Gamma_{[k]}}\right)\Pi_d^{(n+r)}$$

Proof. For the implication $(1) \implies (2)$, consider an arbitrary $X \in (\mathsf{PPTBExt}_d^{(n,r)})^\circ$. By definition, we have $\mathrm{Tr}(XW) \geq 0$ for all $W \in \mathsf{PPTBExt}_d^{(n,r)}$. This also implies that for all $\tilde{W} \in \bigcap_{k=0}^{\lfloor (n+r)/2 \rfloor} \mathsf{PPT}_d^{(n+r,k)}$, we have

$$\mathrm{Tr}((X \otimes I_d^{\otimes r})\tilde{W}) = \mathrm{Tr}(X \,\mathrm{Tr}_{[r]}(\tilde{W})) \geq 0.$$

Therefore, $\Pi_d^{(n+r)}(X \otimes I_d^{\otimes r})\Pi_d^{(n+r)} \in \sum_{k=0}^{\lfloor (n+r)/2 \rfloor} \mathsf{Dec}_d^{(n+r,k)} = \mathsf{Dec}_d^{(n+r)}$, see Corollary 9.37. This shows the first claim.

For the reverse direction, we will show that $\mathrm{Tr}(XW) \geq 0$ for all $W \in \mathsf{PPTBExt}_d^{(n,r)}$. If $W \in \mathsf{PPTBExt}_d^{(n,r)}$, then there exists a $\tilde{W} \in \bigcap_{k=0}^{\lfloor (n+r)/2 \rfloor} \mathsf{PPT}_d^{(n+r,k)}$ such that $\mathrm{Tr}_{[r]}(\tilde{W}) = W$. Then, we can show that

$$\mathrm{Tr}(XW) = \mathrm{Tr}((X \otimes I_d^{\otimes r})\tilde{W}) \geq 0.$$

■

If we restrict to $k = 0$ in the theorem above, we eliminate the non-trivial PPT conditions to obtain the following result.

Corollary 9.63. Let $X \in \mathrm{Herm}[\mathcal{M}_d^{\otimes n}]$ be a self-adjoint matrix such that

$$\Pi_d^{(n)} X \Pi_d^{(n)} = X.$$

Then, $X \in \left(\mathsf{BExt}_d^{(n,r)}\right)^\circ := (\mathsf{ExtW}_d^{(n,r)})$ if and only if

$$\Pi_d^{(n+r)} \left(X \otimes I_d^{\otimes r}\right) \Pi_d^{(n+r)} \succeq 0.$$

9.5.1 *Moment hierarchy for CP Tensors*

In general, checking for the copositivity of a matrix is computationally co-NP-complete, while on the dual side, checking for complete positivity of a matrix is NP-hard. Despite this, there is a systematic way to approximate these sets through inner and outer approximations. We will briefly review the two widely used inner approximations for the set of copositive matrices: the SOS hierarchy and the non-negative hierarchy. The membership at any level of the hierarchy can be decided using a semi-definite/linear program. On the dual side, the duals of these hierarchies outer approximate the completely positive matrices. We also discuss the natural extension of these hierarchies to tensors, and in the next section, provide a surprising connection to the extendibility properties in the diagonally symmetric (DS) subspace. Recall the following tensor duality from Theorem 9.46,

$$(\mathsf{Mom}_d^{(n)})^\circ = \mathsf{SOS}_d^{(n)}.$$

Then, we define the following convex cones:

$$\mathsf{MomExt}_d^{(n,r)} := \{\mathrm{tr}_{[r]}(X) \mid X \in \mathsf{Mom}_d^{(n+r)}\}. \tag{112}$$

For a particular $r \geq 0$, this is the convex cone of tensors in $\vee^n \mathbb{R}^d$ that have a moment tensor extension in the larger space $\vee^{(n+r)} \mathbb{R}^d$. Note that any completely positive tensor $Q = \sum_k v_k^{\otimes n}$ with $v_k \in \mathbb{R}_+^d$ has a moment tensor extension for all r, given by

$$\tilde{Q} = \sum_k \frac{1}{|v_k|^r} v_k^{\otimes (n+r)}.$$

Therefore, we have the following infinite hierarchy of sets that approximate completely positive matrices from the outside:

$$\mathsf{CP}_d^{(n)} \subseteq \cdots \subseteq \mathsf{MomExt}_d^{(n,r)} \subseteq \cdots \subseteq \mathsf{MomExt}_d^{(n,1)} \subseteq \mathsf{MomExt}_d^{(n,0)} = \mathsf{Mom}_d^{(n)}.$$

Unsurprisingly, this is dual to the sum of squares hierarchy, which approximates copositive matrices from the inside. This is the content of our next theorem.

Theorem 9.64 (Dual of SOS hierarchy)**.** We have the following conic duality:

$$\forall n, r, d \in \mathbb{N}, \quad \left(\mathsf{MomExt}_d^{(n,r)}\right)^\circ = \mathsf{RSOS}_d^{(n,r)}.$$

Proof. Let us first note that $\mathsf{RSOS}_d^{(n,r)} = \{Q \in \vee^n \mathbb{R}^d \mid \Pi_d^{(n+r,\mathbb{R})}[Q \otimes |e\rangle^{\otimes n}] \in \mathsf{SOS}_d^{(n+r)}\}$. Note also that the trace operation is dual to the tensoring operation with the normalized all-ones tensor:

$$\langle \mathrm{tr}_{[r]}(T), Q\rangle = \langle T, Q \otimes |e\rangle^{\otimes r}\rangle\,.$$

Also if the tensor T is symmetric, we have

$$\langle T, Q \otimes |e\rangle^{\otimes r}\rangle = \langle \Pi_d^{n+r,\mathbb{R}}[T], Q \otimes |e\rangle^{\otimes r}\rangle = \langle T, \Pi_d^{n+r,\mathbb{R}}[Q \otimes |e\rangle^{\otimes r}]\rangle\,.$$

Finally, we have the following equivalences:

$$\begin{aligned}
X \in \left(\mathsf{MomExt}_d^{(n,r)}\right)^\circ &\iff \forall\, Y \in \mathsf{MomExt}_d^{(n,r)}, \quad \langle X, Y\rangle \geq 0 \\
&\iff \forall\, \tilde{Y} \in \mathsf{Mom}_d^{(n+r)}, \quad \left\langle \mathrm{tr}_{[r]}(\tilde{Y}), X\right\rangle \geq 0 \\
&\iff \forall\, \tilde{Y} \in \mathsf{Mom}_d^{(n+r)}, \quad \left\langle \tilde{Y}, \Pi_d^{n+r,\mathbb{R}}\left[X \otimes |e\rangle^{\otimes r}\right]\right\rangle \geq 0. \\
&\iff \Pi_d^{n+r,\mathbb{R}}\left[X \otimes |e\rangle^{\otimes r}\right] \in (\mathsf{Mom}_d^{(n+r)})^\circ = \mathsf{SOS}_d^{(n+r)}.
\end{aligned}$$

This completes the proof. ∎

Analogous to the case of the sum of squares hierarchy, we will characterize the dual of Polya's non-negative hierarchy. To this end, we define the following convex cones of tensors:

$$\mathsf{NNExt}_d^{(n,r)} := \{\mathrm{tr}_{[r]}(X) \mid X \in \mathsf{NN}_d^{(n+r)}\}. \tag{113}$$

These are exactly the convex cones of tensors that have an entrywise positive extension of order $n + r$. Therefore, we have the following new infinite hierarchy of sets that approximate completely positive tensors from the outside:

$$\mathsf{CP}_d^{(n)} \subseteq \cdots \subseteq \mathsf{NNExt}_d^{(n,r)} \subseteq \cdots \subseteq \mathsf{NNExt}_d^{(n,1)} \subseteq \mathsf{NNExt}_d^{(n,0)} = \mathsf{NN}_d^{(n)}.$$

In the next theorem, we present the conic-duality of the non-negative hierarchy. We skip the proof, as it is essentially the same argument as in Theorem 9.64, by replacing "Mom" with "NN".

Theorem 9.65 (Dual of NN hierarchy)**.** We have the following duality:

$$\forall n, r, d \in \mathbb{N}, \quad \left(\mathsf{NNExt}_d^{(n,r)}\right)^\circ = \mathsf{PNN}_d^{(n,r)}.$$

Remark 9.66. The entrywise positive hierarchy that we discuss here has been abstractly studied in the probability literature as "finitely extendable and exchangeable probability measures". We refer to the recent article [KY19], and all references therein, for the finite-dimensional case of this problem.

9.5.2 *Bosonic extendibility: extending the dictionary*

In the previous section, we discussed two important hierarchies (and their duals) that approximate the set of copositive tensors (and completely positive tensors). In this section, we connect these hierarchies to the bosonic extendibility problem in the diagonally symmetric subspace. To this end, we have the following lemma, which states that a diagonally symmetric matrix has an (n, r)-hypergraph extension if and only if there is an extension in the DS subspace. This result follows from the local symmetry properties of the DS subspace, and has already been noted in [GNP25b, BL25]. We provide the proof for completeness.

Lemma 9.67. Let $X \in \mathsf{DS}_d^{(n)}$. Then, the following statements are equivalent:

(1) X has a (PPT) r-bosonic extension.

(2) X has a (PPT) r-bosonic extension that is in $\mathsf{DS}_d^{(n+r)}$.

Proof. We only do the case without the PPT property, as the PPT case is analogous. The reverse implication is trivial. For the forward implication, let $X \in \mathsf{BExt}_d^{(n,r)}$, i.e there exists an extension $\tilde{X} \in \mathcal{M}_d^{\otimes(n+r)}$ with $\Pi_d^{(n+r)} \tilde{X} \Pi_d^{(n+r)} = \tilde{X}$. We claim that the twirl with respect to the diagonal unitary group $\mathcal{DU}_d$

$$\mathcal{T}_{\mathcal{DU}}(\tilde{X}) := \int_{\mathcal{DU}_d} U^{\otimes(n+r)} \tilde{X} \overline{U}^{\otimes(n+r)} \, \mathrm{d}U$$

is also an bosonic extension of X. Indeed, use $[\Pi_d^{(n+r)}, U^{\otimes(n+r)}] = 0$ and compute

$$\begin{aligned}\mathrm{Tr}_{[r]}\left(\mathcal{T}_{\mathcal{DU}}(\tilde{X})\right) &= \int \mathrm{Tr}_{[r]}\left(U^{\otimes(n+r)}\,\tilde{X}\,\overline{U}^{\otimes(n+r)}\right)\mathrm{d}U \\ &= \int U^{\otimes n}\,\mathrm{Tr}_{[r]}(\tilde{X})\,\overline{U}^{\otimes n}\,\mathrm{d}U \\ &= \int U^{\otimes n} X \overline{U}^{\otimes n}\,\mathrm{d}U \\ &= X,\end{aligned}$$

where the last equality follows from the fact that $X \in \mathsf{DS}_d^{(n)}$. ■

Now, we use the previous lemma to establish the main result of this section, the connection between the bosonic-extendibility of mixtures of Dicke states and hierarchies for completely positive tensors. This has already been proven in the recent papers [GNP25b, BL25] for the bipartite case $n = 2$.

Theorem 9.68. Let $X \in \mathsf{DS}_d^{(n)}$. Then, for all level of the hierarchies $r \geq 0$:

(1) $X \in \mathsf{BExt}_d^{(n,r)} \iff Q[X] \in \mathsf{NNExt}_d^{(n,r)}$

(2) $X \in \mathsf{PPTBExt}_d^{(n,r)} \iff Q[X] \in \mathsf{MomExt}_d^{(n,r)}$.

Proof. For the forward implication of item (1), assume that $X \in \mathsf{BExt}_d^{(n,r)}$, Then, by Lemma 9.67, there exists $\tilde{X} \in \mathsf{DS}_d^{(n,r)}$ which is PSD, and thus $Q[\tilde{X}] \in \mathsf{NN}_d^{(m+r)}$. We also have $Q[X] = Q[\mathrm{Tr}_{[r]}(\tilde{X})] = \mathrm{tr}_{[r]}(Q[\tilde{X}])$ where $Q[\tilde{X}] \in \mathsf{NN}_d^{(n+r)}$. This implies that $Q[X] \in \mathsf{NNExt}_d^{(n,r)}$. For the reverse implication, let $Q[X] \in \mathsf{NNExt}_d^{(n,r)}$. There exists $\tilde{Q} \in \mathsf{NN}_d^{(n+r)}$ such that $\mathrm{tr}_{[r]}(\tilde{Q}) = Q$. Then, the state $\tilde{X} \in \mathsf{DS}_d^{(n+r)}$ such that $Q[\tilde{X}] = \tilde{Q}$ is the bosonic extension of X.

The proof of the second item follows from replacing NN by Mom, PSD by PPT, and bosonic extension by PPT bosonic extension in part (1). ■

Remark 9.69. Our proof of the previous theorem is considerably shorter than the proofs in [GNP25b, BL25], as the hard part of the proof was relegated to establishing a more general dictionary in the previous sections of this work.

Finally, we can also establish the dual result for the extendibility witnesses.

Corollary 9.70. The following hold for operators $O \in \mathsf{DS}_d^{(n)}$:

(1) $O \in \mathsf{ExtW}_d^{(n,r)} \iff W[O] \in \mathsf{PNN}_d^{(n,r)}$

(2) $O \in \mathsf{DecExtW}^{(n,r)} \iff W[O] \in \mathsf{RSOS}_d^{(n,r)}$

Remark 9.71. Note that the theorem provides a much more powerful SDP hierarchy to check separability in diagonally symmetric states. The largest slice flattening of a symmetric tensor of $2n$ legs is of size $\binom{n+d-1}{d-1}$. Therefore, to check $Q[X] \in \mathsf{MomExt}_d^{(n,r)}$, we need to check the PSD of the largest matrix of size $\binom{\lfloor \frac{n+r}{2} \rfloor + d-1}{d-1}$.

This result completes the picture of all the hierarchies for bosonic extendibility and their duals, see Fig. 37 for the full picture of correspondences, inclusions, and dualities.

9.6 CONCLUSION

In this article, we present a detailed study of multipartite entanglement in the diagonally symmetric subspace, with a particular focus on PPT entanglement. This forms a crucial subclass of matrices with bosonic symmetry. By defining a tensor-based parametrisation of these states, we translate the entanglement properties of these states as convex cones of symmetric tensors. In particular, the important entanglement-theoretic cones of separable and PPT states can be described equivalently in terms of the complete positivity and moment positivity of the parametrizing tensor. This extends the results in [TAQ+18, Yu16, RPAR+25] to provide a comprehensive theory for this class of states. Our results provide a bridge between the study of multipartite entanglement, semi-algebraic geometry, and optimization theory.

Our results also lead to several interesting corollaries in the DS subspace. Firstly, we show the existence of PPT entangled states in 3 or more qutrits and ququarts, disproving the recent conjecture from [RPAR+25]. Quite surprisingly, the existence of entanglement witnesses turns out to be closely related to the theory of positive polynomials that are not sums of squares. Using this perspective, we develop a dictionary that links extendibility witnesses on the diagonally symmetric subspace with the sum-of-squares (SOS) hierarchy for copositive tensors. This viewpoint not only clarifies the underlying structure of these witnesses, but also extends earlier extendibility results known in the bipartite setting [GNP25b, BL25] to a broader symmetric framework.

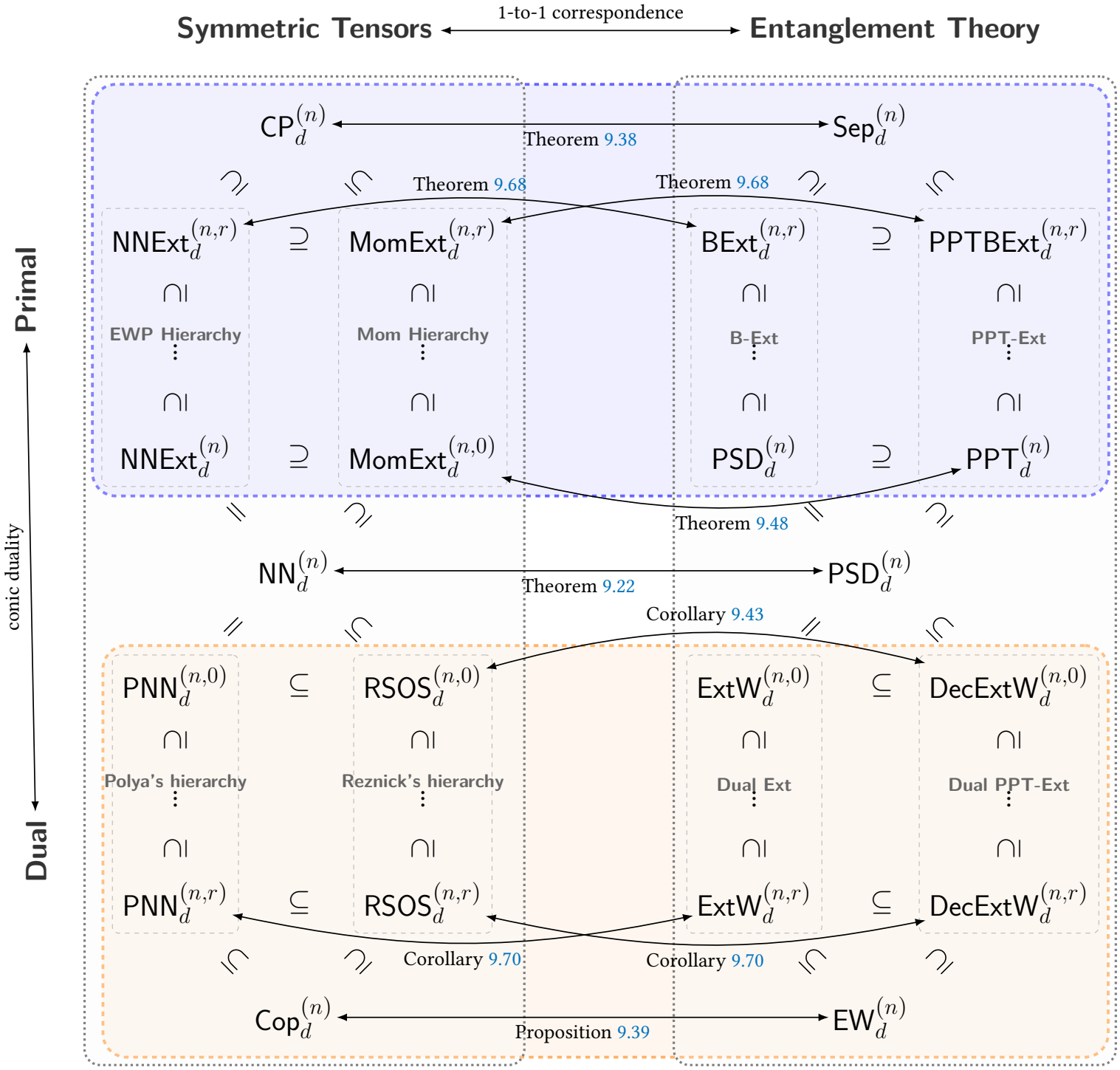


Figure 37: The different sets explored in this work, with their inclusion and duality structures. On the left-hand side, we have sets of symmetric tensors from $\vee^n \mathbb{R}^d$, and on the right-hand side, entanglement properties of the mixtures of Dicke states $\mathrm{DS}_d^{(n)}$. Every set in the diagram is in convex duality with the set that is symmetric with respect to the middle horizontal line.

As a further application, we show that the two-body marginals of pure Dicke states are NPT and therefore necessarily entangled. Our approach yields a shorter and more transparent proof of the corresponding results in [SN25]. More broadly, we expect that the connections developed here between entanglement theory, polynomial positivity, and SOS methods will open several new research directions. We conclude by outlining two concrete avenues for future work.

Firstly, it will be interesting to understand the multipartite states that are invariant under the diagonal unitary group, generalizing the LDUI states from [SN21, JM19]. These bipartite versions of LDUI states can be parameterized using matrix pairs, and entanglement-theoretic properties can be understood as convex cones of matrix pairs. The bipartite mixtures of Dicke states are exactly the LDUI states where these matrices are equal. Therefore, it seems possible that multipartite LDUI states allow a similar description, replacing matrices with *tensors*.

The second question centers on extendibility hierarchies. In this paper, we consider a hierarchy that was well-suited for bosonic states, which we call the (n, r)-hypergraph extendibility. There are other extendibility hierarchies introduced for quantum states in the literature. Since bosonic states are permutation symmetric (i.e. they satisfy $P_\pi \rho = \rho P_\pi$ for all $\pi \in S_n$), can one imagine another extendibility hierarchy in which the extensions are required to be permutation symmetric instead of bosonic? Is there a gap between this hierarchy and the one we consider for bosonic states?

9.7 ACKNOWLEDGMENTS

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9.8 PROOF OF THE DECOMPOSABILITY RESULT

Proof of Theorem 9.42. We shall prove separately the two items in the statement.

Proof of the Item 1.

Consider $O \in \mathsf{Dec}_d^{(n,k)}$ for some integer $k \leq n/2$, and let $p := p_{W[O]}$ the associated polynomial. Our goal is to show that the polynomial p belongs to the cone

$$\mathrm{cone}\{x^\alpha q \mid |\alpha| \in \{n, n-2, n-4 \ldots n-2k\}, q \in \Sigma_d^{(n-|\alpha|)}\}.$$

From $O \in \mathsf{Dec}_d^{n,k}$, we have

$$p(|z|^2) = \langle z^{\otimes n} | P^{\Gamma_{[k]}} | z^{\otimes n} \rangle$$

for some positive senmidefinite matrix P. Using the spectral decomposition of P, we can write

$$p(|z|^2) = \sum_{i=1}^{r} \langle z^{\otimes n}| \, |t_i\rangle\langle t_i|^{\Gamma_{[k]}} \, |z^{\otimes n}\rangle$$

for tensors $t_i \in (\mathbb{R}^d)^{\otimes n}$. By linearity, it is enough to prove the claim for the polynomial corresponding to the general term above, so, without loss of generality, we can assume that $O = |t\rangle\langle t|^{\Gamma[k]}$ for some real tensor t. On the one hand, we have

$$\begin{aligned} p(|z|^2) &= \langle W[O], (|z|^2)^{\otimes n} \rangle \\ &= \sum_{i \in [d]^n} W[O]_i |z_{i_1}|^2 \cdots |z_{i_n}|^2 \\ &= \sum_{\alpha \in \mathbb{N}_d^{(n)}} \binom{n}{\alpha} W[O]_{(\alpha)} \bar{z}^\alpha z^\alpha, \end{aligned} \tag{114}$$

where

$$\mathbb{N}_d^{(n)} := \{\alpha \in \mathbb{Z}^d \mid \alpha_i \geq 0 \, \forall i \in [d] \text{ and } \sum_i \alpha_i = n\}$$

is the set of d-tuples of non-negative integers that sum up to n and corresponds to the types of multi-indices $i \in [d]^n$.

On the other hand, using the form of O and moving the partial transposition on the "z" factors, we also have:

$$p(|z|^2) = \langle z^{\otimes n}| \, |t\rangle\langle t|^{\Gamma_{[k]}} \, |z^{\otimes n}\rangle = \langle \bar{z}^{\otimes k} \otimes z^{\otimes (n-k)}| \, |t\rangle\langle t| \, |\bar{z}^{\otimes k} \otimes z^{\otimes (n-k)}\rangle = |\langle \bar{z}^{\otimes k} \otimes z^{\otimes (n-k)} | t \rangle|^2.$$

In the last scalar product above, we have

$$\bar{z}^{\otimes k} \otimes z^{\otimes (n-k)} \in \vee^k \mathbb{C}^d \otimes \vee^{n-k} \mathbb{C}^d,$$

hence we can assume, without loss of generality, $t \in \vee^k \mathbb{R}^d \otimes \vee^{n-k} \mathbb{R}^d$, by projecting it on the corresponding tensor product of symmetric subspaces of $\mathbb{R}^d$. We can now write

$$
\begin{aligned}
p(|z|^2) &= \sum_{i,j\in[d]^n} \bar{z}_{i_1}\cdots\bar{z}_{i_k} z_{i_{k+1}}\cdots z_{i_n} t_{i_1\cdots i_n} z_{j_1}\cdots z_{j_k}\bar{z}_{j_{k+1}}\cdots\bar{z}_{j_n} t_{j_1\cdots j_n} \\
&= \sum_{\substack{\alpha',\beta'\in\mathbb{N}_d^{(k)} \\ \alpha'',\beta''\in\mathbb{N}_d^{(n-k)}}} \binom{k}{\alpha'}\binom{n-k}{\alpha''}\binom{k}{\beta'}\binom{n-k}{\beta''} \bar{z}^{\alpha'+\beta''} z^{\beta'+\alpha''} t_{(\alpha'),(\alpha'')} t_{(\beta'),(\beta'')} \\
&= \sum_{\substack{\alpha',\beta'\in\mathbb{N}_d^{(k)} \\ \alpha'',\beta''\in\mathbb{N}_d^{(n-k)} \\ \alpha'+\beta''=\beta'+\alpha''}} \binom{k}{\alpha'}\binom{n-k}{\alpha''}\binom{k}{\beta'}\binom{n-k}{\beta''} \bar{z}^{\alpha'+\beta''} z^{\beta'+\alpha''} t_{(\alpha'),(\alpha'')} t_{(\beta'),(\beta'')}
\end{aligned}
$$

where the last equality follows from Eq. (114) which allows us to discard terms with $\alpha' + \beta'' \neq \beta' + \alpha''$.

From the last formula for $p(|z|^2)$ we would like to extract a decomposition as in the statement, as a product of a monomial in $|z|^2$ and a sum-of-squares polynomial q evaluated at $|z|^2$. To this end, define the following d-tuples of non-negative integers:

$$
\begin{aligned}
\mu' &:= \min(\alpha', \beta') \qquad (115)\\
\mu'' &:= \min(\alpha'', \beta'') \\
\mu &:= \min(\alpha', \beta', \alpha'', \beta'') = \min(\mu', \mu'') \\
\delta' &:= \mu' - \mu \\
\delta'' &:= \mu'' - \mu \\
\hat{\alpha}' &:= \alpha' - \delta' \\
\hat{\alpha}'' &:= \alpha'' - \delta'' \\
\hat{\beta}' &:= \beta' - \delta' \\
\hat{\beta}'' &:= \beta'' - \delta'', \qquad (116)
\end{aligned}
$$

where the $\min$ operation is taken entry-wise. We have, for example,

$$
\hat{\alpha}'_i = \alpha'_i - (\min(\alpha'_i, \beta'_i) - \min(\alpha'_i, \beta'_i, \alpha''_i, \beta''_i)) \geq \alpha'_i - \min(\alpha'_i, \beta'_i) \geq 0.
$$

Importantly, note that for every $i \in [d]$, we either have $\mu'_i = \mu_i$ or $\mu''_i = \mu_i$; in other words, the supports of the vectors δ' and δ'' are disjoint. We shall write this as $\delta'\delta'' = 0$ using the entry-wise product of vectors.

We shall now prove the following very important fact:

$$
\hat{\alpha}' = \hat{\alpha}'' \quad \text{and} \quad \hat{\beta}' = \hat{\beta}''. \qquad (117)
$$

For the α's, fix some coordinate $i \in [d]$ and denote by the Latin letter the i-th coordinate of the respective Greek letter (e.g. $\hat{b}'' = \hat{\beta}''_i$). From the constraint $\alpha' + \beta'' = \beta' + \alpha''$, we obtain $a' + b'' = b' + a''$. This means that there exist rational numbers c, x, y such that

$$a' = c + x \quad b'' = c - x \quad b' = c + y \quad a'' = c - y.$$

We have then $m' = c + \min(x, y)$ and $m'' = c - \max(x, y)$; recall that $m = \min(m', m'')$. We now have

$$\hat{a}' = c + x - (c + \min(x, y)) + m \quad \text{and} \quad \hat{a}'' = c - y - (c - \max(x, y)) + m$$

and thus

$$\hat{a}' - \hat{a}'' = x + y - \min(x, y) - \max(x, y) = 0.$$

A similar argument shows $\hat{b}' = \hat{b}''$, proving the claim. From now on, we shall write

$$\hat{\alpha} := \hat{\alpha}' = \hat{\alpha}''$$
$$\hat{\beta} := \hat{\beta}' = \hat{\beta}''.$$

From the claim in Eq. (117), we obtain the following constraints on the non-negative vectors δ', δ'':

$$|\delta'| \leq k$$
$$|\delta''| \leq n - k$$
$$|\delta''| - |\delta'| = n - 2k.$$

Going back to the formula for $p(|z|^2)$, we can now write

$$p(|z|^2) = \sum_{\substack{\alpha', \beta' \in \mathbb{N}_d^{(k)} \\ \alpha'', \beta'' \in \mathbb{N}_d^{(n-k)} \\ \alpha' + \beta'' = \beta' + \alpha''}} \binom{k}{\hat{\alpha} + \delta'} \binom{n-k}{\hat{\alpha} + \delta''} \binom{k}{\hat{\beta} + \delta'} \binom{n-k}{\hat{\beta} + \delta''} (|z|^2)^{\hat{\alpha} + \hat{\beta} + \delta' + \delta''} t_{(\hat{\alpha}+\delta'),(\hat{\alpha}+\delta'')} t_{(\hat{\beta}+\delta'),(\hat{\beta}+}$$

where the 4-tuple $(\delta', \delta'', \hat{\alpha}, \hat{\beta})$ is a function of the 4-tuple $(\alpha', \beta', \alpha'', \beta'')$.

We prove now a second crucial fact: the following two sets S and T are in bijection:

$$S := \{(\alpha', \beta', \alpha'', \beta'') \in \mathbb{N}^d \mid |\alpha'| = |\beta'| = k,\ |\alpha''| = |\beta''| = n - k,\ \alpha' + \beta'' = \beta' + \alpha''\}$$

$$T := \{(\delta', \delta'', \hat{\alpha}, \hat{\beta}) \in \mathbb{N}^d \mid |\delta'| \leq k,\ |\delta''| \leq n - k,\ |\delta''| - |\delta'| = n - 2k,\ \delta' \delta'' = 0,$$
$$|\hat{\alpha}| = |\hat{\beta}| = k - |\delta'| = n - k - |\delta''|\}.$$

Note that some conditions in the definition of T are superfluous, but we prefer to write them for clarity. To prove the claim, we shall construct two maps $\varphi : T \to S$, $\psi : S \to T$ and prove that $\psi \circ \varphi = \mathrm{id}_T$ and $\varphi \circ \psi = \mathrm{id}_S$. We introduce

$$\begin{aligned} \varphi : T &\to S \\ (\delta', \delta'', \hat{\alpha}, \hat{\beta}) &\mapsto (\underbrace{\hat{\alpha} + \delta'}_{\alpha'}, \underbrace{\hat{\beta} + \delta'}_{\beta'}, \underbrace{\hat{\alpha} + \delta''}_{\alpha''}, \underbrace{\hat{\beta} + \delta''}_{\beta''}) \end{aligned}$$

and $\psi : S \to T$ which defines $(\delta', \delta'', \hat{\alpha}, \hat{\beta})$ as functions of $(\alpha', \beta', \alpha'', \beta'')$ following Eqs. (115)–(116) and Eq. (117).

First, we need to show that the maps φ, ψ are well-defined. In the case of φ, the only non-trivial property that one needs to check is

$$\alpha' + \beta'' = \hat{\alpha} + \hat{\beta} + \delta' + \delta'' = \beta' + \alpha''.$$

In the case of ψ, all the properties (including $\delta'\delta'' = 0$) have been checked previously, in the main proof.

We now show $\psi \circ \varphi = \mathrm{id}_T$. Let $(\delta', \delta'', \hat{\alpha}, \hat{\beta}) \in T$ and denote $(\alpha', \beta', \alpha'', \beta'') := \varphi(\delta', \delta'', \hat{\alpha}, \hat{\beta})$, $(\tilde{\delta}', \tilde{\delta}'', \hat{\tilde{\alpha}}, \hat{\tilde{\beta}}) := \psi(\alpha', \beta', \alpha'', \beta'')$. We use Eqs. (115)–(116) to compute

$$\mu' := \min(\alpha', \beta') = \min(\hat{\alpha} + \delta', \hat{\beta} + \delta') = \min(\hat{\alpha}, \hat{\beta}) + \delta'.$$

Similarly, $\mu'' = \min(\hat{\alpha}, \hat{\beta}) + \delta''$ and thus, using now $\delta'\delta'' = 0$, $\mu = \min(\hat{\alpha}, \hat{\beta})$. We conclude that

$$\tilde{\delta}' := \mu' - \mu = \delta' \quad \text{and} \quad \tilde{\delta}'' := \mu'' - \mu = \delta''.$$

Similarly,

$$\hat{\tilde{\alpha}} = \alpha' - \tilde{\delta}' = \hat{\alpha} \quad \text{and} \quad \hat{\tilde{\beta}} = \beta' - \tilde{\delta}' = \hat{\beta},$$

proving $\psi \circ \varphi = \mathrm{id}_T$.

Let us now show $\varphi \circ \psi = \mathrm{id}_S$. Consider $(\alpha', \beta', \alpha'', \beta'') \in S$ and set $(\delta', \delta'', \hat{\alpha}, \hat{\beta}) := \psi(\alpha', \beta', \alpha'', \beta'')$ and then $(\tilde{\alpha}', \tilde{\beta}', \tilde{\alpha}'', \tilde{\beta}'') := \varphi(\delta', \delta'', \hat{\alpha}, \hat{\beta})$. We have

$$\tilde{\alpha}' = \hat{\alpha} + \delta' = \alpha'$$

and similarly for the other 3 elements; here, we implicitly use the result in Eq. (117). This proves the claim that the sets S and T are in bijection.

Having proved the second claim, we can now index the sum formula for $p(|z|^2)$ by the 4-tuple $(\delta', \delta'', \hat{\alpha}, \hat{\beta})$:

$$\begin{aligned}
p(|z|^2) = & \sum_{(\delta',\delta'',\hat{\alpha},\hat{\beta})\in T} \binom{k}{\hat{\alpha}+\delta'}\binom{n-k}{\hat{\alpha}+\delta''}\binom{k}{\hat{\beta}+\delta'}\binom{n-k}{\hat{\beta}+\delta''} \\
& \quad \times (|z|^2)^{\hat{\alpha}+\hat{\beta}+\delta'+\delta''} \, t_{(\hat{\alpha}+\delta'),\,(\hat{\alpha}+\delta'')} \, t_{(\hat{\beta}+\delta'),\,(\hat{\beta}+\delta'')} \\
= & \sum_{\substack{\delta',\delta''\in\mathbb{N}^d \\ |\delta'|\le k,\,|\delta''|\le n-k \\ |\delta''|-|\delta'|=n-2k \\ \delta'\delta''=0}} (|z|^2)^{\delta'+\delta''} \sum_{\substack{\hat{\alpha},\hat{\beta}\in\mathbb{N}^d \\ |\hat{\alpha}|=|\hat{\beta}|=k-|\delta'|}} \binom{k}{\hat{\alpha}+\delta'}\binom{n-k}{\hat{\alpha}+\delta''} \\
& \quad \times \binom{k}{\hat{\beta}+\delta'}\binom{n-k}{\hat{\beta}+\delta''} (|z|^2)^{\hat{\alpha}+\hat{\beta}} \, t_{(\hat{\alpha}+\delta'),\,(\hat{\alpha}+\delta'')} \, t_{(\hat{\beta}+\delta'),\,(\hat{\beta}+\delta'')} \\
= & \sum_{\substack{\delta',\delta''\in\mathbb{N}^d \\ |\delta'|\le k,\,|\delta''|\le n-k \\ |\delta''|-|\delta'|=n-2k \\ \delta'\delta''=0}} (|z|^2)^{\delta'+\delta''} \Bigg[\sum_{\substack{\hat{\alpha}\in\mathbb{N}^d \\ |\hat{\alpha}|=k-|\delta'|}} \binom{k}{\hat{\alpha}+\delta'}\binom{n-k}{\hat{\alpha}+\delta''} \\
& \quad \times (|z|^2)^{\hat{\alpha}} \, t_{(\hat{\alpha}+\delta'),\,(\hat{\alpha}+\delta'')} \Bigg]^2 \\
= & \sum_{l=0}^{k} \sum_{\substack{\delta',\delta''\in\mathbb{N}^d \\ |\delta'|=k-l,\,|\delta''|=n-k-l \\ \delta'\delta''=0}} (|z|^2)^{\delta'+\delta''} \Bigg[\sum_{\substack{\hat{\alpha}\in\mathbb{N}^d \\ |\hat{\alpha}|=l}} \binom{k}{\hat{\alpha}+\delta'}\binom{n-k}{\hat{\alpha}+\delta''} \\
& \quad \times (|z|^2)^{\hat{\alpha}} \, t_{(\hat{\alpha}+\delta'),\,(\hat{\alpha}+\delta'')} \Bigg]^2 .
\end{aligned}$$

Since two polynomials that are identical on non-negative integers are the same, we have proven the result:

$$p(x) = \sum_{l=0}^{k} \sum_{\substack{\delta',\delta''\in\mathbb{N}^d \\ |\delta'|=k-l \\ |\delta''|=n-k-l \\ \delta'\delta''=0}} x^{\overbrace{\delta'+\delta''}^{\text{total degree } n-2l}} \, q_{\delta',\delta''}(x)^2$$

where

$$q_{\delta',\delta''}(x) = \sum_{\substack{\hat{\alpha}\in\mathbb{N}^d \\ |\hat{\alpha}|=k-|\delta'|=n-k-|\delta''|}} \binom{k}{\hat{\alpha}+\delta'}\binom{n-k}{\hat{\alpha}+\delta''} t_{(\hat{\alpha}+\delta'),(\hat{\alpha}+\delta'')} x^{\hat{\alpha}}$$

Proof of the Item 2.

Assume that $p_{W[O]}(x) = x^\alpha \psi^2$ where $\psi \in \mathbb{H}[x]_{d,k}$. We expand the polynomial ψ in the basis of monomials $x^\beta, \beta \in \mathbb{N}_d^{(k)}$.

$$\psi(x) = \sum_{\beta \in \mathbb{N}_d^{(k)}} c_\beta x^\beta \implies \psi(x)^2 = \sum_{\beta,\beta' \in \mathbb{N}_d^{(k)}} c_\beta c_{\beta'} x^{\beta+\beta'}.$$

We now evaluate the polynomial for $z \odot \bar{z}$ where $z \in \mathbb{C}^d$.

$$p_{W[O]}(z \odot \bar{z}) = |z|^{2\alpha} \sum_{\beta,\beta' \in \mathbb{N}_d^{(k)}} c_\beta c_{\beta'} |z|^{2\beta+2\beta'}.$$

Let $\delta, \delta' \in \mathbb{N}^d$ such that $\delta + \delta' = \alpha$. We then can rewrite the previous expression as

$$p_{W[O]}(z \odot \bar{z}) = |\sum_{\beta \in \mathbb{N}_d^{(k)}} c_\beta \bar{z}^{\delta+\beta} z^{\delta'+\beta}|^2.$$

Consider the following vector.

$$|\varphi\rangle := \sum_{\beta \in \mathbb{N}_d^{(k)}} c_\beta \left(|1\rangle^{\otimes \beta_1+\delta_1} \cdots |d\rangle^{\otimes \beta_d+\delta_d} \otimes |1\rangle^{\otimes (\beta_1+\delta'_d)} \cdots |d\rangle^{\otimes (\beta_d+\delta'_d)} \right) \in (\mathbb{C}^d)^{\otimes n},$$

This allows us to rewrite the term inside the modulus as an inner product with the product vector in z and $\bar{z}$.

$$\sum_{\beta \in \mathbb{N}_d^{(k)}} c_\beta \bar{z}^{\delta+\beta} z^{\delta'+\beta} = \langle z^{\otimes k+|\delta|} \otimes \bar{z}^{\otimes n-k-|\delta|} | \varphi \rangle .$$

Therefore, finally, we have the following series of equalities.

$$p_{W[O]}(z \odot \bar{z}) = |\sum_{\beta \in \mathbb{N}_d^{(k)}} c_\beta \bar{z}^{\delta+\beta} z^{\delta'+\beta}| = |\langle z^{\otimes k+|\delta|} \otimes \bar{z}^{\otimes n-k-|\delta|} | \varphi \rangle|^2 = \langle z^{\otimes n}| \, |\varphi\rangle\langle\varphi|^{\Gamma_{[k+|\delta|]}} \, |z^{\otimes n}\rangle .$$

Since $|\alpha| = n - 2k$, for any l satisfying $0 \leq l \leq n - 2k$, there exists a $\delta \leq \alpha$ such that $|\delta| = l$. Defining $l' := k + l$, this also implies that for all $k \leq l' \leq n - k$, there exists a $|\varphi\rangle \in (\mathbb{C}^d)^{\otimes n}$ such that

$$\langle z^{\otimes n}| \operatorname{diag}[W[O]] |z^{\otimes n}\rangle = p_{W[O]}(z \odot \bar{z}) = \langle z^{\otimes n}| \, |\varphi\rangle\langle\varphi|^{\Gamma_{[l']}} \, |z^{\otimes n}\rangle .$$

This proves the claim.

■

9.9 PROOF OF QUBIT PPT CRITERION

We will study the following cone of SOS tensors for $d = 2$.

$$\mathsf{SOS}_2^{(n)} := \{T \mid p_T(x) \in \mathrm{cone}\{x^\alpha \psi \mid |\alpha| \in \{n, n-2, n-4 \ldots n-2\lfloor n/2 \rfloor\}, \psi \in \Sigma_2^{(n-|\alpha|)}\}\}.$$

We will show that some of the terms are superfluous. In particular, we claim that α can be taken to be $\max(\alpha) \leq 1$. So, for the case of n even, we have,

$$\mathsf{SOS}_2^{(n)} = \{T \mid p_T(x) \in \mathrm{cone}\{x^\alpha \psi \mid \alpha \in \{(1,1),(0,0)\}, \psi \in \Sigma_2^{(n-|\alpha|)}\}\},$$

and in the case of n odd, we have,

$$\mathsf{SOS}_2^{(n)} = \{T \mid p_T(x) \in \mathrm{cone}\{x^\alpha \psi \mid \alpha \in \{(0,1),(1,0)\}, \psi \in \Sigma_2^{(n-|\alpha|)}\}\}.$$

We show the proof for n even. Let $x^\alpha \psi$ be an arbitrary term such that $\Sigma_2^{(n-|\alpha|)}$. Also $|\alpha|$ is even. Let $p : \mathbb{N} \to \{0,1\}$ denote the parity function. Then,

$$x^\alpha \psi = x_1^{\alpha_1} x_2^{\alpha_2} \psi = x_1^{p(\alpha_1)} x_2^{p(\alpha_2)} \underbrace{x_1^{\alpha_1 - p(\alpha_1)} x_2^{\alpha_2 - p(\alpha_2)} \psi}_{\in \Sigma_2^{n-p(\alpha_1)-p(\alpha_2)}}$$

Since $p(\alpha_1) + p(\alpha_2) = p(\alpha_1 + \alpha_2) = 0 \mod 2$, either both are 0 or both are 1. Hence, each term is equivalent to $x^\alpha \psi$ where $\Sigma_2^{n-|\alpha|}$ where $\alpha = (0,0)$ or $\alpha = (1,1)$. The proof for the odd case can be done similarly.

By following the essential argument as Theorem 9.44, the argument above implies that the dual of $\mathsf{SOS}_2^{(n)}$ is equivalent to checking positivity of only *two* moment matrices, one for each α.

For the even case, $n = 2m$, the explicit moment matrices in terms of the tensors can be obtained as

$$M^{(0,0)}(T) = \begin{pmatrix} T_{(2m,0)} & T_{(2m-1,1)} & T_{(2m-2,2)} & \cdots & T_{(m,m)} \\ T_{(2m-1,1)} & T_{(2m-2,2)} & T_{(2m-3,3)} & \cdots & T_{(m-1,m+1)} \\ T_{(2m-2,2)} & T_{(2m-3,3)} & T_{(2m-4,4)} & \cdots & T_{(m-2,m+2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_{(m,m)} & T_{(m-1,m+1)} & T_{(m-2,m+2)} & \cdots & T_{(0,2m)} \end{pmatrix}.$$

$$M^{(1,1)}(T) = \begin{pmatrix} T_{(2m-1,1)} & T_{(2m-2,2)} & T_{(2m-3,3)} & \cdots & T_{(m,m)} \\ T_{(2m-2,2)} & T_{(2m-3,3)} & T_{(2m-4,4)} & \cdots & T_{(m-1,m+1)} \\ T_{(2m-3,3)} & T_{(2m-4,4)} & T_{(2m-5,5)} & \cdots & T_{(m-2,m+2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_{(m,m)} & T_{(m-1,m+1)} & T_{(m-2,m+2)} & \cdots & T_{(1,2m-1)} \end{pmatrix}.$$

These matrices of size of order n were also obtained in [Yu16, Theorem 1]. These matrices give necessary and sufficient conditions for the mixture of Dicke state X to be PPT by Theorem 9.48, and hence, in effect, also separable by Theorem 9.50.

Theorem 9.72. Let $X \in \mathrm{Herm}[\mathsf{DS}_2^{(2m)}]$. Then,

$$X \in \mathsf{Sep}_2^{(2m)} \iff M^{(1,1)}(Q[X]) \succeq 0 \text{ and } M^{(0,0)}(Q[X]) \succeq 0.$$

Conditions for n odd can be derived analogously to the case above.

Part III

CONCLUSION

10

Summary and Open Questions

10.1 SUMMARY IN ENGLISH

In this thesis, we study the structure of entanglement and entanglement witnesses in symmetric bipartite and multipartite quantum states, by connecting them to various topics in real algebraic geometry, graph theory, tensor analysis, and polynomial optimization.

Firstly, we consider the entanglement properties of quantum states with cyclic sign invariance, and characterize the geometry of separable and PPT states in the bosonic subspace. This is done by studying the the circulant completely positive matrices and doubly non-negative matrices for $d = 5$, with some progress towards $d = 6$ and $d = 7$; showing the rich geometrical structure of these states. A new class of quantum states was identified, where the PPT and separability can be characterized for all dimensions.

Secondly, we look at some constructions of PPT entangled states using non rank-1 generated matrices in the sets of doubly non-negative, correlation, and sparse PSD matrices.

Thirdly, we study the positivity property of DUC (Diagonal Unitary Covariant) quantum maps. After analysing some structural properties of the pairs of matrices that parametrize these maps, we present a new construction of positive indecomposable map using copositive matrices. We provide some explicit examples by constructing graph-based maps, and characterise decomposability and positivity properties in terms of the graph parameters. Bosonic extendibility of (mixture of) Dicke states was also analysed using SOS hierarchies for copositive matrices.

Finally, we analyse entanglement in multipartite mixture of Dicke states by translating their entanglement properties in terms of properties of real tensors. This allows us to identify PPT entangled states in 3 qutrits, and also generalize some results from the qubit case. Examples of bosonic indecomposable maps can be constructed from positive polynomials that are not sum of squares; and sum of square hierarchies can be used to approximate such witnesses.

10.2 SUMMARY IN FRENCH

Dans cette thèse, nous avons étudié la structure de l'intrication et des témoins d'intrication dans les états quantiques symétriques bipartites et multipartites, en les reliant à divers sujets de géométrie algébrique réelle, de théorie des graphes, d'analyse tensorielle et d'optimisation polynomiale.

Premièrement, nous considérons les propriétés d'intrication des états quantiques possédant une invariance cyclique de signe, et caractérisons la géométrie des états séparables et PPT dans le sous-espace bosonique. Cela est réalisé en étudiant les matrices circulantes complètement positives et les matrices doublement non négatives pour $d = 5$, avec des avancées partielles pour $d = 6$ et $d = 7$, mettant en évidence la riche structure géométrique de ces états. Une nouvelle classe d'états quantiques a été identifiée, pour laquelle les propriétés PPT et de séparabilité peuvent être caractérisées en toute dimension.

Deuxièmement, nous examinons certaines constructions d'états intriqués PPT utilisant des matrices non engendrées par des matrices de rang 1 dans les ensembles de matrices doublement non négatives, de corrélation et de matrices creuses semi-définies positives.

Troisièmement, nous étudions la propriété de positivité des applications quantiques DUC (covariantes par transformations unitaires diagonales). Après avoir analysé certaines propriétés structurelles des paires de matrices qui paramétrisent ces applications, nous présentons une nouvelle construction d'application positive indécomposable utilisant des matrices copositives. Nous fournissons des exemples explicites en construisant des applications associées à des graphes, et caractérisons les propriétés de décomposabilité et de positivité en fonction des paramètres du graphe. L'extensibilité bosonique de mélanges d'états de Dicke a également été analysée à l'aide de hiérarchies SOS pour les matrices copositives.

Enfin, nous étudions l'intrication dans les mélanges multipartites d'états de Dicke en traduisant leurs propriétés d'intrication en termes de propriétés de tenseurs réels. Cela nous permet d'identifier des états intriqués PPT à 3 qutrits, et également d'étendre certains résultats du cas qubit. Des exemples d'applications bosoniques indécomposables peuvent être construits à partir de polynômes positifs qui ne sont pas somme de carrés ; et des hiérarchies de sommes de carrés peuvent être utilisées pour approximer de tels témoins.

10.3 FUTURE DIRECTIONS

Finally, we present some perspectives and related future directions related to the four contributions in this thesis.

1. In Chapter 6, we completely characterized the geometry of the *circulant* completely positive and copositive matrices for $d = 5$, and partial geometries for $d = 6, 7$. It would be interesting to characterize the geometry fully for $d = 6, 7$ and higher dimensions if possible, to gain more insight into the intricate structure of the completely positive and copositive cones. Also, recall that the independence number can be rephrased as an optimization problem over the copositive cone using the Motzkin-Straus theorem [MS65]:

$$\alpha(G) = \max\{t \mid t(I_d + A_G) - J_d \in \mathrm{Cop}_d\}.$$

   For circulant graphs G, it is known that the independence number $\alpha(G)$ is still NP-hard to compute [CGV98], which should imply a similar hardness for membership in the circulant copositive cone.

2. The Gurvits-Barnum ball is the largest ball in the set of separable states [GB02], centered around the maximally mixed state. In the convex geometry literature, this is known as the Chebyshev center of a convex set (the center of the largest inscribed ball in the convex set). Can similar results be obtained for the sets of bosonic separable states and completely positive matrices? In particular, what are the Chebyshev centers of these sets? Some research along this direction has been done by considering the absolutely separable states [LSEBM25] in the bosonic subspace.

3. In Chapter 8, we discuss the construction of positive indecomposable maps using copositive matrices. Firstly, it would be interesting to understand the k-positivity of this class of maps, and of the Markov-Choi maps [CKL92, Ha03]. This is dually connected to PPT entangled states with high Schmidt numbers [HLLMH18, PV19, KG24]. Secondly, it would be valuable to understand whether examples of positive indecomposable maps can be connected to the PSD incompletable matrices, which were shown to be witnesses for PPT entangled states in Chapter 7.

4. The convex set of bipartite separable states is a semialgebraic set that is not a spectrahedral shadow except when $d \cdot d' \leq 6$ [Faw21]. The same is true for the copositive matrices [BKT22], when it is not equal to SPN matrices and the cone of positive polynomials, when it is not equal to SOS. This motivates the following questions : Is the convex set of separable bosonic states also *not* a spectrahedral shadow for $n = 2, d \geq 3$ and $n \geq 4, d = 2$ since it is not equal to the set of PPT states? What about the $3 \times 3 \times 3$ copositive tensors? Note that for $d = 2$, the copositive tensors are equal to sums of squares of tensors, and hence semidefinite representable.

5. We showed that the extendibility of multipartite mixtures of Dicke states is connected to moment tensor hierarchies in Chapter 9. Firstly, it would be interesting to study

the convergence rates of such hierarchies, similarly to the results in [BL26, FF21, LJ25]. Secondly, it would be interesting to study the extendibility of bosonic states (and mixtures of Dicke states) with local symmetries, to study concretely how this class of states displays monogamy of entanglement [Ter04, ACG+26]. The case of extendibility of *random* bosonic states also deserves scrutiny, and might involve similar methods as in [Lan16].

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