# Semidefinite hierarchies for diagonal unitary invariant bipartite quantum states

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**Abstract**

We investigate questions about the cone $\mathrm{SEP}_n$ of separable bipartite states, consisting of the Hermitian matrices acting on $\mathbb{C}^n \otimes \mathbb{C}^n$ that can be written as conic combinations of rank one matrices of the form $xx^* \otimes yy^*$ with $x, y \in \mathbb{C}^n$. Bipartite states that are not separable are said to be entangled. Detecting quantum entanglement is a fundamental task in quantum information and a hard computational problem. We explore the Doherty-Parrilo-Spedaglieri (DPS) hierarchy of semidefinite conic approximations for $\mathrm{SEP}_n$ when the bipartite states have some additional structural properties: first, (i) for states with diagonal unitary invariance, and second (ii) for states with Bose symmetry. In case (i) we show that the DPS hierarchy can be block diagonalized, which, combining with its moment reformulation, leads to a substantially more efficient implementation. In case (ii), we give a characterization of the dual hierarchy, in terms of sums of squares of Hermitian complex polynomials, extending a known result in the generic case. It turns out that the completely positive cone $\mathrm{CP}_n$, its dual cone $\mathrm{COP}_n$, and their sums-of-squares based conic approximations $\mathcal{K}_n^{(t)}$, play a central role in these two settings (i),(ii). We clarify these connections and test the block diagonal relaxations on classes of examples.

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# 1 Introduction

In quantum information theory, a bipartite quantum state corresponds to a Hermitian positive semidefinite matrix[1] $\rho_{AB}$ acting on a tensor product space $\mathbb{C}^{n_A} \otimes \mathbb{C}^{n_B}$. Each of the two Hilbert spaces $\mathbb{C}^{n_A}$ and $\mathbb{C}^{n_B}$ corresponds to a part of a bipartite quantum system, also referred to as its A- and B-registers; the notation $\rho_{AB}$ is meant to reflect this fact and is commonly used in quantum information theory. Then, the state $\rho_{AB}$ is said to be *separable* when it can written as a sum of tensor product states, of the form $X \otimes Y$ with $X \in \mathrm{Herm}_+^{n_A}$ and $Y \in \mathrm{Herm}_+^{n_B}$, in which case $\rho_{AB}$ acts 'separately' on each register of the quantum system. When $\rho_{AB}$ is not separable it is said to be *entangled*. Entanglement is a physical resource that can be used to carry out more efficiently on a quantum computer certain tasks in computation, communication, teleportation, etc. We refer, e.g., to the books [NC00, Wat18] for background in quantum information theory. From now on we assume $n_A = n_B = n$, but we may sometimes still use the letters $n_A$, $n_B$ to stress the roles of the two A- and B-registers in the system. The set of separable states in $\mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ can alternatively be described as

$$\mathrm{SEP}_n = \mathrm{cone}\{xx^* \otimes yy^* : x, y \in \mathbb{C}^n, \|x\| = \|y\| = 1\} \subseteq \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n). \tag{1}$$

Testing whether a given bipartite state is separable or entangled is a fundamental problem in quantum information theory, which has been shown to be computationally hard (Gurvits [Gur03]).

Doherty, Parrilo and Spedaglieri [DPS02, DPS04] introduced a hierarchy of semidefinite relaxations $\mathrm{DPS}_n^{(t)}$ (for $t \geq 1$) for the separable cone $\mathrm{SEP}_n$, having the property that it is *complete*: if a state $\rho_{AB}$ is entangled, then $\rho_{AB} \notin \mathrm{DPS}_n^{(t)}$ for some order $t$, i.e., entanglement is detected at some finite level of the DPS hierarchy. Testing membership in the relaxation $\mathrm{DPS}_n^{(t)}$ amounts to testing feasibility of a semidefinite program involving $t+1$ matrices of size $n^{t+1}$, thus rapidly increasing with the relaxation order $t$. This motivates investigating more economical relaxations when dealing with classes of bipartite states that enjoy some structural properties.

In this paper we investigate the following structural properties: when the bipartite state is *invariant under some diagonal unitaries*, leading to classes of bipartite states coined in the literature as $\mathrm{CLDUI}_n$, $\mathrm{LDUI}_n$ and $\mathrm{LDOI}_n$, and when the bipartite state is *Bose symmetric*. For separable bipartite states enjoying some of these structural properties, there are interesting connections with the cone $\mathrm{CP}_n$ of completely positive matrices, a well-studied matrix cone in matrix theory and

[1] We consider here *unnormalized* states, i.e., we do not require that $\rho_{AB}$ has trace one. This restriction, which is common in quantum information, is however just a matter of scaling.

optimization. Some natural extensions of $\mathrm{CP}_n$ have been introduced in quantum information theory, known as $\mathrm{PCP}_n$ and $\mathrm{TCP}_n$, consisting of all pairwise (triplewise) completely positive matrices (exact definitions follow below). Via conic duality there are also intimate links to positive polynomials and their characterizations in terms of sums of squares of polynomials. This leads in particular to connections with the copositive cone $\mathrm{COP}_n$, the dual cone of $\mathrm{CP}_n$, and some of its semidefinite approximation hierarchies.

**Diagonal unitary invariant bipartite states**

Following Johnston and MacLean [JM19] and Singh and Nechita [SN21], we say that a bipartite state $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ is *conjugate local diagonal unitary invariant* [2] (CLDUI, for short) if

$$\rho_{AB} = (U \otimes \overline{U})\rho_{AB}(U \otimes \overline{U})^* \quad \text{for all } U \in \mathcal{DU}_n. \tag{2}$$

Here, $\mathcal{DU}_n$ is the set of diagonal unitaries, which consists of the matrices $U = \mathrm{Diag}(u)$ for $u \in \mathbb{T}^n$, where $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$. Analogously, $\rho_{AB}$ is *local diagonal unitary invariant* (LDUI) if

$$\rho_{AB} = (U \otimes U)\rho_{AB}(U \otimes U)^* \quad \text{for all } U \in \mathcal{DU}_n \tag{3}$$

and $\rho_{AB}$ is *local diagonal orthogonal invariant* (LDOI) if it satisfies

$$\rho_{AB} = (O \otimes O)\rho_{AB}(O \otimes O)^* \quad \text{for all } O = \mathrm{Diag}(o) \text{ with } o \in \{\pm 1\}^n. \tag{4}$$

Let $\mathrm{CLDUI}_n$, $\mathrm{LDUI}_n$ and $\mathrm{LDOI}_n$ denote the sets of bipartite states with the relevant invariance properties, so that $\mathrm{CLDUI}_n \cup \mathrm{LDUI}_n \subseteq \mathrm{LDOI}_n$. If, in (2) and (3), one would ask invariance under *all unitaries* (instead of all diagonal unitaries), then one gets the class of (CLDUI) Werner states [Wer89] and (LDUI) isotropic states [HH99]. As observed in [JM19, SN21] and recalled in (5)-(7) below, CLDUI, LDUI, and LDOI states have a very special sparsity pattern.

A matrix $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ is indexed by $[n]^2$, whose elements are the sequences $(i, j)$ in $[n_A] \times [n_B]$, simply denoted as $ij$ for compact notation; so[3], $\rho_{AB} = ((\rho_{AB})_{ij,kl})_{i,k\in[n_A],j,l\in[n_B]}$. Its *support* $\mathrm{supp}(\rho_{AB})$ is defined as the set of positions corresponding to nonzero entries of $\rho_{AB}$, thus consisting of the pairs $(ij, kl) \in [n]^2 \times [n]^2$ with $(\rho_{AB})_{ij,kl} \neq 0$. Define the sets

$$\Omega_n = \{(ij, ij) : i, j \in [n]\} \cup \{(ii, jj) : i, j \in [n]\},$$
$$\Phi_n = \{(ij, ij) : i, j \in [n]\} \cup \{(ij, ji) : i, j \in [n]\}.$$

For a matrix $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$, the following equivalences hold:

$$\rho_{AB} \text{ is CLDUI} \iff \mathrm{supp}(\rho_{AB}) \subseteq \Omega_n, \tag{5}$$
$$\rho_{AB} \text{ is LDUI} \iff \mathrm{supp}(\rho_{AB}) \subseteq \Phi_n, \tag{6}$$
$$\rho_{AB} \text{ is LDOI} \iff \mathrm{supp}(\rho_{AB}) \subseteq \Omega_n \cup \Phi_n. \tag{7}$$

As an illustration, we give the (easy) argument for (5). Let $U = \mathrm{Diag}(u)$ with $u \in \mathbb{T}^n$, and let $i, j, k, l \in [n]$. Then, we have $((U \otimes \overline{U})\rho_{AB}(U \otimes \overline{U})^*)_{ij,kl} = u_i\overline{u_j}\ \overline{u_k}u_l(\rho_{AB})_{ij,kl}$, which is equal to $(\rho_{AB})_{ij,kl}$ if $(i, k) = (j, l)$ or $(i, j) = (k, l)$. At any other position, there exists $u \in \mathbb{T}^n$ such that $u_i\overline{u_j}\ \overline{u_k}u_l \neq 1$, which implies $(\rho_{AB})_{ij,kl} = 0$. This shows (5) and the argument is similar for (6)-(7).

[2] The name reflects the fact that each $U$ is 'diagonal unitary' and 'conjugate local' refers to the fact that $U$ acts on the A-register while its conjugate $\overline{U}$ acts on the B-register.

[3] The letters $n_A$, $n_B$ are used to stress the different roles of the indices, but recall $n_A = n_B = n$.

Hence, the nonzero entries of an LDOI matrix $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ are fully captured by a triplet of matrices $(X, Y, Z) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \times \mathrm{Herm}^n$, obtained by setting

$$X = ((\rho_{AB})_{ij,ij})_{i,j=1}^n, \quad Y = ((\rho_{AB})_{ii,jj})_{i,j=1}^n, \quad Z = ((\rho_{AB})_{ij,ji})_{i,j=1}^n; \tag{8}$$

note that $\mathrm{diag}(X) = \mathrm{diag}(Y) = \mathrm{diag}(Z)$ holds. Conversely, given $(X, Y, Z) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \times \mathrm{Herm}^n$ with $\mathrm{diag}(X) = \mathrm{diag}(Y) = \mathrm{diag}(Z)$, one can define a matrix $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ via relation (8), with zero entries at all other positions; following [SN21], this matrix is denoted $\rho_{(X,Y,Z)}$. For the reader's convenience, its explicit description reads

$$\begin{aligned}
&\rho_{(X,Y,Z)} \\
&= \sum_{i,j=1}^{n} X_{ij} e_i e_i^* \otimes e_j e_j^* + \sum_{i\neq j\in[n]} Y_{ij} e_i e_j^* \otimes e_i e_j^* + \sum_{i\neq j\in[n]} Z_{ij} e_i e_j^* \otimes e_j e_i^* \\
&= \sum_{i,j=1}^{n} X_{ij} (e_i \otimes e_j)(e_i \otimes e_j)^* + \sum_{i\neq j\in[n]} Y_{ij} (e_i \otimes e_i)(e_j \otimes e_j)^* \\
&\quad + \sum_{i\neq j\in[n]} Z_{ij} (e_i \otimes e_j)(e_j \otimes e_i)^*.
\end{aligned} \tag{9}$$

Hence, $\rho_{(X,Y,Z)}$ is LDOI by construction. Set $d = \mathrm{diag}(X) = \mathrm{diag}(Y) = \mathrm{diag}(Z) \in \mathbb{R}^n$. When $Y$ is diagonal, set $\rho_{(X,\cdot,Z)} = \rho_{(X,\mathrm{Diag}(d),Z)}$, which is LDUI by construction, and when $Z$ is diagonal, set $\rho_{(X,Y)} = \rho_{(X,Y,\mathrm{Diag}(d))}$, which is CLDUI by construction. In other words, $\rho_{(X,Y,Z)}$ can be written (after suitably permuting its rows/columns) as a block-diagonal matrix of the form

$$\rho_{(X,Y,Z)} \simeq Y \oplus \oplus_{1\leq i<j\leq n} \begin{pmatrix} X_{ij} & Z_{ij} \\ Z_{ji} & X_{ji} \end{pmatrix}. \tag{10}$$

Hence, $\rho_{(X,Y,Z)} \succeq 0$ if and only if $Y \succeq 0$ and each of the above $2 \times 2$ matrices is positive semidefinite. Furthermore, $\mathrm{Tr}[\rho_{(X,Y,Z)}] = 1$ (i.e. $\rho_{(X,Y,Z)}$ is a normalized quantum state) if and only if $\sum_{i,j\in[n]} X_{i,j} = 1$.

Observe that going from the CLDUI sparsity pattern to the LDUI sparsity pattern amounts to "taking the partial transpose $T_B$ with respect to the B-register" (see (18)). Roughly, this means switching the second indices, i.e., mapping position $(ih, jk)$ to position $(ik, jh)$. In particular,

$$\rho_{(X,Y,Z)}^{T_B} = \rho_{(X,Z,Y)}, \quad \rho_{(X,Y)}^{T_B} = \rho_{(X,\cdot,Y)}. \tag{11}$$

So, the CLDUI and LDOI sparsity structures can be seen as the main players, but additional symmetry structure can be added to LDUI states as we see below.

### (Pairwise/triplewise) completely positive matrices

Following [JM19, SN21], define the cone $\mathrm{PCP}_n$ (resp., the cone $\mathrm{TCP}_n$) consisting of all matrix pairs $(X, Y)$ for which the bipartite state $\rho_{(X,Y)}$ is separable (resp., all matrix triplets $(X, Y, Z)$ for which $\rho_{(X,Y,Z)}$ is separable). It turns out that these two cones can be seen as generalizations of the classical *completely positive cone* $\mathrm{CP}_n$, defined as

$$\mathrm{CP}_n = \mathrm{conv}\{xx^T : x \in \mathbb{R}_+^n\}. \tag{12}$$

Indeed, the following links between the cones $\mathrm{CP}_n$, $\mathrm{PCP}_n$ and $\mathrm{TCP}_n$ are shown in [JM19, SN21] (recalled in Lemma 2.10 with a short proof). For a matrix $X \in \mathcal{S}^n$,

$$\begin{aligned} X \in \mathrm{CP}_n &\Longleftrightarrow (X, X) \in \mathrm{PCP}_n \;\; (\text{i.e., } \rho_{(X,X)} \in \mathrm{SEP}_n) \\ &\Longleftrightarrow (X, X, X) \in \mathrm{TCP}_n \;\; (\text{i.e., } \rho_{(X,X,X)} \in \mathrm{SEP}_n). \end{aligned} \tag{13}$$

Accordingly, elements of $\mathrm{PCP}_n$ ($\mathrm{TCP}_n$) are called *pairwise (triplewise) completely positive.*

### Bose symmetric bipartite states

Let $\mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n) \subseteq \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ denote the set of *Bose symmetric* (or simply *symmetric*) bipartite states $\rho_{AB}$, i.e., satisfying the following permutation invariance property:

$$(\rho_{AB})_{ij,kl} = (\rho_{AB})_{ij,lk} \text{ for all } i, j, k, l \in [n].$$

Hence, any $\rho_{AB} \in \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n)$ leaves $S^2(\mathbb{C}^n)$ invariant and vanishes on $(S^2(\mathbb{C}^n))^\perp$, so that $\mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n) \simeq \mathrm{Herm}(S^2(\mathbb{C}^n))$. Clearly, any state $xx^* \otimes xx^*$ is Bose symmetric and, in fact, these states generate the cone $\mathrm{SEP}_n^{\mathrm{BS}}$, defined as the set of separable Bose symmetric states:

$$\mathrm{SEP}_n^{\mathrm{BS}} := \mathrm{SEP}_n \cap \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n) = \mathrm{cone}\{xx^* \otimes xx^* : x \in \mathbb{S}^{n-1}\}. \tag{14}$$

(See Lemma 2.3 for a short argument.) Note that Bose symmetric states with LDOI pattern arise in the following way, as directly follows using relation (8): for a bipartite state $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$,

$$\begin{aligned} &\rho_{AB} \in \mathrm{LDOI}_n \cap \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n) \Longleftrightarrow \\ &\rho_{AB} = \rho_{(X,Y,X)} \text{ for some } X \in \mathcal{S}^n, Y \in \mathrm{Herm}^n \text{ with } \mathrm{diag}(X) = \mathrm{diag}(Y). \end{aligned} \tag{15}$$

We will give a class of examples in Section 4.3 as an illustration for the case $n = 3$.

### Our contributions and organization of the paper

The above connections suggest the following natural questions:
• Is it possible to adapt the DPS hierarchy in order to test separability of CLDUI (or LDUI, LDOI) bipartite quantum states in a more economical way?
• Is there a link between the DPS hierarchy for separable bipartite states and the well-known hierarchy of semidefinite relaxations for the cone $\mathrm{CP}_n$ (and its dual, the copositive cone $\mathrm{COP}_n$)?
These questions form the main motivation for our work. We address the first question in Section 3 and the second one in Section 4.

In Section 3 we show that the sparsity structure of CLDUI (LDUI, LDOI) states can be transported to every level of the DPS hierarchy. In a nutshell, we show that the matrices involved in the semidefinite program modeling the DPS relaxation at any given level $t$ inherit the sparsity structure of the original bipartite state (Theorem 3.1) and, moreover, that they enjoy a block-diagonal structure (Theorem 3.9). As an application, solving these semidefinite programs is much more efficient, which makes it possible to compute the relaxations at higher order. In Corollary 3.11, we give an estimate on the size of the matrices involved in the semidefinite programs modeling the level $t$ DPS relaxation in the tensor setting and, in Lemma 5.4, we indicate the maximum block size when reformulating the relaxation in the moment framework. We also refer to Tables 4, 5, 6 that show the comparative explicit matrix sizes for small $n$ and $t$ (when reformulating the SDP in the polynomial optimization framework). We report about computational experiments in Section 5.3.

It turns out that the second question – about links between the hierarchy of conic approximations for $\mathrm{COP}_n$ and the DPS hierarchy – was considered in the recent paper [GNP25], of which we learned while completing the present manuscript. We revisit this question in Section 4, where we additionally offer some sharpenings and more compact arguments. The analysis relies in a crucial manner on the dual objects, the dual cone of $\mathrm{SEP}_n$ and the copositive cone $\mathrm{COP}_n$ that tie naturally with positive polynomials and sums of squares. In particular, we show a characterization of the dual of the variation (31) of the DPS hierarchy adapted to Bose symmetric states (Theorem 4.1), which fully mirrors an earlier result of Fang and Fawzi [FF20] for general bipartite states. Based on this characterization, one can then easily establish a correspondence between the hierarchy of inner conic approximations $\mathcal{K}_n^{(t)}$ for the copositive cone $\mathrm{COP}_n$, and the dual of the symmetry-adapted DPS hierarchy (Theorem 4.4), thereby essentially recovering a recent result of [GNP25].

The paper is organized as follows. In Section 2 we introduce the main concepts and provide background facts on the main players in the paper, including the cones $\mathrm{CP}_n$, $\mathrm{SEP}_n$, $\mathrm{DPS}_n^{(t)}$, $\mathrm{PCP}_n$ and their duals, and we review basic properties of bipartite states with diagonal unitary invariance. In Section 3, we investigate how to exploit the sparsity structure of CLDUI (LDUI, LDOI) states in order to design an adapted, more economical variation of the DSP hierarchy; we show that this leads to a reformulation involving matrices with a block-diagonal structure. Section 4 is devoted to Bose symmetric bipartite states; we first give a characterization of the dual symmetry-adapted DPS hierarchy, which we then use to establish a correspondence between the hierarchy of cones $\mathcal{K}_n^{(t)}$ and the symmetry-adapted DPS hierarchy. In Section 5 we discuss several issues regarding the practical implementation of the DPS hierarchy. We first indicate how to reformulate it in the 'moment setting', which is the right setting permitting to remove the redundancies that are inherent to the 'tensor setting' in which the DPS hierarchy is originally defined. This applies to general bipartite states, as well as to bipartite states with some diagonal unitary invariance. After that, we report on numerical experiments that have been carried out on classes of bipartite states with LDOI sparsity structure, motivated by the so-called $\mathrm{PPT}^2$ conjecture from quantum information theory.

# 2 Preliminaries and background results

## 2.1 Preliminaries on notation

We begin with introducing notation on matrices, tensors, and polynomials, used throughout the paper. Thereafter, we group basic definitions and preliminary results about the various objects that are the main players in the paper. This includes the DPS hierarchy and the associated dual cones, a semidefinite hierarchy for the copositive cone and the associated dual cones for (pairwise) completely positive matrices, and basic facts on bipartite states with diagonal unitary invariance. So, this section offers a road map through the main players of the paper and can serve as a gentle introduction to the subject.

### Matrices and tensors

For integers $1 \leq k \leq n$, set $[k:n] = \{k, k+1, \ldots, n-1, n\}$ and $[n] = [1:n]$, and let $\mathfrak{S}_n$ denote the group of permutations of the set $[n]$. Let $\mathbb{T} \subseteq \mathbb{C}$ denote the set of complex numbers $z$ with squared modulus $|z|^2 = \overline{z}z = 1$. We use the notation $\mathbf{i} = \sqrt{-1} \in \mathbb{T}$. For a complex number $z \in \mathbb{C}$, $\mathrm{Re}(z) = (z + \overline{z})/2$ denotes its real part; the notation extends to vectors and matrices by taking the entrywise real part. Let $e_1, \ldots, e_n$ denote the standard unit vectors that form an orthonormal basis of $\mathbb{K}^n$, for $\mathbb{K} = \mathbb{R}, \mathbb{C}$. For $u \in \mathbb{K}^n$, $\|u\| = \sqrt{u^*u}$ is the Euclidean norm, where $u^* = \overline{u}^T$ denotes the conjugate transpose of $u$. Let $\mathbb{S}^{n-1} = \{u \in \mathbb{C}^n : \|u\| = 1\}$ denote the unit sphere in $\mathbb{C}^n$.

We use the trace inner product $\langle X, Y\rangle = \mathrm{Tr}(X^*Y)$ for matrices $X, Y \in \mathbb{K}^{n\times n}$, with $X^* = \overline{X}^T$ denoting the conjugate transpose of $X$. A matrix $X$ is Hermitian if $X^* = X$ and positive semidefinite, denoted as $X \succeq 0$, if all its eigenvalues are nonnegative. Let $\mathrm{Herm}^n$ (resp., $\mathcal{S}^n$) denote the set of $n \times n$ Hermitian (resp., real symmetric) matrices and $\mathrm{Herm}^n_+$ (resp., $\mathcal{S}^n_+$) its subcone of positive semidefinite matrices. For a matrix $X \in \mathbb{C}^{n\times n}$, $\ker X$ denotes its kernel (all vectors $w \in \mathbb{C}^n$ such that $Xw = 0$). Moreover, $\mathrm{diag}(X) = (X_{ii})_{i=1}^n$ denotes the vector consisting of its diagonal entries and, for a vector $x \in \mathbb{C}^n$, $\mathrm{Diag}(x) \in \mathbb{C}^{n\times n}$ denotes the diagonal matrix with $X_{ii} = x_i$ for $i \in [n]$, and $D_X = \mathrm{Diag}(\mathrm{diag}(X))$ denotes the diagonal matrix with same diagonal entries as $X$. We let $I_n$, $J_n$ denote, respectively, the identity matrix and the all-ones matrix of size $n \times n$.

The support of a matrix $X \in \mathrm{Herm}^n$ is the set $\mathrm{supp}(X) = \{(i, j) \in [n]^2 : i \neq j, X_{i,j} \neq 0\}$ consisting of the off-diagonal positions corresponding to nonzero entries. Then, $X$ is said to be supported on a graph $G = ([n], E)$ if $\mathrm{supp}(X) \subseteq E$, i.e., $X_{i,j} = 0$ if $(i, j)$ is not an edge of $G$.

We use the symbol '$\circ$' to denote the Hadamard product and '$\otimes$' to denote the tensor product. Given two vectors $u, v \in \mathbb{C}^n$, their Hadamard product is $u \circ v = (u_iv_i)_{i=1}^n \in \mathbb{C}^n$. The definition applies analogously to matrices: $A \circ B = (A_{ij}B_{ij})_{i\in[m],j\in[n]}$ for $A, B \in \mathbb{C}^{m\times n}$. Given vectors $u \in \mathbb{C}^{n_1}$, $v \in \mathbb{C}^{n_2}$, their tensor product is $u \otimes v \in \mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2}$ with entries $(u \otimes v)_{i_1i_2} = u_{i_1}v_{i_2}$ for $i_1 \in [n_1], i_2 \in [n_2]$. Analogously, given matrices $A \in \mathbb{C}^{m_1\times n_1}, B \in \mathbb{C}^{m_2\times n_2}$, their tensor product is $A \otimes B \in \mathbb{C}^{m_1\times n_1} \otimes \mathbb{C}^{m_2\times n_2}$ with entries $(A \otimes B)_{(i_1,i_2),(j_1,j_2)} = A_{i_1,j_1}B_{i_2,j_2}$ for $(i_1, i_2) \in [m_1] \times [m_2]$ and $(j_1, j_2) \in [n_1] \times [n_2]$. Given $A \in \mathbb{C}^{n\times n}$, the following (easy) observation will be often used later:

$$A \circ uu^* = \mathrm{Diag}(u)A\mathrm{Diag}(u)^* \quad \text{for any } u \in \mathbb{C}^n. \tag{16}$$

Given $X \in \mathrm{Herm}^n$, $Y \in \mathrm{Herm}^m$,

$$X \oplus Y = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} \in \mathrm{Herm}^{n+m}$$

is their direct sum, which has a block-diagonal form. Such block-diagonal structure is useful since $X \oplus Y \succeq 0$ if and only if $X, Y \succeq 0$, where the latter is easier to test as it involves smaller matrices.

We will deal with bipartite states, i.e., matrices that act on a tensor product space $\mathbb{C}^n \otimes \mathbb{C}^n$. While $\mathbb{C}^n \otimes \mathbb{C}^n$ can be identified with $\mathbb{C}^{n^2}$, we also use the notation $\mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$, $\mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)_+$ (instead of $\mathrm{Herm}^{n^2}$, $\mathrm{Herm}^{n^2}_+$) when it is important to stress the tensor product structure. This notation will be especially useful when considering states that act on a tensor product space of the form $(\mathbb{C}^n)^{\otimes t}$ (for some $t \geq 1$). Then, it is convenient (and common in quantum information) to refer to the various copies of $\mathbb{C}^n$ as the *registers* of the quantum system $(\mathbb{C}^n)^{\otimes t}$.

Consider the tensor space $(\mathbb{C}^n)^{\otimes t}$ (for $t \geq 1$). A $t$-tensor $v \in (\mathbb{C}^n)^{\otimes t}$ is indexed by sequences $\underline{i} = (i_1, \ldots, i_t) \in [n]^t$, so $v = (v_{\underline{i}})_{\underline{i}\in[n]^t}$. For compact notation, we also use the notation $\underline{i} = i_1 \ldots i_t$ for sequences in $[n]^t$. For an integer $1 \leq s \leq t$, we let $\underline{ij} \in [n]^t$ denote the concatenation of $\underline{i} \in [n]^s$ and $\underline{j} \in [n]^{t-s}$. Given a sequence $\underline{i} = i_1 \ldots i_t \in [n]^t$, we let $\{\underline{i}\} = \{i_1, \ldots, i_t\} \subseteq [n]$ denote the associated multiset, and define $\alpha(\underline{i}) = (\alpha(\underline{i})_k)_{k=1}^n \in \mathbb{N}^n$, where $\alpha(\underline{i})_k$ denotes the number of occurrences of the symbol $k$ in the multiset $\{\underline{i}\}$. Then, $|\alpha(\underline{i})| = \sum_{k=1}^n \alpha(\underline{i})_k = t$. Moreover, two sequences $\underline{i}, \underline{j} \in [n]^t$ correspond to the same multiset, i.e., $\{\underline{i}\} = \{\underline{j}\}$, precisely when $\alpha(\underline{i}) = \alpha(\underline{j})$.

Any permutation $\sigma \in \mathfrak{G}_t$ of the set $[t]$ acts on $[n]^t$ by setting $\underline{i}^\sigma = i_{\sigma(1)} \ldots i_{\sigma(t)}$ for $\underline{i} \in [n]^t$, it also acts on $(\mathbb{C}^n)^{\otimes t}$ by setting $v^\sigma = (v_{\sigma(\underline{i})})_{\underline{i}\in[n]^t}$ for $v \in (\mathbb{C}^n)^{\otimes t}$, and on $\mathrm{Herm}((\mathbb{C}^n)^{\otimes t})$ by setting $\rho^\sigma = (\rho_{\underline{i}^\sigma,\underline{j}^\sigma})_{\underline{i},\underline{j}\in[n]^t}$ for $\rho \in \mathrm{Herm}((\mathbb{C}^n)^{\otimes t})$. Then, $v \in (\mathbb{C}^n)^{\otimes t}$ is called a *symmetric tensor* if $v^\sigma = v$ for all $\sigma \in \mathfrak{G}_t$. Let $\mathcal{S}^t(\mathbb{K}^n)$ denote the subspace of symmetric $t$-tensors and $\Pi_t : (\mathbb{K}^n)^{\otimes t} \to \mathcal{S}^t(\mathbb{K}^n)$ denotes the orthogonal projection onto the symmetric subspace $\mathcal{S}^t(\mathbb{K}^n)$.

A matrix $\rho \in \mathrm{Herm}((\mathbb{C}^n)^{\otimes t})$ is said to be *Bose symmetric* (also called *bosonic* in the quantum information literature) if $\rho^\sigma = \rho$ for all $\sigma \in \mathfrak{G}_t$, i.e., $\rho\ e_{i_1} \otimes \ldots \otimes e_{i_t} = \rho\ e_{i_{\sigma(1)}} \otimes \ldots \otimes e_{i_{\sigma(t)}}$ for all $\sigma \in \mathfrak{G}_t$ and $\underline{i} \in [n]^t$. Equivalently, $\rho$ is Bose symmetric if $\rho\Pi_t = \rho$ (or $\Pi_t\rho = \rho$, or $\Pi_t\rho\Pi_t = \rho$, since $\rho$ is Hermitian). Let $\mathrm{BS}((\mathbb{C}^n)^{\otimes t}) \subseteq \mathrm{Herm}((\mathbb{C}^n)^{\otimes t})$ denote the set of Hermitian Bose symmetric matrices. So, any $\rho \in \mathrm{BS}_t((\mathbb{C}^n)^{\otimes t})$ leaves $\mathcal{S}^t(\mathbb{C}^n)$ invariant and vanishes on its orthogonal complement. This fact justifies the identifications $\mathrm{BS}((\mathbb{C}^n)^{\otimes t}) \simeq \mathrm{Herm}(S^t(\mathbb{C}^n))$ and $(\mathrm{BS}((\mathbb{C}^n)^{\otimes t})^\perp \simeq \mathrm{Herm}((S^t(\mathbb{C}^n))^\perp)$. In the same way, $\mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$ denotes the subspace of Hermitian matrices in $\mathrm{Herm}((\mathbb{C}^n)^{\otimes(t+1)})$ that leave $\mathbb{C}^n \otimes S^t(\mathbb{C}^n)$ invariant and vanish on its orthogonal complement $\mathbb{C}^n \otimes (S^t(\mathbb{C}^n))^\perp$.

For a matrix acting on a tensor product space, one can define the *partial trace* and the *partial transpose* with respect to a subset of registers. We first introduce these notions for the case of a tensor space $\mathbb{C}^{n_A} \otimes \mathbb{C}^{n_B}$. Let $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^{n_A} \otimes \mathbb{C}^{n_B})$. Then, *tracing out the B-register* produces the matrix $\mathrm{Tr}_B(\rho_{AB}) \in \mathrm{Herm}(\mathbb{C}^{n_A})$, with entries

$$\mathrm{Tr}_B(\rho_{AB})_{i,j} = \langle \mathrm{Tr}_B(\rho_{AB}), e_i e_j^T \rangle = \langle \rho_{AB}, e_i e_j^T \otimes I_{n_B} \rangle = \sum_{k \in [n_B]} (\rho_{AB})_{ik,jk} \tag{17}$$

for $i, j \in [n_A]$. *Taking the partial transpose with respect to the B-register* produces $\rho_{AB}^{T_B} \in \mathrm{Herm}(\mathbb{C}^{n_A} \otimes \mathbb{C}^{n_B})$, with entries

$$(\rho_{AB}^{T_B})_{ih,jk} = (\rho_{AB})_{ik,jh} \quad \text{for } i, j \in [n_A], h, k \in [n_B]. \tag{18}$$

**Example 2.1.** *For $t = 2$, the vectors $D_{ii} = e_i \otimes e_i$ ( for $i \in [n]$) and $D_{ij} = (e_i \otimes e_j + e_j \otimes e_i)/\sqrt{2}$ (for $1 \leq i < j \leq n$) form an orthonormal basis of $\mathcal{S}^2(\mathbb{C}^n)$, known as the* Dicke basis. *The* Dicke states *$D_{ij}D_{ij}^*$ ($1 \leq i \leq j \leq n$) are clearly Bose symmetric. Moreover, they span the space $\mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n) \cap \mathrm{LDUI}_n$, also known as the set of* mixed Dicke states *[GNP25] (called* diagonally symmetric states *in [MATS21, TAQ+18]). This follows from (15) combined with the fact that, for any $X \in \mathcal{S}^n$, $\rho_{(X,\cdot,X)}$ can be decomposed as*

$$\rho_{(X,\cdot,X)} = \sum_{i=1}^{n} X_{ii} D_{ii} D_{ii}^* + \sum_{1 \leq i < j \leq n} X_{ij} D_{ij} D_{ij}^*.$$

*Each state $D_{ii}D_{ii}^* = e_i e_i^* \otimes e_i e_i^*$ is clearly separable. However, for $i < j$, the state $D_{ij}D_{ij}^*$ is entangled, and it is known as the* maximally entangled state. *That the state $D_{ij}D_{ij}^*$ is entangled follows from the fact that its partial transpose is not positive semidefinite, as shown below for $n = 2$. Then, $D_{12} = (e_1 \otimes e_1 + e_2 \otimes e_2)/\sqrt{2}$,*

$$D_{12}D_{12}^* = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (D_{12}D_{12}^*)^{T_B} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \not\succeq 0,$$

*where the matrices are indexed by $11, 12, 21, 22$ (in that order). Note that $D_{12}D_{12}^*$ is LDUI and its partial transpose $(D_{12}D_{12}^*)^{T_B}$ is CLDUI (as expected). Moreover, $D_{12}D_{12}^*$ is Bose symmetric, but its partial transpose $(D_{12}D_{12}^*)^{T_B}$ is not (since its columns indexed by 12 and 21 are distinct). Note also that $\mathrm{Tr}_B(D_{12}D_{12}^*) = \frac{1}{2}I_2$.*

The partial trace and partial transpose extend naturally to a tensor product space of the form $\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}$ (with $t \geq 1$), as will be the setting for the DPS hierarchy in Section 2.2 below. Consider

$\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$, where the notation is meant to stress the role of the first A-register $\mathbb{C}^n$ combined with $t$ copies of the B-register $\mathbb{C}^n$. Then, one can trace out or take the partial trace with respect to any subset of the $t+1$ registers. In the application to the DPS hierarchy, we will do this for a subset of the $B$-registers. Assume we are given an integer $s \in [t]$ and we apply these operations w.r.t. the last $s$ B-registers; this amounts to consider $\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}$ as the bipartite system $\mathbb{C}^{n_A} \otimes \mathbb{C}^{n_B}$ with $\mathbb{C}^{n_A} \sim \mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes(t-s)}$ and $\mathbb{C}^{n_B} \sim (\mathbb{C}^n)^{\otimes s}$, in which case relations (17) and (18) specialize as follows. Then, $\mathrm{Tr}_{B[t-s+1:t]}(\rho_{AB[t]}) \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes(t-s)})$ denotes the matrix obtained from $\rho_{AB[t]}$ by *tracing out the last $s$ B-registers*, thus with entries

$$(\mathrm{Tr}_{B[t-s+1:t]}(\rho_{AB[t]}))_{i_0\underline{i},j_0\underline{j}} = \sum_{\underline{k}\in[n]^s} (\rho_{AB[t]})_{i_0\underline{i}\underline{k},j_0\underline{j}\underline{k}} \tag{19}$$

for $(i_0,\underline{i}),(j_0,\underline{j}) \in [n]\times[n]^{t-s}$. Similarly, $\rho_{AB[t]}^{T_{B[t-s+1:t]}} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$ is the matrix obtained from $\rho_{AB[t]}$ by taking the *partial transpose with respect to the last $s$ B-registers*, thus with entries

$$(\rho_{AB[t]}^{T_{B[t-s+1]}})_{i_0\underline{i}\underline{h},j_0\underline{j}\underline{k}} = (\rho_{AB[t]})_{i_0\underline{j}\underline{h},j_0\underline{i}\underline{k}} \text{ for } (i_0,\underline{i},\underline{h}),(j_0,\underline{j},\underline{k}) \in [n]\times[n]^{t-s}\times[n]^s. \tag{20}$$

Hence, $\mathrm{Tr}_B = \mathrm{Tr}_{B[1:1]}$ and $T_B = T_{B[1:1]}$ if $s=t=1$. For instance, if $\rho_{AB[t]} = xx^* \otimes (yy^*)^{\otimes t}$, then

$$\begin{aligned} \mathrm{Tr}_{B[t-s+1:t]}(\rho_{AB[t]}) &= xx^* \otimes (yy^*)^{\otimes(t-s)}\|y\|^{2s}, \\ \rho_{AB[t]}^{T_{B[t-s+1:t]}} &= xx^* \otimes (yy^*)^{\otimes(t-s)} \otimes (\overline{yy}^*)^{\otimes s}. \end{aligned} \tag{21}$$

**Polynomials**

We will use polynomials in real variables and in complex variables, so we introduce both settings. Throughout, $\mathbb{R}[x]=\mathbb{R}[x_1,\ldots,x_n]$ denotes the polynomial ring in $n$ variables $x=(x_1,\ldots,x_n)$, with real coefficients. For an integer $d\geq 0$, $\mathbb{R}[x]_d$ denotes the space of homogeneous polynomials of degree $d$, of the form $p=\sum_{\alpha\in\mathbb{N}^n,|\alpha|=d} p_\alpha x^\alpha$, and $\mathbb{R}[x]_{\leq d} = \cup_{k=0}^d \mathbb{R}[x]_k$ is the set of polynomials with degree at most $d$. Here, $|\alpha| = \sum_{i=1}^n \alpha_i$ and $x^\alpha = \prod_{i=1}^n x_i^{\alpha_i}$ for $\alpha\in\mathbb{N}^n$. A polynomial $p\in\mathbb{R}[x]$ is said to be a *sum of squares* (*sos*, for short) if $p=\sum_{\ell=1}^m q_\ell^2$ for some $q_\ell\in\mathbb{R}[x]$ and $m\geq 1$. Then, $p$ has even degree $2d$, $q_\ell$ has degree at most $d$, and each $q_\ell$ is homogeneous of degree $d$ if $p$ is homogeneous. As is well-known, a polynomial $p$ of degree $2d$ is sos if and only if the following semidefinite program is feasible: there exists a positive semidefinite matrix $Q\in\mathcal{S}^N$ ($N=\binom{n+d}{d}$) such that the polynomial identity $p=\langle Q,(x^{\alpha+\beta})_{\alpha,\beta\in\mathbb{N}^n,|\alpha|,|\beta|\leq d}\rangle$ holds.

We will also consider the ring $\mathbb{C}[x,\overline{x}]$ of polynomials in $n$ complex variables $x=(x_1,\ldots,x_n)$ and their conjugates $\overline{x}=(\overline{x}_1,\ldots,\overline{x}_n)$. So, $p\in\mathbb{C}[x,\overline{x}]$ is of the form $p=\sum_{\alpha,\alpha'\in\mathbb{N}^n} p_{\alpha,\alpha'} x^\alpha \overline{x}^{\alpha'}$ (with finitely many nonzero coefficients). The largest value of $|\alpha|+|\alpha'|$ such that $p_{\alpha,\alpha'}\neq 0$ is the *total degree* of $p$. One can also consider the degree in $x$ and the degree in $\overline{x}$. For integers $d,d'\geq 0$, $\mathbb{C}[x,\overline{x}]_{d,d'}$ consists of the homogeneous polynomials $p$ with degree $d$ in $x$ and $d'$ in $\overline{x}$, i..e, with $p_{\alpha,\alpha'}=0$ if $(|\alpha|,|\alpha'|)\neq(d,d')$. A polynomial $p\in\mathbb{C}[x,\overline{x}]$ is said to be *Hermitian* if $p=\overline{p}$ holds. For instance, $p=x+\overline{x}$ is Hermitian, but $q=\mathbf{i}x+\overline{x}$ is not Hermitian since $\overline{q}=-\mathbf{i}\overline{x}+x\neq q$.

A (Hermitian) polynomial $p\in\mathbb{C}[x,\overline{x}]$ is said to be a *real-sum of squares* (abbreviated as *r-sos*) if $p=\sum_{\ell=1}^m q_\ell^2$ for some Hermitian polynomials $q_\ell\in\mathbb{C}[x,\overline{x}]$. Equivalently, $p$ is r-sos if and only if $p=\sum_\ell h_\ell\overline{h_\ell}$ for some polynomials $h_\ell\in\mathbb{C}[x,\overline{x}]$. For instance, $p=x\overline{x}=\left(\frac{x+\overline{x}}{2}\right)^2+\left(\frac{x-\overline{x}}{2\mathbf{i}}\right)^2$ is r-sos. Here, we stress 'real'-sos in order to distinguish from the other (more restricted) notion of *complex-sum of squares* (*c-sos*), where $p\in\mathbb{C}[x,\overline{x}]$ is c-sos if $p=\sum_\ell h_\ell\overline{h_\ell}$ for some $h_\ell\in\mathbb{C}[x]$. Again, one can check whether a polynomial $p\in\mathbb{C}[x,\overline{x}]$ is r-sos by means of a semidefinite program.

Any polynomial $p(x,\overline{x}) \in \mathbb{C}[x,\overline{x}]$ can be transformed into a pair of polynomials in $\mathbb{R}[x_{\mathrm{Re}}, x_{\mathrm{Im}}]$ in the real variables $x_{\mathrm{Re}}, x_{\mathrm{Im}} \in \mathbb{R}^n$ via the transformation $x = x_{\mathrm{Re}} + \mathbf{i}x_{\mathrm{Im}}$. In this way, each $p \in \mathbb{C}[x,\overline{x}]$ corresponds to a unique pair $(p_{\mathrm{Re}}, p_{\mathrm{Im}}) \in \mathbb{R}[x_{\mathrm{Re}}, x_{\mathrm{Im}}]^2$ via

$$\begin{aligned} p_{\mathrm{Re}}(x_{\mathrm{Re}}, x_{\mathrm{Im}}) &= \mathrm{Re}(p(x_{\mathrm{Re}} + \mathbf{i}x_{\mathrm{Im}}, x_{\mathrm{Re}} - \mathbf{i}x_{\mathrm{Im}})), \\ p_{\mathrm{Im}}(x_{\mathrm{Re}}, x_{\mathrm{Im}}) &= \mathrm{Im}(p(x_{\mathrm{Re}} + \mathbf{i}x_{\mathrm{Im}}, x_{\mathrm{Re}} - \mathbf{i}x_{\mathrm{Im}}), \end{aligned}$$

and we have the identity

$$p(x,\overline{x}) = p(x_{\mathrm{Re}} + \mathbf{i}x_{\mathrm{Im}}, x_{\mathrm{Re}} - \mathbf{i}x_{\mathrm{Im}}) = p_{\mathrm{Re}}(x_{\mathrm{Re}}, x_{\mathrm{Im}}) + \mathbf{i}p_{\mathrm{Im}}(x_{\mathrm{Re}}, x_{\mathrm{Im}}). \tag{22}$$

So, $p_{\mathrm{Re}} = \mathrm{Re}(p)$ is the real part of $p$ and $p_{\mathrm{Im}} = \mathrm{Im}(p)$ is its imaginary part. Then, $p$ is Hermitian (i.e., $p = \overline{p}$) precisely when $\mathrm{Im}(p) = 0$. In particular, the polynomial $p\overline{p}$ is Hermitian and equality

$$\mathrm{Re}(p\overline{p}) = p_{\mathrm{Re}}^2 + p_{\mathrm{Im}}^2 \tag{23}$$

holds. Based on this one can verify the following well-known correspondence: for a Hermitian polynomial $p \in \mathbb{C}[x,\overline{x}]$,

$$p \text{ is r-sos} \iff \text{its real part } p_{\mathrm{Re}} \in \mathbb{R}[x_{\mathrm{Re}}, x_{\mathrm{Im}}] \text{ is sos} \tag{24}$$

(which explains the terminology 'real'-sos). See, e.g., [GLS21, Appendix A] for a detailed exposition.

For the application to the DPS hierarchy, one needs a second group $y = (y_1, \ldots, y_n)$ of $n$ complex variables and their conjugates $\overline{y} = (\overline{y}_1, \ldots, \overline{y}_n)$. So, we will use the ring $\mathbb{C}[x,\overline{x},y,\overline{y}]$ of polynomials in these variables, where a polynomial $p \in \mathbb{C}[x,\overline{x},y,\overline{y}]$ is of the form $p = \sum_{\alpha,\alpha',\beta,\beta' \in \mathbb{N}^n} p_{\alpha,\alpha',\beta,\beta'} x^\alpha \overline{x}^{\alpha'} y^\beta \overline{y}^{\beta'}$ (with finitely many nonzero coefficients) and one can consider the separate degrees in each of $x$, $\overline{x}$, $y$ and $\overline{y}$. For instance, for a matrix $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$, the polynomial $F_M = \langle M, (x \otimes y)(x \otimes y)^* \rangle$ (as in (37) below) is Hermitian and belongs to $\mathbb{C}[x,\overline{x},y,\overline{y}]_{1,1,1,1}$.

## 2.2 The DPS hierarchy for bipartite separable states

We define the hierarchy of semidefinite relaxations, denoted[4] as $\mathrm{DPS}_n^{(t)}$, that were introduced by Doherty, Parrilo and Spedaglieri [DPS02, DPS04] to approximate the cone $\mathrm{SEP}_n$ of separable states (as in (1)). Consider a bipartite state $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$. Assume that $\rho_{AB}$ is separable, i.e., there exist vectors $x_\ell, y_\ell \in \mathbb{S}^{n-1}$ and scalars $\lambda_\ell > 0$, satisfying

$$\rho_{AB} = \sum_{\ell=1}^m \lambda_\ell \; x_\ell x_\ell^* \otimes y_\ell y_\ell^*.$$

For any integer $t \geq 1$, one can define the following "extended state"

$$\rho_{AB[t]} = \sum_{\ell=1}^m \lambda_\ell \; x_\ell x_\ell^* \otimes (y_\ell y_\ell^*)^{\otimes t},$$

obtained by replacing each factor $y_\ell y_\ell^*$ by its $t$-th tensor product $(y_\ell y_\ell^*)^{\otimes t}$. Then, $\rho_{AB[t]}$ belongs to $\mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$ and it satisfies the following conditions. First, it is invariant under permuting

[4] Here, we follow the notation used in [FF20], also for extended states $\rho_{AB[t]}$ and the partial transpose $T_{B[s]}$. In the quantum information literature, the DPS relaxation is also denoted by (a variation of) $\mathrm{PPTBExt}_n^{(t)}$; see, e.g., [GNP25], where the authors refer to the notion of *star-extendibility*, connecting to [ACG+23].

the $t$ B-registers:

$$\begin{aligned}
&(I_n \otimes \Pi_t)\ \rho_{AB[t]}\ (I_n \otimes \Pi_t) = \rho_{AB[t]};\ \text{equivalently,}\ \rho_{AB[t]}\ (I_n \otimes \Pi_t) = \rho_{AB[t]},\\
&\text{i.e., } (\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}} = (\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}^\sigma} \text{ for all } \sigma \in \mathfrak{S}_t,\ i_0, j_0 \in [n],\ \underline{i}, \underline{j} \in [n]^t;\\
&\text{in other words, } \rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n)).
\end{aligned} \tag{25}$$

Second, taking the partial transpose of any subset of the $t$ B-registers preserves positive semidefiniteness (recall (21)). In view of the permutation invariance property (25), one may restrict to taking the partial transpose with respect to the first $s$ B-registers, denoted as $T_{B[s]}$, leading to

$$\rho_{AB[t]}^{T_{B[s]}} \succeq 0 \ \text{ for all } s = 0, 1, \ldots, t. \tag{26}$$

If $s = 0$, then no partial transpose is taken; so, (26) for $s = 0$ amounts to asking $\rho_{AB[t]} \succeq 0$. Finally, if we trace out the last $t - 1$ B-registers, then we recover the initial state $\rho_{AB}$:

$$\mathrm{Tr}_{B[2:t]}(\rho_{AB[t]}) = \rho_{AB}. \tag{27}$$

Now, define the relaxation $\mathrm{DPS}_n^{(t)}$ of order $t$ as

$$\begin{aligned}
\mathrm{DPS}_n^{(t)} = \{\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n) : \exists \rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})\\
\text{satisfying } (25), (26), (27)\}.
\end{aligned} \tag{28}$$

Any $\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$ satisfying (25)-(27) certifies membership of $\rho_{AB}$ in the set $\mathrm{DPS}_n^{(t)}$, we call it a $\mathrm{DPS}^{(t)}$-*certificate* for $\rho_{AB}$.

For $t = 1$, no 'state extension' takes place and $\rho_{AB} \in \mathrm{DPS}_n^{(1)}$ if and only if $\rho_{AB} \succeq 0$ and $\rho_{AB}^{T_B} \succeq 0$; the latter condition is known as the *PPT (positive partial transpose) condition* (see [HHH96, Hor97]). From the above discussion, $\mathrm{SEP}_n \subseteq \mathrm{DPS}_n^{(t)}$ for all $t \geq 1$, and $\mathrm{DPS}_n^{(t+1)} \subseteq \mathrm{DPS}_n^{(t)}$ (since tracing out the last register in a $\mathrm{DPS}^{(t+1)}$-certificate produces a $\mathrm{DPS}^{(t)}$-certificate for $\rho_{AB}$). In [DPS02, DPS04] it is shown that the hierarchy is *complete*; that is,

$$\bigcap_{t \geq 1} \mathrm{DPS}_n^{(t)} = \mathrm{SEP}_n. \tag{29}$$

An alternative proof of completeness, based on the moment approach in polynomial optimization, can be found in [GLS21]. In Section 5, we will recall how this alternative approach also leads to a more economical description of the DPS hierarchy. Also the weaker hierarchy that requires (26) only for $s = 0$ (i.e., $\rho_{AB[t]} \succeq 0$) is complete (see [CKMR07], with a proof based on quantum de Finetti theorems).

Observe that if $\rho_{AB[t]}$ is a $\mathrm{DPS}^{(t)}$-certificate for $\rho_{AB}$, then its complex conjugate $\overline{\rho_{AB[t]}}$ is a $\mathrm{DPS}^{(t)}$-certificate for the conjugate $\overline{\rho_{AB}}$ of $\rho_{AB}$. The next lemma follows then as an easy application.

**Lemma 2.2.** *Assume that $\rho_{AB}$ belongs to $\mathrm{DPS}_n^{(t)}$ with $\mathrm{DPS}_n^{(t)}$-certificate $\rho_{AB[t]}$. Then, its real part $\Re(\rho_{AB}) = \frac{1}{2}(\rho_{AB} + \overline{\rho_{AB}})$ belongs to $\mathrm{DPS}_n^{(t)}$ with real-valued $\mathrm{DPS}_n^{(t)}$-certificate $\Re(\rho_{AB[t]})$.*

Note that the analogous result does *not* hold for $\mathrm{SEP}_n$: while a real-valued separable state $\rho_{AB}$ admits a real-valued $\mathrm{DPS}^{(t)}$-certificate for every $t$, it can be that any separable decomposition $\rho_{AB} = \sum x_\ell x_\ell^* \otimes y_\ell y_\ell^*$ requires some complex atoms $x_\ell, y_\ell \in \mathbb{C}^n \setminus \mathbb{R}^n$. We will see such an example in Section 4.3 (see Remark 4.7).

For Bose symmetric separable states, one can naturally strengthen the DPS hierarchy. We begin with giving a short argument for the description (14) of the set $\mathrm{SEP}_n^{\mathrm{BS}}$.

**Lemma 2.3.** *The set of Bose symmetric separable bipartite states is given by*

$$\mathrm{SEP}_n^{\mathrm{BS}} := \mathrm{SEP}_n \cap \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n) = \mathrm{cone}\{xx^* \otimes xx^* : x \in \mathbb{S}^{n-1}\}.$$

*Proof.* Assume $\rho_{AB} \in \mathrm{SEP}_n \cap \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n)$. Say, $\rho_{AB} = \sum_{\ell=1}^m \lambda_\ell \; x_\ell x_\ell^* \otimes y_\ell y_\ell^*$ for some $\lambda_\ell > 0$ and $x_\ell, y_\ell \in \mathbb{S}^{n-1}$. As $\rho_{AB}$ is Bose symmetric, the vector $e_i \otimes e_j - e_j \otimes e_i$ belongs to the kernel of $\rho_{AB}$ for all $i \neq j \in [n]$. Hence, this vector also belongs to the kernel of $x_\ell x_\ell^* \otimes y_\ell y_\ell^*$ for each $\ell$. This implies that $(x_\ell)_i(y_\ell)_j = (x_\ell)_j(y_\ell)_i$ for all $i \neq j \in [n]$, and thus $x_\ell = \pm y_\ell$ (as both are unit vectors). $\square$

Hence, any separable Bose symmetric state $\rho_{AB} = \sum_\ell \lambda_\ell (x_\ell x_\ell^*)^{\otimes 2}$ admits a $\mathrm{DPS}^{(t)}$-certificate $\rho_{AB[t]} = \sum_\ell \lambda_\ell (x_\ell x_\ell^*)^{\otimes(t+1)}$ satisfying a stronger symmetry property, namely, invariance under permuting *all* $t+1$ registers, including the A-register, instead of just the $t$ B-registers as in relation (25); that is, one may assume $\rho_{AB[t]} \in \mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)}) \simeq \mathrm{Herm}(S^{t+1}(\mathbb{C}^n))$. Note that for any $\rho_{AB[t]} \in \mathrm{BS}((\mathbb{C}^n)^{t+1})$, using the fact that the transpose of a Hermitian positive semidefinite matrix is positive semidefinite, condition (26) is equivalent to

$$\rho_{AB[t]}^{T_{B[s]}} \succeq 0 \quad \text{ for } s = 0, 1, \ldots, \lfloor (t+1)/2 \rfloor. \tag{30}$$

This leads to the (symmetric) variation[5] of the set $\mathrm{DPS}_n^{(t)}$, which we denote $\widetilde{\mathrm{DPS}}_n^{(t)}$, defined by

$$\begin{aligned}\widetilde{\mathrm{DPS}}_n^{(t)} = \{\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n) : \exists \rho_{AB[t]} \in \mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)}) \text{ satisfying (30)} \\ \text{and } \rho_{AB} = \mathrm{Tr}_{B[2:t]}(\rho_{AB[t]})\}.\end{aligned} \tag{31}$$

For any order $t \geq 1$, we have

$$\mathrm{SEP}_n^{\mathrm{BS}} \subseteq \widetilde{\mathrm{DPS}}_n^{(t+1)} \subseteq \widetilde{\mathrm{DPS}}_n^{(t)} \subseteq \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n), \;\; \widetilde{\mathrm{DPS}}_n^{(t)} \subseteq \mathrm{DPS}_n^{(t)} \cap \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n). \tag{32}$$

The right-most inclusion is an equality for $t = 1$ (since no state extension takes place); it remains an open question to show that the inclusion is strict for $t \geq 2$ and $n \geq 5$. Completeness of the DPS hierarchy for $\mathrm{SEP}_n$ (recall (29)) implies completeness of the $\widetilde{\mathrm{DPS}}$ hierarchy for $\mathrm{SEP}_n^{\mathrm{BS}}$:

$$\bigcap_{t \geq 1} \widetilde{\mathrm{DPS}}_n^{(t)} = \mathrm{SEP}_n^{\mathrm{BS}}.$$

Next, we turn to the description of the dual objects for $\mathrm{CP}_n$, $\mathrm{SEP}_n$ and $\mathrm{DPS}_n^{(t)}$, and we will consider the dual of $\widetilde{\mathrm{DPS}}_n^{(t)}$ in Section 4.

## 2.3 Dual cones for $\mathrm{CP}_n$, $\mathrm{SEP}_n$ and $\mathrm{DPS}_n^{(t)}$

The dual cone of the completely positive cone $\mathrm{CP}_n$ is the copositive cone $\mathrm{COP}_n$, defined as

$$\begin{aligned}\mathrm{COP}_n &= \{A \in \mathcal{S}^n : x^T A x \geq 0 \text{ for all } x \in \mathbb{R}^n_+\} \\ &= \{A \in \mathcal{S}^n : (x^{\circ 2})^T A x^{\circ 2} \geq 0 \text{ for all } x \in \mathbb{R}^n\},\end{aligned} \tag{33}$$

where $x^{\circ 2} = x \circ x = (x_i^2)_{i=1}^n$ for $x \in \mathbb{R}^n$. So, any matrix $A \in \mathcal{S}^n$ defines a homogeneous $n$-variate polynomial with degree 4,

$$f_A = (x^{\circ 2})^T A x^{\circ 2} = \sum_{i,j=1}^n x_i^2 x_j^2 A_{ij} \in \mathbb{R}[x]_4, \tag{34}$$

[5] This relaxation corresponds to the set $\mathrm{PPTBExt}_n^{K_{t+1}}$ from [GNP25, Section 8.2], consisting of the $K_{t+1}$-*PPT bosonic extendible states*, corresponding to *complete graph extendibility* in [ACG+23].

and this polynomial is globally nonnegative precisely when $A$ is a copositive matrix. A sufficient condition for $f_A$ to be globally nonnegative is when the polynomial $\|x\|^{2t} f_A$ is sos for some integer $t \geq 0$. Motivated by this, Parrilo [Par00] and de Klerk and Pasechnik [dKP02] define the cones

$$\mathcal{K}_n^{(t)} = \big\{ A \in \mathcal{S}^n : \|x\|^{2t} f_A = \|x\|^{2t} \cdot (x^{\circ 2})^T A x^{\circ 2} \text{ is sos} \big\}. \tag{35}$$

These cones form a hierarchy of semidefinite inner approximations for $\mathrm{COP}_n$ and satisfy

$$\mathcal{K}_n^{(t)} \subseteq \mathcal{K}_n^{(t+1)} \subseteq \mathrm{COP}_n, \quad \mathrm{int}(\mathrm{COP}_n) \subseteq \bigcup_{t\geq 0} \mathcal{K}_n^{(t)} \subseteq \mathrm{COP}_n,$$

where the inclusion $\mathrm{int}(\mathrm{COP}_n) \subseteq \bigcup_{t\geq 0} \mathcal{K}_n^{(t)}$ follows from Reznick [Rez95]. As a consequence, the dual cones $(\mathcal{K}_n^{(t)})^*$ form a complete hierarchy of semidefinite outer approximations for $\mathrm{CP}_n$, i.e.,

$$\mathrm{CP}_n \subseteq (\mathcal{K}_n^{(t+1)})^* \subseteq (\mathcal{K}_n^{(t)})^*, \quad \mathrm{CP}_n = \bigcap_{t\geq 0} (\mathcal{K}_n^{(t)})^*. \tag{36}$$

Here are some known facts about the cones $\mathcal{K}_n^{(t)}$ and their duals, as background information. For $t = 0$, we have $(\mathcal{K}_n^{(0)})^* = \mathcal{S}_+^n \cap \mathbb{R}_+^{n\times n}$. Hence, $(\mathcal{K}_n^{(0)})^*$ consists of the matrices that are positive semidefinite and entrywise nonnegative, known as *doubly nonnegative* matrices. Equivalently, $\mathcal{K}_n^{(0)}$ consists of the matrices that can be written as sum of a positive semidefinite matrix and an entrywise nonnegative matrix (see [Par00, dKP02]). For $n \leq 4$, equality $\mathrm{CP}_n = (\mathcal{K}_n^{(0)})^*$ holds, or, equivalently, $\mathrm{COP}_n = \mathcal{K}_n^{(0)}$ [Dia62]. For $n \geq 5$, the inclusion $\mathcal{K}_n^{(t)} \subseteq \mathrm{COP}_n$ is strict for any $t \geq 0$ [DDGH13]. Moreover, equality $\bigcup_{t\geq 0} \mathcal{K}_5^{(t)} = \mathrm{COP}_5$ holds [SV24] and the inclusion $\bigcup_{t\geq 0} \mathcal{K}_n^{(t)} \subseteq \mathrm{COP}_n$ is strict for $n \geq 6$ [LV23].

We now turn to the dual cone of the separable cone $\mathrm{SEP}_n$. For a matrix $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$, consider the associated polynomial $F_M$ in $2n$ complex variables $x = (x_1, \dots, x_n)$, $y = (y_1, \dots, y_n)$ and their conjugates $\overline{x} = (\overline{x}_1, \dots, \overline{x}_n)$, $\overline{y} = (\overline{y}_1, \dots, \overline{y}_n)$, defined as

$$F_M = \langle M, (x \otimes y)(x \otimes y)^* \rangle = \langle M, xx^* \otimes yy^* \rangle \in \mathbb{C}[x, \overline{x}, y, \overline{y}]_{1,1,1,1}. \tag{37}$$

Then, the dual of $\mathrm{SEP}_n$ is defined as

$$\mathrm{SEP}_n^* = \{ M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n) : F_M = (x \otimes y)^* M (x \otimes y) \geq 0 \ \forall x, y \in \mathbb{C}^n \}. \tag{38}$$

Note indeed that, since $F_M$ is homogeneous (of degree 1) in each of $x, \overline{x}, y, \overline{y}$, $F_M$ is globally nonnegative if and only if $F_M$ is nonnegative on the bi-sphere $\mathbb{S}^{n-1} \times \mathbb{S}^{n-1}$.

Any nonzero matrix $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ provides a hyperplane in the space $\mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$, with normal $M$. The corresponding half-space, consisting of the states $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ satisfying $\langle M, \rho_{AB} \rangle \geq 0$, contains $\mathrm{SEP}_n$ precisely when $M \in \mathrm{SEP}_n^*$. For this reason, $M$ is also called an *entanglement witness* since it separates some entangled states, i.e., $\langle M, \rho_{AB} \rangle < 0$ for some $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n) \setminus \mathrm{SEP}_n$.

A sufficient condition for $F_M$ to be globally nonnegative is when the polynomial $\|y\|^{2t} F_M$ is r-sos for some integer $t \geq 0$. Fang and Fawzi [FF20] characterize the matrices $M$ satisfying this property for a given order $t$ and show that this corresponds precisely to the dual of the DPS hierarchy. To state their result, let $\mathcal{W}_{n,s}^{(t)}$ denote the set of matrices satisfying condition (26) for given $s$, i.e.,

$$\mathcal{W}_{n,s}^{(t)} = \{ \rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}) : \rho_{AB[t]}^{T_{B[s]}} \succeq 0 \} \quad \text{for } s = 0, 1, \dots, t. \tag{39}$$

**Theorem 2.4.** *[FF20] Consider a matrix $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ and an integer $t \geq 1$. The following assertions are equivalent.*

*(i)* $M \in (\mathrm{DPS}_n^{(t)})^*$.

*(ii)* *The polynomial* $\|y\|^{2(t-1)} F_M \in \mathbb{C}[x, \overline{x}, y, \overline{y}]_{1,1,2t,2t}$ *is r-sos.*

*(iii)* *There exist matrices* $B, W_0, W_1, \ldots, W_t \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$ *such that*

$$M \otimes I_n^{\otimes(t-1)} = B + \sum_{s=0}^{t} W_s$$

*with* $B \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))^\perp$ *and* $W_s \in \mathcal{W}_{n,s}^{(t)}$ *for* $s = 0, 1, \ldots, t$.

Note the analogy between the description of the approximation hierarchy $\mathcal{K}_n^{(t)}$ for the copositive cone $\mathrm{COP}_n$ and the approximation hierarchy $(\mathrm{DPS}_n^{(t)})^*$ for the dual separable cone $\mathrm{SEP}_n^*$; in particular, compare relation (35) and Theorem 2.4(ii). As we will see in Section 4, there is a formal relationship between these objects, which can be shown when restricting to Bose symmetric states.

### 2.4 Diagonal unitary invariant states

We return to the class of CLDUI states. Recall the two equivalent characterizations through the invariance property (2) and through the sparsity pattern (5). Following [JM19], we now consider a third characterization via the projection[6] $\Pi_{\mathrm{CLDUI}_n} : \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n) \to \mathrm{CLDUI}_n$ given by

$$\Pi_{\mathrm{CLDUI}_n}(\rho_{AB}) = \int_{\mathcal{DU}_n} (U \otimes \overline{U}) \rho_{AB} (U \otimes \overline{U})^* dU, \tag{40}$$

where we integrate with regards to the Haar measure. Since this integration can be seen as forming the group average of the operation in (2), this map is indeed the projection onto the $\mathrm{CLDUI}_n$ subspace. Now, clearly we have

$$\rho_{AB} \in \mathrm{CLDUI}_n \iff \Pi_{\mathrm{CLDUI}_n}(\rho_{AB}) = \rho_{AB}.$$

Two easy but important properties of this projection, collected in the next lemma, are that it preserves positive semidefiniteness and separability.

**Lemma 2.5.** *If* $\rho_{AB}$ *is positive semidefinite (resp., separable), then* $\Pi_{\mathrm{CLDUI}}(\rho_{AB})$ *is positive semidefinite (resp., separable).*

*Proof.* If $\rho_{AB} \succeq 0$, then $\Pi_{\mathrm{CLDUI}}(\rho_{AB}) \succeq 0$ because it is block-diagonal with its diagonal blocks being equal to certain selected principal submatrices of $\rho_{AB}$ (see relation (10)). Given $x, y \in \mathbb{C}^n$, we now show that $\Pi_{\mathrm{CLDUI}}(xx^* \otimes yy^*)$ is separable, using (40). For any $U \in \mathcal{DU}_n$, we have

$$(U \otimes \overline{U})(xx^* \otimes yy^*)(U \otimes \overline{U})^* = Ux(Ux)^* \otimes \overline{U}y(\overline{U}y)^* \in \mathrm{SEP}_n.$$

Since integration can be seen as a limit of finite sums and $\mathrm{SEP}_n$ is a closed cone, it follows that $\Pi_{\mathrm{CLDUI}}(xx^* \otimes yy^*) \in \mathrm{SEP}_n$. □

The projection $\Pi_{\mathrm{CLDUI}}$ also allows to connect two different ways of characterizing the cone of pairwise completely positive matrices, as done in [JM19].

[6] This map is also known as the CLDUI-twirling, see, e.g., [GNP25].

**Theorem 2.6.** *[JM19] Let* $(X, Y) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$ *and assume that* $\mathrm{diag}(X) = \mathrm{diag}(Y)$*. Then,* $(X, Y) \in \mathrm{PCP}_n$ *(i.e., the associated CLDUI matrix* $\rho_{(X,Y)}$ *belongs to* $\mathrm{SEP}_n$*) if and only if*

$$(X, Y) \in \mathrm{cone}\{((x \circ \overline{x})(y \circ \overline{y})^*, (x \circ y)(x \circ y)^*) : x, y \in \mathbb{C}^n\}. \tag{41}$$

*Proof.* The underlying key fact is that, for any $x, y \in \mathbb{C}^n$ and $i, j \in [n]$, we have

$$\begin{aligned}(xx^* \otimes yy^*)_{ij,ij} &= x_i\overline{x}_i y_j\overline{y}_j = ((x \circ \overline{x})(y \circ \overline{y})^*)_{i,j},\\ (xx^* \otimes yy^*)_{ii,jj} &= x_i\overline{x}_j y_i\overline{y}_j = ((x \circ y)(x \circ y)^*)_{ii,jj}.\end{aligned} \tag{42}$$

Assume $(X, Y) \in \mathrm{PCP}_n$, i.e., $\rho_{(X,Y)} \in \mathrm{SEP}_n$. Then, $\rho_{(X,Y)} = \sum_{\ell=1}^m x_\ell x_\ell^* \otimes y_\ell y_\ell^*$ for some $x_\ell, y_\ell \in \mathbb{C}^n$. Using relation (8) combined with (42), we obtain

$$X = \sum_{\ell=1}^m (x_\ell \circ \overline{x}_\ell)(y_\ell \circ \overline{y}_\ell)^*, \ Y = \sum_{\ell=1}^m (x_\ell \circ y_\ell)(x_\ell \circ y_\ell)^*, \tag{43}$$

as desired. Conversely, assume that (43) holds for some $x_\ell, y_\ell \in \mathbb{C}^n$. Then, using relations (5), (8) and (42), we obtain that $\Pi_{\mathrm{CLDUI}_n}(\sum_{l=1}^m x_l x_l^* \otimes y_l y_l^*) = \rho_{(X,Y)}$. Since the projection preserves separability (by Lemma 2.5), this shows $\rho_{(X,Y)} \in \mathrm{SEP}_n$ and thus $(X, Y) \in \mathrm{PCP}_n$, as desired. $\square$

The alternate characterization (41), which is in fact the original definition of $\mathrm{PCP}_n$ in [JM19], further illustrates the connection between the two cones $\mathrm{PCP}_n$ and $\mathrm{CP}_n$. Clearly, every completely positive matrix is both entrywise nonnegative and positive semidefinite. These two properties are now 'split up' between the two arguments of a pairwise completely positive matrix tuple:

$$(X, Y) \in \mathrm{PCP}_n \Longrightarrow X \geq 0 \text{ and } Y \succeq 0,$$

which follows from relation (41). Another necessary condition for $(X, Y) \in \mathrm{PCP}_n$ is

$$|Y_{ij}|^2 \leq X_{ij}X_{ji} \ \text{ for all } i, j \in [n] \tag{44}$$

(coined in [JM19] as "$X$ is almost entrywise larger then $Y$"). Johnston and MacLean [JM19] show this using the description (41) of $\mathrm{PCP}_n$ (and Cauchy-Schwartz inequality). Alternatively, one can show it at the 'state level' since $(X, Y) \in \mathrm{PCP}_n$ if and only if $\rho_{(X,Y)} \in \mathrm{SEP}_n$. This implies $\rho_{(X,Y)}^{T_B} = \rho_{(X,\cdot,Y)} \succeq 0$, which, by relation (10), gives (44) (and $X \geq 0$, $Y \succeq 0$).

The above results and arguments can analogously be cast for the LDUI and LDOI cases. The corresponding projections are given by

$$\Pi_{\mathrm{LDUI}_n}(\rho_{AB}) = \int_{\mathcal{DU}_n} (U \otimes U)\rho_{AB}(U \otimes U)^* dU, \tag{45}$$

$$\Pi_{\mathrm{LDOI}_n}(\rho_{AB}) = \frac{1}{2^n} \sum_{O\in\mathcal{DO}_n} (O \otimes O)\rho_{AB}(O \otimes O)^*. \tag{46}$$

Note that the identity $(\Pi_{\mathrm{CLDUI}_n}(\rho_{AB}))^{T_B} = \Pi_{\mathrm{LDUI}_n}(\rho_{AB}^{T_B})$ indeed holds. Moreover, as $|\mathcal{DO}_n| = 2^n$, the projection onto the $\mathrm{LDOI}_n$ subspace is given by a finite sum.

**Remark 2.7.** *Also for the projections onto the* $\mathrm{CLDUI}_n$ *and* $\mathrm{LDUI}_n$ *subspaces, one could replace the integral over* $\mathcal{DU}_n$ *by a finite sum over a suitably selected finite subset. This follows from a general result by Tchakaloff [Tch57], but can also be easily derived directly as indicated below.*

*For $k \in [n-1]$ let $U_k \in \mathcal{DU}_n$ be the diagonal matrix with entry $\mathbf{i} = \sqrt{-1} \in \mathbb{C}$ at position $(k,k)$ and entry 1 at every other diagonal position. Then, one can easily verify the identities*

$$\begin{aligned} \Pi_{\mathrm{CLDUI}_n}(\rho_{AB}) &= \frac{1}{n-1}\sum_{k=1}^{n-1}(U_k \otimes \overline{U}_k)\rho_{AB}(U_k \otimes \overline{U}_k)^*, \\ \Pi_{\mathrm{LDUI}_n}(\rho_{AB}) &= \frac{1}{n-1}\sum_{k=1}^{n-1}(U_k \otimes U_k)\rho_{AB}(U_k \otimes U_k)^*. \end{aligned} \tag{47}$$

Following [SN21], we have the following alternative characterization for the cone $\mathrm{TCP}_n$, whose proof is analogous to that of Theorem 2.6.

**Theorem 2.8.** *[SN21] Let $(X,Y,Z) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \times \mathrm{Herm}^n$ with $\mathrm{diag}(X) = \mathrm{diag}(Y) = \mathrm{diag}(Z)$. Then, $(X,Y,Z) \in \mathrm{TCP}_n$ (i.e., the associated LDOI matrix $\rho_{(X,Y,Z)}$ belongs to $\mathrm{SEP}_n$) if and only if*

$$(X,Y,Z) \in \mathrm{cone}\{((x\circ\overline{x})(y\circ\overline{y})^*, (x\circ y)(x\circ y)^*, (x\circ\overline{y})(x\circ\overline{y})^*) : x,y \in \mathbb{C}^n\}. \tag{48}$$

**Lemma 2.9.** *[SN21] If $(X,Y,Z) \in \mathrm{TCP}_n$, then $(X,Y),(X,Z) \in \mathrm{PCP}_n$.*

Here too, the proof can be done, either on the 'matrix level' and using the decomposition in (48) (following [SN21]), or on the 'state level' and applying the projections $\Pi_{\mathrm{CLDUI}_n}$ and $\Pi_{\mathrm{LDUI}_n}$ to $\rho_{(X,Y,Z)}$. Finally, we restate the links between the cones $\mathrm{CP}_n$, $\mathrm{PCP}_n$ (from [JM19]) and $\mathrm{TCP}_n$ (from [SN21]), mentioned earlier in (13), together with a short proof.

**Lemma 2.10.** *[SN21] For a matrix $X \in \mathcal{S}^n$, we have*

$$X \in \mathrm{CP}_n \Longleftrightarrow (X,X) \in \mathrm{PCP}_n \Longleftrightarrow (X,X,X) \in \mathrm{TCP}_n.$$

*Proof.* The implication $(X,X,X) \in \mathrm{TCP}_n \Longrightarrow (X,X) \in \mathrm{PCP}_n$ follows from Lemma 2.9. The implication $X \in \mathrm{CP}_n \Longrightarrow (X,X,X) \in \mathrm{TCP}_n$ follows from the fact that, if $X = aa^T$ for some nonnegative $a \in \mathbb{R}^n_+$, then, setting $x = y = \sqrt{a}$ (entrywise) provides a decomposition showing $(X,X,X) \in \mathrm{TCP}_n$ (using the characterization in Theorem 2.8). Finally, assume $(X,X) \in \mathrm{PCP}_n$; we show $X \in \mathrm{CP}_n$. As $(X,X) \in \mathrm{PCP}_n$, we have $\rho_{(X,X)} \in \mathrm{SEP}_n$, implying $\rho_{(X,\cdot,X)} = \rho_{(X,X)}^{T_B} \in \mathrm{SEP}_n$. Since $\rho_{(X,\cdot,X)}$ is in addition Bose symmetric it admits a symmetric separable decomposition, of the form $\sum_\ell x_\ell x_\ell^* \otimes x_\ell x_\ell^*$ for some $x_\ell \in \mathbb{C}^n$ (Lemma 2.3). From this follows that $X = \sum_\ell a_\ell a_\ell^T$, where we set $a_\ell = (|(x_\ell)_i|^2)_{i=1}^n \in \mathbb{R}^n_+$, thus showing $X \in \mathrm{CP}_n$. □

**Remark 2.11.** *Observe that any separable state of the form $\rho_{(X,X,X)}$ admits a real separable decomposition, i.e., involving only real vectors. This follows as a byproduct of the above proof: If $\rho_{(X,X,X)} \in \mathrm{SEP}_n$, then $X \in \mathrm{CP}_n$ and thus $X = \sum_\ell a_\ell a_\ell^T$ for some $a_\ell \in \mathbb{R}^n_+$. Setting $x_\ell = (\sqrt{(a_\ell)_i})_{i=1}^n \in \mathbb{R}^n$, we obtain $\rho_{(X,X,X)} = \Pi_{\mathrm{LDOI}_n}(\sum_\ell x_\ell x_\ell^* \otimes x_\ell x_\ell^*)$. Combined with the fact that the projection $\Pi_{\mathrm{LDOI}_n}$ can be formulated as an average by real-valued matrices (see (46)), we obtain a separable decomposition by real vectors, as desired. This argument does not extend to the CLDUI or LDUI cases, since then the averaging is by complex-valued matrices (see (45), (47)). Indeed, in Section 4.3 (see Remark 4.7), one can see a real-valued separable CLDUI state of the form $\rho_{(X,X)}$ that does not admit a real separable decomposition.*

### 2.5 Dual cone of $\mathrm{PCP}_n$

As $\mathrm{PCP}_n$ is a cone in $\mathbb{R}^{n\times n} \times \mathrm{Herm}^n$, its dual cone is defined as

$$\mathrm{PCP}_n^* = \{(S,T) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n : \langle (S,T),(X,Y)\rangle \geq 0 \text{ for all } (X,Y) \in \mathrm{PCP}_n\},$$

where $\langle (S,T),(X,Y)\rangle = \langle S,X\rangle + \langle T,Y\rangle$ is the standard inner product in the product space. In order to define the dual of $\mathrm{PCP}_n$ at the 'state level' we make the following definition.

**Definition 2.12.** *Given a pair $(S,T) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$, define the following matrix*

$$M_{S,T} = \sum_{i,j=1}^{n} S_{ij} e_i e_i^* \otimes e_j e_j^* + \sum_{i,j=1}^{n} T_{ij} e_j e_i^* \otimes e_j e_i^* \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n). \tag{49}$$

So, $M_{S,T} \in \mathrm{CLDUI}_n$ by construction. Given a pair $(X,Y) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$ with $\mathrm{diag}(X) = \mathrm{diag}(Y)$, recall from (10) the associated bipartite state $\rho_{(X,Y)} \in \mathrm{CLDUI}_n$, defined as

$$\rho_{(X,Y)} = \sum_{i,j=1}^{n} X_{ij} e_i e_i^* \otimes e_j e_j^* + \sum_{i,j=1, i\neq j}^{n} Y_{ij} e_i e_j^* \otimes e_i e_j^* \in \mathrm{CLDUI}_n. \tag{50}$$

Then, one can easily verify that

$$\langle M_{S,T}, \rho_{(X,Y)}\rangle = \langle S,X\rangle + \langle T,Y\rangle = \langle (S,T),(X,Y)\rangle. \tag{51}$$

Moreover, one can verify the following polynomial identity:

$$\langle M_{S,T}, xx^* \otimes yy^*\rangle = \langle S, (x\circ\overline{x})(y\circ\overline{y})^*\rangle + \langle T, (x\circ y)(x\circ y)^*\rangle. \tag{52}$$

The characterization of the dual cone $\mathrm{PCP}_n^*$ now follows easily.

**Lemma 2.13.** *For a pair $(S,T) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$, $(S,T) \in \mathrm{PCP}_n^*$ if and only if $M_{S,T} \in \mathrm{SEP}_n^*$, i.e., the polynomial $\langle M_{S,T}, xx^* \otimes yy^*\rangle$ is globally nonnegative.*

*Proof.* By combining (52) and the characterization (41) of $\mathrm{PCP}_n$, it follows that the polynomial $\langle M_{S,T}, xx^* \otimes yy^*\rangle$ is globally nonnnegative (i.e., $M_{S,T} \in \mathrm{SEP}_n^*$) if and only $(S,T) \in \mathrm{PCP}_n^*$. ☐

**Remark 2.14.** *Note that the matrix $M_{S,T}$ in (49) remains unchanged under redistributing diagonal entries between $S$ and $T$, i.e., $M_{S,T} = M_{S+D,T-D}$ for any diagonal matrix $D$. Recall the notation $D_T = \mathrm{Diag}(\mathrm{diag}(T))$ for any square matrix $T$. By replacing $(S,T)$ by $(S+D,T-D)$ with $D = (D_T - D_S)/2$, one can assume that $S$ and $T$ have the same diagonal. Moreover, by replacing $(S,T)$ by $(S+D_T, T-D_T)$, one can move all diagonal entries to the first argument, in which case one gets $M_{S,T} = M_{S+D_T,T-D_T} = \rho_{(S+D_T,T^T+D_S)}$ and*

$$\rho_{(A,B)} = M_{A,B^T-D_B} \text{ for any } (A,B) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \text{ with } \mathrm{diag}(A) = \mathrm{diag}(B). \tag{53}$$

*We find it more convenient to keep the notation $M_{S,T}$ that can be freely used for* any *$S,T$ and permits to distinguish between the primal side (where states $\rho_{(X,Y)}$ live) and the dual side (where matrices $M_{S,T}$ live). We now compare the cone $\mathrm{PCP}_n^*$ with the cone $\mathrm{PCOP}_n$ (of* pairwise copositive matrices*) recently introduced in [GNP25, Def. 3.1].*

*As in [GNP25], set $\mathbb{R}^{n\times n} \times_{\mathbb{R}^n} \mathrm{Herm}^n = \{(A,B) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n : \mathrm{diag}(A) = \mathrm{diag}(B)\}$. Then, $\mathrm{PCOP}_n$ is defined as the set of matrix pairs $(A,B) \in \mathbb{R}^{n\times n} \times_{\mathbb{R}^n} \mathrm{Herm}^n$ for which the polynomial $\langle A, (x\circ\overline{x})(y\circ\overline{y})^*\rangle + \langle B - D_B, (x\circ y)(x\circ y)^*\rangle$ is globally nonnegative. Hence, we have*

$$(A,B) \in \mathrm{PCOP}_n \Longleftrightarrow M_{A,B-D_B} \in \mathrm{SEP}_n^*, \quad \textit{i.e.,} \quad (A, B - D_B) \in \mathrm{PCP}_n^*.$$

*In [GNP25, Prop. 3.2] it is shown that* $\mathrm{PCOP}_n$ *is the dual of* $\mathrm{PCP}_n$*. The (minor) difference with our setting is that the dual is taken with respect to the variation of the standard inner product, where the diagonal entries are 'counted only once'; that is, defining the scalar product of two matrix pairs* $(A,B),(A',B') \in \mathbb{R}^{n\times n} \times_{\mathbb{R}^n} \mathrm{Herm}^n$ *as* $\langle A, A'\rangle + \langle B - D_B, B' - D_{B'}\rangle$*.*

Here are some basic results about $\mathrm{PCP}_n^*$ (also mentioned in [GNP25]) that we will need later.

**Lemma 2.15.** *(i) If* $(X,Y) \in \mathrm{PCP}_n$*, then* $(X^T, Y^T) \in \mathrm{PCP}_n$*.*

*(ii) If* $(S,T) \in \mathrm{PCP}_n^*$*, then* $(S^T, T^T) \in \mathrm{PCP}_n^*$*.*

*(iii) If* $(S,T) \in \mathrm{PCP}_n^*$*, then* $S + S^T + T + T^T \in \mathrm{COP}_n$*.*

*Proof.* (i),(ii) follow using the definitions. For (iii), note that $(S,T) \in \mathrm{PCP}_n^*$ implies that the polynomial in (52) is globally nonnegative; by evaluating it at $y = \overline{x}$, one gets the desired result. ☐

**Lemma 2.16.** *(i) If* $(S,T) \in \mathrm{PCP}_n^*$*, then* $S_{ij} + S_{ji} \geq 0$ *(for* $i \neq j \in [n]$*) and* $S_{ii} + T_{ii} \geq 0$ *(for* $i \in [n]$*).*

*(ii) Let* $S \in \mathbb{C}^{n\times n}$*. Then,* $(S,S) \in \mathrm{PCP}_n^* \iff S \in \mathcal{S}^n \cap \mathbb{R}_+^{n\times n}$*.*

*Proof.* (i) follows by taking the inner product of $(S,T)$ with the matrix pairs $(e_ie_j^* + e_je_i^*, 0)$ and $(e_ie_i^*, e_ie_i^*)$ that both belong to $\mathrm{PCP}_n$. We show (ii). If $(S,S) \in \mathrm{PCP}_n^*$, then $S$ is symmetric (since real, Hermitian) and $S \geq 0$ by (i). Conversely, assume $S \in \mathcal{S}^n$ and $S \geq 0$. For $(X,Y) \in \mathrm{PCP}_n$,

$$\langle (S,S), (X,Y)\rangle = \sum_{i=1}^n S_{ii}(X_{ii} + Y_{ii}) + \sum_{1\leq i<j\leq n} S_{ij}(X_{ij} + X_{ji} + Y_{ij} + Y_{ji}).$$

The first sum is nonnegative since $S, X \geq 0$ and $\mathrm{diag}(Y) = \mathrm{diag}(X)$. Also the second sum is nonnnegative: by (44), we have $\mathrm{Re}(Y_{ij})^2 \leq |Y_{ij}|^2 \leq X_{ij}X_{ji}$, implying $\mathrm{Re}(Y_{ij}) \geq -\sqrt{X_{ij}X_{ji}}$ and thus $X_{ij} + X_{ji} + Y_{ij} + Y_{ji} = X_{ij} + X_{ji} + 2\mathrm{Re}(Y_{ij}) \geq (\sqrt{X_{ij}} - \sqrt{X_{ji}})^2 \geq 0$. So, $(S,S) \in \mathrm{PCP}_n^*$. ☐

More results about the cone $\mathrm{PCOP}_n$ can be found in [GNP25]. In particular, it is shown in [GNP25, Theorem 3.9, Corollary 3.10] that, for a pair $(A,B) \in \mathbb{R}^{n\times n} \times_{\mathbb{R}^n} \mathrm{Herm}^n$, $A \geq 0$ and $\tilde{A} + \mathrm{Re}(U^*(B - D_B)U) \in \mathrm{COP}_n$ for all $U \in \mathcal{DU}_n$ implies $(A,B) \in \mathrm{PCOP}_n$, after setting $\tilde{A} = (\sqrt{A_{ij}A_{ji}})_{i,j=1}^n$. Moreover, this implication holds as an equivalence if $A$ is real symmetric. In addition, when $B$ is real symmetric, it suffices to consider real-valued $U \in \mathcal{DU}_n$ in the previous claim.

# 3 The DPS hierarchy for diagonal unitary invariant states

In this section we investigate how to adapt the DPS hierarchy for bipartite states having some diagonal unitary invariance, with the aim of obtaining more economical relaxations. We first focus on the class $\mathrm{CLDUI}_n$ and then indicate how the results easily extend to the classes $\mathrm{LDUI}_n$, $\mathrm{LDOI}_n$.

## 3.1 An extended sparsity pattern for DPS certificates of CLDUI states

Here, we show that any separable bipartite state $\rho_{AB} \in \mathrm{CLDUI}_n$ admits a $\mathrm{DPS}^{(t)}$-certificate that enjoys invariance and sparsity properties inherited from those of the state $\rho_{AB}$. For this, for an integer $t \geq 1$, define the set

$$\begin{aligned}\mathrm{CLDUI}_n^{(t)} = \{&\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}) : \\ &\rho_{AB[t]} = (U \otimes \overline{U}^{\otimes t})\rho_{AB[t]}(U \otimes \overline{U}^{\otimes t})^* \ \forall U \in \mathcal{DU}_n\}\end{aligned} \tag{54}$$

and let $\Pi_{\mathrm{CLDUI}_n^{(t)}}$ denote the projection onto $\mathrm{CLDUI}_n^{(t)}$. So, for $t = 1$, we recover $\mathrm{CLDUI}_n$ and, for $t \geq 1$, the definition follows the analogous recipe, motivated by the fact that the $t$ copies of the B-register should all be treated in the same way (in order to preserve invariance under any permutation of these $t$ registers).

Our aim is to prove the following result, which claims that any state in $\mathrm{CLDUI}_n \cap \mathrm{DPS}_n^{(t)}$ admits a $\mathrm{DPS}^{(t)}$-certificate in $\mathrm{CLDUI}_n^{(t)}$ and after that we will see that such certificate enjoys a block-diagonal structure.

**Theorem 3.1.** *Assume that $\rho_{AB} \in \mathrm{DPS}_n^{(t)}$ with $\mathrm{DPS}^{(t)}$-certificate $\rho_{AB[t]}$. Then, $\Pi_{\mathrm{CLDUI}_n}(\rho_{AB}) \in \mathrm{DPS}_n^{(t)}$ with $\mathrm{DPS}^{(t)}$-certificate $\Pi_{\mathrm{CLDUI}_n^{(t)}}(\rho_{AB[t]})$. Therefore, if $\rho_{AB} \in \mathrm{CLDUI}_n$, then $\rho_{AB}$ admits a $\mathrm{DPS}^{(t)}$-certificate that belongs to $\mathrm{CLDUI}_n^{(t)}$.*

In order to prove Theorem 3.1 we first collect structural results about the set $\mathrm{CLDUI}_n^{(t)}$. Recall from relation (5) that $\rho_{AB} \in \mathrm{CLDUI}_n$ if and only if $\mathrm{supp}(\rho_{AB}) \subseteq \Omega_n$. As in the case $t = 1$, the set $\mathrm{CLDUI}_n^{(t)}$ allows for alternate descriptions through its sparsity pattern and the associated projection. For this, we now define the following 'extended' sparsity pattern:

$$\Omega_n^{(t)} = \{(i_0\underline{i}, j_0\underline{j}) \in [n]^{t+1} \times [n]^{t+1} : \{i_0\underline{j}\} = \{j_0\underline{i}\}, \text{ i.e., } \alpha(i_0\underline{j}) = \alpha(j_0\underline{i})\}. \tag{55}$$

For $\underline{i} \in [n]^t$, recall that $\alpha(\underline{i}) \in \mathbb{N}^n$, with $k$-th entry the number of occurrences of $k$ in the multiset $\{\underline{i}\} = \{i_1, \ldots, i_t\}$. So, $\alpha(i_0\underline{j}) = e_{i_0} + \alpha(\underline{j})$. Setting $t = 1$ recovers the original set $\Omega_n$, i.e., we have

$$\Omega_n^{(1)} = \{(ij, kl) \in [n]^2 \times [n]^2 : \{il\} = \{jk\}\} = \Omega_n.$$

Moreover, as in the case $t = 1$ (Remark 2.7), in definition (54) it suffices to require invariance under a finite subset of $\mathcal{DU}_n$.

**Lemma 3.2.** *Let $\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$. Then, the following assertions are equivalent.*

*(i)* $\rho_{AB[t]} \in \mathrm{CLDUI}_n^{(t)}$, *i.e.*, $\rho_{AB[t]} = (U \otimes \overline{U}^{\otimes t})\rho_{AB[t]}(U \otimes \overline{U}^{\otimes t})^*$ *for* $U \in \mathcal{DU}_n$.

*(ii)* $\rho_{AB[t]} = (U_k \otimes \overline{U_k}^{\otimes t})\rho_{AB[t]}(U_k \otimes \overline{U_k}^{\otimes t})^*$ *for all $k \in [n-1]$, where $U_k$ is the diagonal matrix with $(U_k)_{k,k} = \omega$ and all other diagonal entries equal to 1, and we set*[7] $\omega := e^{\frac{2\pi \mathbf{i}}{t+2}}$.

*(iii)* $\mathrm{supp}(\rho_{AB[t]}) \subseteq \Omega_n^{(t)}$.

*Proof.* The implication (i) $\Longrightarrow$ (ii) is obvious. Assume (ii) holds, we show (iii). First, note that for any $U \in \mathcal{DU}_n$ with $u = \mathrm{diag}(U)$, and any index pair $(i_0\underline{i}, j_0\underline{j}) \in [n]^{t+1} \times [n]^{t+1}$, by (16), one has

$$\begin{aligned} ((U \otimes \overline{U}^{\otimes t})\rho_{AB[t]}(U \otimes \overline{U}^{\otimes t})^*)_{i_0\underline{i}, j_0\underline{j}} &= (\rho_{AB[t]})_{i_0\underline{i}, j_0\underline{j}} \cdot u_{i_0}\overline{u}_{i_1} \ldots \overline{u}_{i_t}\overline{u}_{j_0}u_{j_1} \ldots u_{j_t} \\ &= (\rho_{AB[t]})_{i_0\underline{i}, j_0\underline{j}} \cdot u^{\alpha(i_0\underline{j})}\overline{u}^{\alpha(j_0\underline{i})}. \end{aligned} \tag{56}$$

Consider an index pair $(i_0\underline{i}, j_0\underline{j}) \notin \Omega_n^{(t)}$. Then, $\alpha(i_0\underline{j})_k \neq \alpha(j_0\underline{i})_k$ for some index $k$ that can be chosen in $[n-1]$ since $|\alpha(i_0\underline{j})| = |\alpha(j_0\underline{i})|$. W.l.o.g. we may assume $\ell := \alpha(j_0\underline{i})_k - \alpha(i_0\underline{j})_k > 0$. Moreover, $\ell \leq t + 1$ (since $|\alpha(j_0\underline{i})| = t + 1$). Note that this implies that $\omega^\ell \neq 1$. Now, we apply (56) to the

[7]Alternatively, one could choose $\omega = e^{\frac{2\pi \mathbf{i}}{\lambda}}$ for some $\lambda \in \mathbb{R} \setminus \mathbb{Q}$, which would give a finite representation independent of the parameter $t$.

matrix $U = U_k$; then, the value in (56) is equal to $(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}} \cdot \omega^{\alpha(i_0\underline{j})_k - \alpha(j_0\underline{i})_k} = (\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}} \cdot \omega^\ell$, which is equal to $(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}}$ only if $(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}} = 0$, since $\omega^\ell \neq 1$. So, (iii) holds.

Finally, assume (iii) holds, we show (i). In view of (56) it suffices to show that the value in (56) is equal to $(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}}$ when $(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}} \neq 0$. But, then, $(i_0\underline{i}, j_0\underline{j}) \in \Omega_n^{(t)}$, which gives $\alpha(i_0\underline{i}) = \alpha(j_0\underline{i})$ and thus $u^{\alpha(i_0\underline{j})}\overline{u}^{\alpha(j_0\underline{i})} = 1$. Hence, the value in (56) equals $(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}}$, as desired. ☐

As for $t = 1$, the projection onto the $\mathrm{CLDUI}_n^{(t)}$ subspace is given by

$$\Pi_{\mathrm{CLDUI}_n^{(t)}}(\rho_{AB[t]}) = \int_{\mathcal{DU}_n} (U \otimes \overline{U}^{\otimes t})\rho_{AB[t]}(U \otimes \overline{U}^{\otimes t})^* dU. \tag{57}$$

In view of Lemma 3.2, the projection can also be seen as the map that preserves the entries indexed by $\Omega_n^{(t)}$ and places 0 everywhere else. Moreover, the integral can be replaced by a finite sum over the $n-1$ matrices $U_k$ from Lemma 3.2.

The following lemma is the key ingredient for the proof of Theorem 3.1, which is given thereafter. Its proof relies on the sparsity structure of $\mathrm{CLDUI}_n^{(t)}$ from Lemma 3.2 and the integral formulation (57) of the corresponding projector.

**Lemma 3.3.** *Let $W \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$ and consider an integer $0 \leq s \leq t$.*

*(i) If $W \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$, then $\Pi_{\mathrm{CLDUI}_n^{(t)}}(W) \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$.*

*(ii) If $W \in \mathcal{W}_{n,s}^{(t)}$, then $\Pi_{\mathrm{CLDUI}_n^{(t)}}(W) \in \mathcal{W}_{n,s}^{(t)}$.*

*Proof.* (i) Assume $W \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$; we show $\widetilde{W} := \Pi_{\mathrm{CLDUI}_n^{(t)}}(W) \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$. For this, let $i_0\underline{i}, j_0\underline{j} \in [n]^{t+1}$ and $\sigma \in \mathfrak{G}_t$. By assumption, $W_{i_0\underline{i},j_0\underline{j}} = W_{i_0\underline{i},j_0\sigma(\underline{j})}$; we need to show that the same holds for $\widetilde{W}$. By Lemma 3.2, the support of $\widetilde{W}$ is contained in the set $\Omega_n^{(t)}$. So, it suffices now to observe that $(i_0\underline{i}, j_0\underline{j}) \in \Omega_n^{(t)} \iff (i_0\underline{i}, j_0\underline{j}^\sigma) \in \Omega_n^{(t)}$, since $\{i_0\underline{j}\}$ and $\{i_0\underline{j}^\sigma\}$ are the same multisets.

(ii) Assume $W \in \mathcal{W}_{n,s}^{(t)}$, i.e., $W^{T_{B[s]}} \succeq 0$ (by (39)). Let $U \in \mathcal{DU}_n$ and $u = \mathrm{diag}(U)$. Then,

$$\begin{aligned}
(U \otimes \overline{U}^{\otimes t})W(U \otimes \overline{U}^{\otimes t})^* &= W \circ (uu^* \otimes (\overline{u}\,\overline{u}^*)^{\otimes t}),\\
(W \circ (uu^* \otimes (\overline{u}\,\overline{u}^*)^{\otimes t}))^{T_{B[s]}} &= W^{T_{B[s]}} \circ (uu^* \otimes (\overline{u}\,\overline{u}^*)^{\otimes t})^{T_{B[s]}}\\
&= W^{T_{B[s]}} \circ ((uu^*)^{\otimes(s+1)} \otimes (\overline{u}\,\overline{u}^*)^{\otimes(t-s)})\\
&= (U^{\otimes(s+1)} \otimes \overline{U}^{\otimes(t-s)})W^{T_{B[s]}}(U^{\otimes(s+1)} \otimes \overline{U}^{\otimes(t-s)})^*
\end{aligned}$$

(using (16) at the first and last lines). Using both equations gives

$$(\Pi_{\mathrm{CLDUI}_n^{(t)}}(W))^{T_{B[s]}} = \int_{\mathcal{DU}_n} (U^{\otimes(s+1)} \otimes \overline{U}^{\otimes(t-s)})W^{T_{B[s]}}(U^{\otimes(s+1)} \otimes \overline{U}^{\otimes(t-s)})^* dU.$$

As $W^{T_{B[s]}} \succeq 0$, we obtain that each integrand is positive semidefinite, and thus $(\Pi_{\mathrm{CLDUI}_n^{(t)}}(W))^{T_{B[s]}} \succeq 0$. ☐

*Proof of Theorem 3.1.* Assume $\rho_{AB} \in \mathrm{DPS}^{(t)}$ with $\mathrm{DPS}^{(t)}$-certificate $\rho_{AB[t]}$. We show $\widetilde{\rho_{AB[t]}} = \Pi_{\mathrm{CLDUI}_n}(\rho_{AB[t]})$ is a $\mathrm{DPS}_n^{(t)}$-certificate of $\widetilde{\rho_{AB}} = \Pi_{\mathrm{CLDUI}_n}(\rho_{AB})$. So, $\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$, $\rho_{AB[t]} \in \mathcal{W}_{n,s}^{(t)}$ for all integers $0 \leq s \leq t$, and $\mathrm{Tr}_{B[2:t]}(\rho_{AB[t]}) = \rho_{AB}$. By Lemma 3.3 we have

$\widetilde{\rho_{AB[t]}} \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$ and $\widetilde{\rho_{AB[t]}} \in \mathcal{W}_{n,s}^{(t)}$ for any $0 \le s \le t$. There remains to show that $\mathrm{Tr}_{B[2:t]}(\widetilde{\rho_{AB[t]}}) = \widetilde{\rho_{AB}}$. For this, let $i,j,k,l \in [n]$ and $\underline{h} \in [n]^{t-1}$. Note that

$$(ij,kl) \in \Omega_n \text{ if and only if } (ij\underline{h}, kl\underline{h}) \in \Omega_n^{(t)}, \tag{58}$$

because $\{ij\} = \{kl\}$ if and only if $\{ij\underline{h}\} = \{kl\underline{h}\}$. Using the definition of the partial trace, $(\mathrm{Tr}_{B[2:t]}(\widetilde{\rho_{AB[t]}}))_{ij,kl}$ is equal to

$$\sum_{\underline{h}\in[n]^{t-1}} (\widetilde{\rho_{AB[t]}})_{ij\underline{h},jk\underline{h}} = \begin{cases} (\mathrm{Tr}_{B[2:t]}(\rho_{AB[t]}))_{ij,kl} & \text{if } (ij,kl) \in \Omega_n, \\ 0 & \text{else.} \end{cases}$$

Since $\mathrm{Tr}_{B[2:t]}(\rho_{AB[t]}) = \rho_{AB}$ this is in fact precisely the definition of $\widetilde{\rho_{AB}}$. $\square$

The result of Theorem 3.1 has an immediate counterpart on the dual side: any matrix in $(\mathrm{DPS}_n^{(t)})^* \cap \mathrm{CLDUI}_n$ admits a certificate as in Theorem 2.4(iii) with, in addition, $B, W_s \in \mathrm{CLDUI}_n^{(t)}$.

**Corollary 3.4.** *If $M \in (\mathrm{DPS}_n^{(t)})^*$, then $\Pi_{\mathrm{CLDUI}_n}(M) \otimes I_n^{\otimes(t-1)}$ belongs to*

$$\mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))^\perp \cap \mathrm{CLDUI}_n^{(t)} + \sum_{s=0}^{t} \mathcal{W}_{n,s}^{(t)} \cap \mathrm{CLDUI}_n^{(t)}$$

*and thus $\Pi_{\mathrm{CLDUI}}(M) \in (\mathrm{DPS}_n^{(t)})^*$.*

*Proof.* Assume that $M \in (\mathrm{DPS}_n^{(t)})^*$. Then, by Theorem 2.4(iii), there exist $B \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))^\perp$ and $W_s \in \mathcal{W}_{n,s}^{(t)}$ such that $M \otimes I_n^{\otimes(t-1)} = B + \sum_{s=0}^t W_s$. Taking the projection onto $\mathrm{CLDUI}_n^{(t)}$ at both sides, we get

$$\begin{aligned} \Pi_{\mathrm{CLDUI}_n}(M) \otimes I_n^{\otimes(t-1)} &= \Pi_{\mathrm{CLDUI}_n^{(t)}}(M \otimes I_n^{\otimes(t-1)}) \\ &= \Pi_{\mathrm{CLDUI}_n^{(t)}}(B) + \sum_{s=0}^{t} \Pi_{\mathrm{CLDUI}_n^{(t)}}(W_s), \end{aligned}$$

where the first equality follows using (58). By Lemma 3.3(ii), we have that $\Pi_{\mathrm{CLDUI}_n^{(t)}}(W_s) \in \mathcal{W}_{n,s}^{(t)}$ for each $s$. To conclude, we use Lemma 3.3(i) to show that $\Pi_{\mathrm{CLDUI}_n^{(t)}}(B) \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))^\perp$. Indeed, if $W \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$, then $\Pi_{\mathrm{CLDUI}_n^{(t)}}(W) \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$ and thus we have $\langle \Pi_{\mathrm{CLDUI}_n^{(t)}}(B), W\rangle = \langle B, \Pi_{\mathrm{CLDUI}_n^{(t)}}(W)\rangle = 0$ holds, as desired. $\square$

### 3.2 Exploiting sparsity of DPS certificates for CLDUI states

As we now see, matrices in the set $\mathrm{CLDUI}_n^{(t)}$ have a block-diagonal structure. For convenience, let $G_n^{(t)}$ denote the (undirected) graph with vertex set $[n]^{t+1}$ and edge set $\Omega_n^{(t)}$. So, any matrix $W \in \mathrm{CLDUI}_n^{(t)}$ has a sparsity pattern that is contained in the graph $G_n^{(t)}$, i.e., $\mathrm{supp}(W) \subseteq \Omega_n^{(t)}$. An easy but very useful fact is that the graph $G_n^{(t)}$ is a disjoint union of cliques.

**Lemma 3.5.** *The graph $G_n^{(t)} = ([n]^{t+1}, \Omega_n^{(t)})$ is a disjoint union of cliques. Hence, any matrix $W \in \mathrm{CLDUI}_n^{(t)}$ is block-diagonal, of the form $W = \oplus_C W[C]$, where the direct sum is over the maximal cliques of $G_n^{(t)}$.*

*Proof.* Assume $i_0\underline{i}$ is adjacent to both $j_0\underline{j}$ and $k_0\underline{k}$ in $G_n^{(t)}$, we show that $(j_0\underline{j})$ is adjacent to $(k_0\underline{k})$. By assumption, $\alpha(i_0\underline{j}) = \alpha(j_0\underline{i})$ and $\alpha(i_0\underline{k}) = \alpha(k_0\underline{i})$. This implies

$$\alpha(j_0\underline{k}) - \alpha(k_0\underline{j}) = (\alpha(j_0\underline{i}) - \alpha(i_0\underline{j})) + (\alpha(i_0\underline{k}) - \alpha(k_0\underline{i})) = 0$$

(since $\alpha(\cdot)$ is linear under the concatenation of sequences), which shows that $(j_0\underline{j}, k_0\underline{k}) \in \Omega_n^{(t)}$. The second claim follows as an immediate consequence. $\square$

So, if $W \in \mathrm{CLDUI}_n^{(t)}$, then $W \succeq 0$ if and only if $W[C] \succeq 0$ for all the maximal cliques $C$ of $G_n^{(t)}$. This generalizes what we saw earlier in (10) for the case $t = 1$ . The analogous result also holds for testing positive semidefiniteness of partial transposes, i.e., membership in the set $\mathcal{W}_{n,s}^{(t)}$ for $s \in [t]$.

Let $1 \le s \le t$ be an integer. Given a sequence $\underline{i} = i_1 \dots i_t \in [n]^t$ we define the subsequences $\underline{i}[s] = i_1 \dots i_s \in [n]^s$ and $i[s+1:t] = i_{s+1} \dots i_t \in [n]^{t-s}$, which are, respectively, the $s$-prefix and $(t-s)$-suffix of $\underline{i}$. Consider the function

$$\begin{aligned} T_{B[s]} : [n]^{t+1} \times [n]^{t+1} &\to [n]^{t+1} \times [n]^{t+1} \\ (i_0\underline{i}, j_0\underline{j}) &\mapsto (i_0\underline{j}[s]\underline{i}[s+1:t], j_0\underline{i}[s]\underline{j}[s+1:t]) \end{aligned}$$

that swaps the $s$-prefices of $\underline{i}$ and $\underline{j}$. Then, the entry of $W^{T_{B[s]}}$ indexed by the pair $(i_0\underline{i}, j_0\underline{j})$ is equal to the entry of $W$ indexed by the pair $T_{B[s]}((i_0\underline{i}, j_0\underline{j}))$. Now, we define the set

$$\Omega_{n,s}^{(t)} := \{(i_0\underline{i}, j_0\underline{j}) \in [n]^{t+1} \times [n]^{t+1} : T_{B[s]}((i_0\underline{i}, j_0\underline{j})) \in \Omega_n^{(t)}\}$$

and, accordingly, $G_{n,s}^{(t)}$ is the graph with vertex set $[n]^{t+1}$ and edge set $\Omega_{n,s}^{(t)}$. So, the partial transpose $W^{T_{B[s]}}$ in the first $s$ $B$-registers of a matrix $W$ in $\mathrm{CLDUI}_n^{(t)}$ has a sparsity pattern contained in $G_{n,s}^{(t)}$.

**Lemma 3.6.** *For any $s \in [t]$, the graph $G_{n,s}^{(t)} = ([n]^{t+1}, \Omega_{n,s}^{(t)})$ is a disjoint union of cliques. Hence, if $W \in \mathrm{CLDUI}_n^{(t)}$, then $W^{T_{B[s]}}$ is block-diagonal, of the form $W^{T_{B[s]}} = \oplus_C W^{T_{B[s]}}[C]$, where the direct sum is over the maximal cliques of $G_{n,s}^{(t)}$.*

*Proof.* Let $i_0\underline{i}$ be adjacent to $j_0\underline{j}$ and $k_0\underline{k}$ in $G_{n,s}^{(t)}$. Then, $\alpha(i_0\underline{i}[s]\underline{j}[s+1:t]) = \alpha(j_0\underline{j}[s]\underline{i}[s+1:t])$ and $\alpha(i_0\underline{i}[s]\underline{k}[s+1:t]) = \alpha(k_0\underline{k}[s]\underline{i}[s+1:t])$. Hence,

$$\begin{aligned} &\alpha(k_0\underline{k}[s]\underline{j}[s+1:t]) - \alpha(j_0\underline{j}[s]\underline{k}[s+1:t]) = \\ &\quad (\alpha(k_0\underline{k}[s]\underline{i}[s+1:t]) - \alpha(i_0\underline{i}[s]\underline{k}[s+1:t])) \\ &\quad + (\alpha(i_0\underline{i}[s]\underline{j}[s+1:t]) - \alpha(j_0\underline{j}[s]\underline{i}[s+1:t])) \end{aligned}$$

is equal to 0, and thus $j_0\underline{j}$ is adjacent to $k_0\underline{k}$ in $G_{n,s}^{(t)}$. $\square$

**Corollary 3.7.** *For a matrix $W \in \mathrm{CLDUI}_n^{(t)}$ and $0 \le s \le t$, $W^{T_{B[s]}} \succeq 0$ if and only if $W^{T_{B[s]}}[C] \succeq 0$ for all the maximal cliques $C$ of $G_{n,s}^{(t)}$ (setting $G_{n,0}^{(t)} = G_t^{(t)}$).*

**Example 3.8.** *As an illustration we describe the maximal cliques of the graphs $G_n^{(t)}$ and $G_{n,s}^{(t)}$ for the case $n = 3$, $t = 2$, $s = 1, 2$, in which case the graphs have $n^{t+1} = 27$ vertices. Denote the adjacency relation in the graph $G_3^{(2)}$ (resp., the graph $G_{3,s}^{(2)}$) with $\simeq$ (resp., with $\overset{s}{\simeq}$). Then, $i_0i_1i_2 \simeq j_0j_1j_2$ if $\{i_0\underline{j}\} = \{j_0\underline{i}\}$ as multisets, $i_0i_1i_2 \overset{1}{\simeq} j_0j_1j_2$ if and only if $i_0j_1i_2 \simeq j_0i_1j_2$, and*

$i_0i_1i_2 \overset{2}{\simeq} j_0j_1j_2$ *if and only if* $i_0j_1j_2 \simeq j_0i_1i_2$. *For instance,* $121 \simeq 112$, $111 \overset{1}{\simeq} 122$, $112 \overset{2}{\simeq} 121$, *and* $113 \simeq 223$, $123 \overset{1}{\simeq} 213$, $123 \overset{2}{\simeq} 213$. *The maximal cliques of the graphs* $G_3^{(2)}$, $G_{3,1}^{(2)}$ *and* $G_{3,2}^{(2)}$ *are listed, respectively, in Tables 1, 2, 3. One can see that* $G_3^{(2)}$ *and* $G_{3,1}^{(2)}$ *each have twelve maximal cliques (including three of size 5, three of size 2, six of size 1), and* $G_{3,2}^{(2)}$ *has ten maximal cliques (including one of size 6, six of size 3, and three of size 1).*

*We will return to the case* $(n,t) = (3,2)$ *in Example 5.3 of Section 5.2, where we will use the moment approach to reformulate the DPS hierarchy for CLDUI states in a more compact manner.*

| Block size | Number of blocks | Indexed by maximal cliques of $G_3^{(2)}$ |
|---|---|---|
| 5×5 | 3 | {111, 212, 221, 313, 331}<br>{222, 121, 112, 323, 332}<br>{333, 131, 113, 232, 223} |
| 2×2 | 3 | {123, 132}<br>{213, 231}<br>{312, 321} |
| 1×1 | 6 | {122}, {133}, {211}, {233}, {311}, {322} |

Table 1: Block structure of $\rho_{AB[2]} \in \mathrm{CLDUI}_3^{(2)}$

| Block size | Number of blocks | Indexed by maximal cliques of $G_{3,1}^{(2)}$ |
|---|---|---|
| 5×5 | 3 | {111, 122, 133, 212, 313}<br>{222, 211, 233, 121, 323}<br>{333, 311, 322, 131, 232} |
| 2×2 | 3 | {123, 213}<br>{231, 321}<br>{312, 132} |
| 1×1 | 6 | {112}, {113}, {221}, {223}, {331}, {332} |

Table 2: Block structure of $\rho_{AB[2]}^{T_B[1]}$ for $\rho_{AB[2]} \in \mathrm{CLDUI}_3^{(2)}$

| Block size | Number of blocks | Indexed by maximal cliques of $G_{3,2}^{(2)}$ |
|---|---|---|
| 6×6 | 1 | {123, 132, 213, 231, 312, 321} |
| 3×3 | 6 | {122, 212, 221}<br>{133, 313, 331}<br>{211, 121, 112}<br>{233, 323, 332}<br>{311, 131, 113}<br>{322, 232, 223} |
| 1×1 | 3 | {111}, {222}, {333} |

Table 3: Block structure of $\rho_{AB[2]}^{T_B[1:2]}$ for $\rho_{AB[2]} \in \mathrm{CLDUI}_3^{(2)}$

### 3.3 Generalizations to LDUI and LDOI states

The previous results for CLDUI states extend in a straightforward way to LDUI and LDOI states. The respective 'extended' invariance classes are given by

$$\begin{aligned}
\mathrm{LDUI}_n^{(t)} &:= \{\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}) : \\
&\qquad \rho_{AB[t]} = (U \otimes U^{\otimes t})\rho_{AB[t]}(U \otimes U^{\otimes t})^* \ \forall U \in \mathcal{DU}_n\}, \\
\mathrm{LDOI}_n^{(t)} &:= \{\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}) : \\
&\qquad \rho_{AB[t]} = (O \otimes O^{\otimes t})\rho_{AB[t]}(O \otimes O^{\otimes t})^* \ \forall O \in \mathcal{DO}_n\},
\end{aligned}$$

where in the definition of $\mathrm{LDUI}_n^{(t)}$ one can restrict the invariance under $n-1$ selected matrices (as in Lemma 3.3(ii)). The sparsity patterns of $\mathrm{LDUI}_n^{(t)}$ and $\mathrm{LDOI}_n^{(t)}$ are captured, respectively, by

$$\begin{aligned}
\Phi_n^{(t)} &:= \{(i_0\underline{i}, j_0\underline{j}) \in [n]^{t+1} \times [n]^{t+1} : \alpha(i_0\underline{i}) = \alpha(j_0\underline{j})\}, \\
\Psi_n^{(t)} &:= \{(i_0\underline{i}, j_0\underline{j}) \in [n]^{t+1} \times [n]^{t+1} : \alpha(i_0\underline{i}j_0\underline{j}) \equiv 0 \bmod 2\},
\end{aligned} \tag{59}$$

and the respective projections are given by

$$\begin{aligned}
\Pi_{\mathrm{LDUI}_n^{(t)}}(\rho_{AB[t]}) &= \int_{\mathcal{DU}_n} (U \otimes U^{\otimes t})\rho_{AB[t]}(U \otimes U^{\otimes t})^* dU, \\
\Pi_{\mathrm{LDOI}_n^{(t)}}(\rho_{AB[t]}) &= \frac{1}{2^n} \sum_{O \in \mathcal{DO}_n} (O \otimes O^{\otimes t})\rho_{AB[t]}(O \otimes O^{\otimes t})^*.
\end{aligned}$$

We now have all the prerequisites to adapt Theorem 3.1 for LDUI and LDOI states. The proof is similar, thus omitted.

**Theorem 3.9.** *Assume that $\rho_{AB} \in \mathrm{DPS}^{(t)}$ with $\mathrm{DPS}^{(t)}$-certificate $\rho_{AB[t]}$. Then, $\Pi_{\mathrm{LDUI}_n}(\rho_{AB}) \in \mathrm{DPS}^{(t)}$ (resp., $\Pi_{\mathrm{LDOI}_n}(\rho_{AB}) \in \mathrm{DPS}^{(t)}$) with $\mathrm{DPS}^{(t)}$-certificate $\Pi_{\mathrm{LDUI}_n^{(t)}}(\rho_{AB[t]})$ (resp., $\Pi_{\mathrm{LDOI}_n^{(t)}}(\rho_{AB[t]})$).*

Again, this theorem has an immediate counterpart on the dual side for $(\mathrm{DPS}_n^{(t)})^*$: the analog of Corollary 3.4 holds replacing CLDUI, respectively, by LDUI or LDOI.

Also the analogs of Lemmas 3.5, 3.6 hold: each of the graphs $([n]^{t+1}, \Psi_n^{(t)})$ and $([n]^{t+1}, \Phi_n^{(t)})$ is a disjoint union of cliques and the same holds for the graphs attached to taking partial transposes. (The LDUI case follows from the CLDUI case up to a transposition and the proof in the LDOI case is in fact even easier since it involves a parity argument). In summary, matrices in $\mathrm{LDUI}_n^{(t)}$ or $\mathrm{LDOI}_n^{(t)}$ and their partial transposes all have a block-diagonal structure.

We now give in Lemma 3.10 an upper bound on the size of the blocks occurring in a matrix in $\mathrm{LDOI}_n^{(t)}$, by upper bounding the maximum size of a clique in the graph $([n]^{t+1}, \Psi_n^{(t)})$. Note that this bound also applies to the maximum clique size in the graph corresponding to taking partial transposes, because the definition of edges in $\Psi_n^{(t)}$ is 'global' in the sense that it depends only on the concatenated sequence $\alpha(i_0\underline{i}j_0\underline{j})$. In addition, the bound from Lemma 3.10 also applies to the graphs $([n]^{t+1}, \Phi_n^{(t)})$, $G_n^{(t)} = ([n]^{t+1}, \Omega_n^{(t)})$ (and their analogs corresponding to taking partial transposes) that model the sparsity patterns of matrices in $\mathrm{LDUI}_n^{(t)}$ and $\mathrm{CLDUI}_n^{(t)}$, because they are subgraphs of the graph $([n]^{t+1}, \Psi_n^{(t)})$.

**Lemma 3.10.** *The maximum size of a clique in the graph $([n]^{t+1}, \Psi_n^{(t)})$ is at most $t!n^{\lceil t/2 \rceil}$.*

We omit the proof since, later in Lemma 5.4 of Section 5, we will prove a similar statement adapted to the more economical moment framework. By the above discussion, Corollary 3.11 below follows as a direct application of Lemma 3.10.

**Corollary 3.11.** *If $W \in \mathrm{LDOI}_n^{(t)}$ then, for any $0 \le s \le t$, $W^{T_{B[s]}}$ is a block-diagonal matrix with all its blocks of size at most $t!n^{\lceil t/2 \rceil}$. The same holds if $W \in \mathrm{LDUI}_n^{(t)}$ or $W \in \mathrm{CLDUI}_n^{(t)}$.*

So, for $t = 1$, the maximum block size is $n$ for matrices in $\mathrm{LDOI}_n$, which matches relation (10).

### 3.4 A class of CLDUI examples: exploiting additional structure in DPS certificates

Here, we investigate a class of CLDUI bipartite quantum states (see Definition 3.16) and show *analytically* that their separability is characterized by the DPS hierarchy at level $t = 2$. We will use this characterization in Section 5.3 to generate test states for the $\mathrm{PPT}^2$ conjecture. To be able to analytically analyze $\mathrm{DPS}^{(2)}$-certificates, one needs to exploit additional structural properties of the quantum state at hand (in order to further reduce the block sizes and the number of variables). So, we begin with some results showing how additional properties of a quantum state $\rho_{AB}$ (like having a large kernel, or enjoying some symmetry property) are inherited by its $\mathrm{DPS}^{(t)}$-certificates $\rho_{AB[t]}$. These results are of independent interest and apply to general quantum states.

#### Properties of the kernel

As we now see, any vector in the kernel of a state $\rho_{AB}$ can be used to construct vectors in the kernel of its $\mathrm{DPS}^{(t)}$-certificates. This relies on the partial trace property (27) and positivity $\rho_{AB} \succeq 0$.

**Lemma 3.12.** *Assume that $\rho_{AB} \in \mathrm{DPS}_n^{(t)}$ with $\rho_{AB[t]}$ as $\mathrm{DPS}^{(t)}$-certificate. If $w \in \ker \rho_{AB}$, then $w \otimes e_{k_2} \otimes \ldots \otimes e_{k_t} \in \ker \rho_{AB[t]}$ for all $k_2, \ldots, k_t \in [n]$.*

*Proof.* Since $w \in \ker \rho_{AB}$, we have $\rho_{AB} w = 0$, and thus

$$\begin{aligned} 0 = \langle \rho_{AB}, ww^* \rangle &= \langle \mathrm{Tr}_{B[2:t]}(\rho_{AB[t]}), ww^* \rangle = \langle \rho_{AB[t]}, ww^* \otimes I_n^{\otimes (t-1)} \rangle \\ &= \sum_{k_2, \ldots, k_t = 1}^{n} \langle \rho_{AB[t]}, ww^* \otimes e_{k_2} e_{k_2}^* \otimes \ldots \otimes e_{k_t} e_{k_t}^* \rangle \\ &= \sum_{k_2, \ldots, k_t = 1}^{n} (w \otimes e_{k_1} \otimes \ldots \otimes e_{k_t})^* \rho_{AB[t]} (w \otimes e_{k_1} \otimes \ldots \otimes e_{k_t}). \end{aligned}$$

As $\rho_{AB[t]} \succeq 0$, each summand is nonnegative and thus equal to 0. From this one obtains that $0 = \rho_{AB[t]}(w \otimes e_{k_2} \otimes \ldots \otimes e_{k_t})$, as desired. □

#### Symmetry properties

We now turn to exploiting symmetries of the initial quantum state for its $\mathrm{DPS}^{(t)}$-certificates.

First, let us introduce how the permutation group $\mathfrak{S}_n$ acts on $[n]^t$ and on $\mathrm{Herm}((\mathbb{C}^n)^t$. Any permutation $\theta \in \mathfrak{S}_n$ has an entrywise action on $[n]^t$, by setting $\theta(\underline{i}) = \theta(i_1) \ldots \theta(i_t)$ for $\underline{i} = i_1 \ldots i_t \in [n]^t$. In turn, $\theta$ acts on $\rho \in \mathrm{Herm}((\mathbb{C}^n)^t$, by permuting its rows and columns according to the action of $\theta$ on $[n]^t$, thus producing $\theta(\rho) \in \mathrm{Herm}((\mathbb{C}^n)^{\otimes} t)$, with entries

$$\theta(\rho)_{i_0 \underline{i}, j_0 \underline{j}} = \rho_{\theta(i_0)\theta(\underline{i}), \theta(j_0)\theta(\underline{j})} \text{ for } i_0 \underline{i}, j_0 \underline{j} \in [n]^{t+1}.$$

**Remark 3.13.** *So, a permutation $\theta \in \mathfrak{S}_n$ acts on the values $i_k \in [n]$ and* not *on their indices $k \in [t]$, as was the case earlier, when a permutation $\sigma \in \mathfrak{S}_t$ would produce $\underline{i}^\sigma = i_{\sigma(1)} \dots i_{\sigma(t)} \in [n]^t$ and $\rho^\sigma \in \mathrm{Herm}((\mathbb{C}^n)^{\otimes t})$ with entries $\rho^\sigma_{\underline{i},\underline{j}} = \rho_{\underline{i}^\sigma,\underline{j}^\sigma}$ for $\underline{i},\underline{j} \in [n]^t$. We will use the following observation (that follows using the definitions): for a sequence $\underline{i} = i_1 \dots i_t \in [n]^t$,*

$$\theta(\underline{i}^\sigma) = \theta(i_{\sigma(1)}) \dots \theta(i_{\sigma(t)}) = (\theta(i_1) \dots \theta(i_t))^\sigma = \theta(\underline{i})^\sigma \text{ for any } \theta \in \mathfrak{S}_n, \sigma \in \mathfrak{S}_t. \tag{60}$$

**Lemma 3.14.** *Assume $\rho_{AB} \in \mathrm{DPS}_n^{(t)}$ with $\rho_{AB[t]}$ as $\mathrm{DPS}^{(t)}$-certificate. For any $\theta \in \mathfrak{S}_n$, $\theta(\rho_{AB[t]})$ is a $\mathrm{DPS}^{(t)}$-certificate for $\theta(\rho_{AB})$.*

*Proof.* By assumption, $\rho_{AB[t]}$ satisfies (25), (26), (27), we show that the same holds for $\theta(\rho_{AB[t]})$. First, we show (25). For this, let $\sigma \in \mathfrak{S}_t$ and $i_0\underline{i}, j_0\underline{j} \in [n]^{t+1}$. Then, we have

$$\begin{aligned}\theta(\rho_{AB[t]})_{i_0\underline{i}^\sigma,j_0\underline{j}^\sigma} &= (\rho_{AB[t]})_{\theta(i_0)\theta(\underline{i}^\sigma),\theta(j_0)\theta(\underline{j}^\sigma)} = (\rho_{AB[t]})_{\theta(i_0)(\theta(\underline{i}))^\sigma,\theta(j_0)\theta(\underline{j})^\sigma} \\ &= (\rho_{AB[t]})_{\theta(i_0)\theta(\underline{i}),\theta(j_0)\theta(\underline{j})} = \theta(\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}},\end{aligned}$$

using (60) at the first line and the fact that $\rho_{AB[t]}$ satisfies (25) at the second line. Hence, $\theta(\rho_{AB[t]})$ also satisfies (25).

Condition (26) follows from the fact that the operations of applying $\theta$ and taking the partial transpose commute: $\big(\theta(\rho_{AB[t]})\big)^{T_{B[s]}} = \theta\big(\rho_{AB[t]}^{T_{B[s]}}\big)$, which can be checked by computing

$$\begin{aligned}&\Big( \big(\theta(\rho_{AB[t]})\big)^{T_{B[s]}} \Big)_{i_0\underline{i},j_0\underline{j}} = \big(\theta(\rho_{AB[t]})\big)_{i_0j_1\dots j_s i_{s+1}\dots s_t, j_0 i_1 \dots i_s j_{s+1}\dots j_t} \\ &= (\rho_{AB[t]})_{\theta(i_0j_1\dots j_s i_{s+1}\dots s_t),\theta(j_0i_1\dots i_s j_{s+1}\dots j_t)} = \big(\rho_{AB[t]}^{T_{B[s]}}\big)_{\theta(i_0\underline{i}),\theta(j_0\underline{j})} \\ &= \big(\theta\big(\rho_{AB[t]}^{T_{B[s]}}\big)\big)_{i_0\underline{i},j_0\underline{j}}.\end{aligned}$$

Hence, $\rho_{AB[t]}^{T_{B[s]}} \succeq 0$ implies $\theta(\rho_{AB[t]}^{T_{B[s]}}) \succeq 0$ and thus $(\theta(\rho_{AB[t]}))^{T_{B[s]}} \succeq 0$, as desired.

Finally, condition (27) follows from the fact that the operations of applying $\theta$ and taking the partial trace also commute, which can be checked by computing

$$\begin{aligned}&\big(\mathrm{Tr}_{B[2:t]}\big(\theta(\rho_{AB[t]})\big)\big)_{i_0i_1,j_0j_1} = \sum_{\underline{k}\in[n]^{t-1}} \big(\theta(\rho_{AB[t]})\big)_{i_0i_1\underline{k},j_0j_1\underline{k}} \\ &= \sum_{\underline{k}\in[n]^{t-1}} \big(\rho_{AB[t]}\big)_{\theta(i_0i_1)\theta(\underline{k}),\theta(j_0j_1)\theta(\underline{k})} = \sum_{\underline{h}\in[n]^{t-1}} \big(\rho_{AB[t]}\big)_{\theta(i_0i_1)\underline{h},\theta(j_0j_1)\underline{h}} \\ &= \mathrm{Tr}_{r-2}(\rho_{AB[t]})_{\theta(i_0i_1),\theta(j_0j_1)} = (\rho_{AB})_{\theta(i_0i_1),\theta(j_0j_1)} = \theta(\rho_{AB})_{i_0i_1,j_0j_1},\end{aligned}$$

using the fact that $\rho_{AB[t]}$ satisfies (27) at the last but one equality. □

**Corollary 3.15.** *Assume $\rho_{AB} \in \mathrm{DPS}^{(t)}$ and $\theta(\rho_{AB}) = \rho_{AB}$ for some $\theta \in \mathfrak{S}_t$. Then, $\rho_{AB}$ has a $\mathrm{DPS}^{(t)}$-certificate $\rho_{AB[t]}$ that satisfies $\theta(\rho_{AB[t]}) = \rho_{AB[t]}$.*

*Proof.* Let $\rho_{AB[t]}$ be a $\mathrm{DPS}^{(t)}$-certificate for $\rho_{AB} \in \mathrm{DPS}^{(t)}$. Then, for any integer $k \geq 1$, $\theta^k(\rho_{AB[t]})$ is a $\mathrm{DPS}^{(t)}$-certificate for $\theta^k(\rho_{AB}) = \rho_{AB}$, which follows using Lemma 3.14 and the fact that $\theta(\rho_{AB}) = \rho_{AB}$. Let $m \geq 1$ be an integer such that $\theta^m = id$. Since the set of $\mathrm{DPS}^{(t)}$-certificates for $\rho_{AB}$ is a convex set, one finds that $\widetilde{\rho}_{AB[t]} := \frac{1}{m}\sum_{k=1}^m \theta^k(\rho_{AB[t]})$ is a $\mathrm{DPS}^{(t)}$-certificate for $\rho_{AB}$. Moreover, it satisfies $\theta(\widetilde{\rho}_{AB[t]}) = \widetilde{\rho}_{AB[t]}$. □

**A class of CLDUI bipartite quantum states**

We consider the CLDUI bipartite states $\rho_{a,a'}$ $(a, a' \geq 0)$ in Definition 3.16, generalizing the case $a' = 1/a$ $(a > 0)$ considered in [JM19, Example 3.3]. We show that $\rho_{a,a'}$ is separable if and only if it belongs to $\mathrm{DPS}_3^{(2)}$, or, equivalently, $aa' \geq 1$ (Theorem 3.20). Analytically characterizing membership in $\mathrm{DPS}_3^{(2)}$ is the most technical part, which exploits knowing the maximal cliques of the graph $G_3^{(2)}$ (Table 1) and structural properties of the state $\rho_{a,a'}$ (on symmetry and its kernel). We will use this class of examples later in Section 5.3.

**Definition 3.16.** *For $a, a' \in \mathbb{R}_+$, define the quantum state $\rho_{a,a'} \in \mathrm{CLDUI}_3$ as*

$$\rho_{a,a'} = \left(\begin{array}{ccc|ccc|ccc} 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & a & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & a' & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & a' & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & a & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a' & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \end{array}\right) = \rho_{(X,Y)} \text{ with } X = \begin{pmatrix} 1 & a & a' \\ a' & 1 & a \\ a & a' & 1 \end{pmatrix}, Y = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

*where $\rho_{a,a'}$ is indexed by* $11, 12, 13, 21, 22, 23, 31, 32, 33$, $X = ((\rho_{a,a'})_{ij,ij})_{i,j=1}^3$, $Y = ((\rho_{a,a'})_{ii,jj})_{i,j=1}^3$.

**Lemma 3.17.** *The matrix $\rho_{a,a'}$ belongs to $\mathrm{DPS}_3^{(1)}$ if and only if $a, a' \geq 0$ and $aa' \geq 1$.*

*Proof.* By definition, $\rho_{a,a'} \in \mathrm{DPS}_3^{(1)}$ if and only if $\rho_{a,a'} \succeq 0$ and $\rho_{a,a'}^{T_B} \succeq 0$. This is equivalent to $a, a' \geq 0$ and the block $\left(\begin{smallmatrix} a & 1 \\ 1 & a' \end{smallmatrix}\right)$ being positive semidefinite, i.e., $aa' \geq 1$. □

**Lemma 3.18.** *Assume that $\rho_{a,a'} \in \mathrm{DPS}_3^{(2)}$. Then, $\rho_{a,a'}$ has a $\mathrm{DPS}^{(2)}$-certificate $\rho$ with the following properties: $\rho$ is block-diagonal and each of its blocks is a scalar multiple of the all-ones matrix.*

*Proof.* The existence of a block-diagonal certificate $\rho$ follows from Theorem 3.1 and Corollary 3.7. So, $\rho = \oplus_C \rho[C]$, where the direct sum is over the maximal cliques $C$ of the graph $G_3^{(2)}$ (described in Table 1). We now argue that, for every maximal clique $C$, $\rho[C] = x_C J_{|C|}$ for some $x_C \in \mathbb{R}$. That is, the columns $\rho_{\cdot,i_0i_1i_2}$, $\rho_{\cdot,j_0j_1j_2}$ of $\rho$ indexed by any two elements $i_0i_1i_2, j_0j_1j_2 \in C$ are equal. It suffices to show this for the six cliques of size 2 or 5.

First, we use the property (25) of $\rho$, which claims that $\rho_{\cdot,j_0j_1j_2} = \rho_{\cdot,j_0j_2j_1}$ for any $j_0j_1j_2 \in [3]^3$. This directly settles the case of the cliques of size 2, $\{123, 132\}$, $\{213, 231\}$ and $\{312, 321\}$. Consider now a clique of size 5, say $C = \{111, 212, 221, 313, 331\}$. Then, $\rho_{\cdot,212} = \rho_{\cdot,221}$, $\rho_{\cdot,313} = \rho_{\cdot,331}$ holds. There remains to show that the columns indexed by the elements $111, 221, 331$ are equal. For this, we use the fact that the vectors $w_1 = e_2 \otimes e_2 - e_3 \otimes e_3$ and $w_2 = e_1 \otimes e_1 - e_3 \otimes e_3$ belong to the kernel of $\rho_{a,a'}$. By Lemma 3.12, it follows that $w \otimes e_i \in \ker \rho$ for each $i \in [3]$ and $w \in \{w_1, w_2\}$. From this one obtains that the columns of $\rho$ indexed by the indices $111, 221, 331$ are all identical, as desired. The same reasoning applies to the other two cliques of size 5. □

Next, we further simplify the structure of a $\mathrm{DPS}^{(2)}$-certificate for $\rho_{a,a'}$, by exploiting the fact that $\rho_{a,a'}$ is invariant under the cyclic permutation $\theta = (123) \in \mathfrak{S}_3$, i.e., $\theta(\rho_{a,a'}) = \rho_{a,a'}$.

**Lemma 3.19.** *Assume that $\rho_{a,a'} \in \mathrm{DPS}_3^{(2)}$. Then, $\rho_{a,a'}$ has a $\mathrm{DPS}^{(2)}$-certificate $\rho$ with the following properties: $\rho$ is block-diagonal: $\rho = \oplus_C \rho[C]$, where the blocks are indexed by the maximal cliques $C$ of $G_3^{(2)}$, and* *(i) the three blocks of size 5 are identical: if* $|C| = 5$*, then* $\rho[C] = xJ_5$ *for some* $x \in \mathbb{R}$*,*

*(ii) the three blocks of size 2 are identical: if* $|C| = 2$*, then* $\rho[C] = yJ_2$ *for some* $y \in \mathbb{R}$*,*

*(iii)* $\rho_{122,122} = \rho_{233,233} = \rho_{311,311} =: z \in \mathbb{R}$*,*

*(iv)* $\rho_{133,133} = \rho_{211,211} = \rho_{322,322} =: z' \in \mathbb{R}$*.*

*Proof.* The additional properties in (i)-(iv) follow using the fact that $\rho_{a,a'}$ is invariant under the cyclic permutation $\theta = (123)$. Indeed, by Corollary 3.15, $\rho_{a,a'}$ has a $\theta$-invariant $\mathrm{DPS}^{(2)}$-certificate $\rho \in \mathrm{CLDUI}_3^{(2)}$. We show that this certificate $\rho$ has the desired properties. Observe that $C_1 := \{111, 212, 221, 313, 331\}$, $C_2 := \theta(C)$, $C_3 := \theta^2(C)$ are the three cliques of size 5 in $G_3^{(2)}$ (where $\theta$ is applied element-wise). First, we have

$$\rho_{111,111} = \rho_{\theta(111),\theta(111)} = \rho_{222,222} = \rho_{\theta(222),\theta(222)} = \rho_{333,333}.$$

For $i = 1, 2, 3$, the index $iii$ belongs to the clique $C_i$. By Lemma 3.18, all entries of $\rho[C_i]$ are equal, say to $x_i$, implying $x_i = \rho_{iii,iii}$. Combined with the above relation, one obtains $x_1 = x_2 = x_3 =: x$, showing (i).

(ii) follows analogously, using the fact that $\theta(123) = 231$ and $\theta(231) = 312$, which implies that the scalars determining the blocks $\rho[C_{23}], \rho[C_{31}], \rho[C_{12}]$ are all equal to the same scalar $y$.

For (iii)-(iv), note that the six blocks of size 1 lie in two different orbits: $\theta(122) = 233, \theta(233) = 122$ and $\theta(133) = 211, \theta(211) = 322.$, which implies $\rho[122] = \rho[233] = \rho[122] =: z$ and $\rho[133] = \rho[211] = \rho[322] =: z'$, as desired. ☐

**Theorem 3.20.** *For the state* $\rho_{a,a'}$ *from Definition 3.16, the following are equivalent:*

$$\rho_{a,a'} \in \mathrm{SEP}_3 \iff \rho_{a,a'} \in \mathrm{DPS}_3^{(2)} \iff a \geq 1 \text{ and } a' \geq 1.$$

*Proof.* Assume $\rho_{a,a'} \in \mathrm{DPS}_3^{(2)}$, we show $a, a' \geq 1$. Let $\rho$ be a $\mathrm{DPS}^{(2)}$-certificate for $\rho_{a,a'}$ that satisfies the properties claimed in Lemma 3.19. Since $\rho$ satisfies (27), we get

$$1 = (\rho_{a,a'})_{11,11} = \mathrm{Tr}_B(\rho)_{11,11} = \rho_{111,111} + \rho_{112,112} + \rho_{113,113} = 3x,$$

which implies $x = \frac{1}{3}$. Similarly, we get

$$a = \mathrm{Tr}_B(\rho)_{12,12} = x + z + y, \quad a' = \mathrm{Tr}_B(\rho)_{21,21} = y + z' + x,$$

which implies $z = a - y - \frac{1}{3}$ and $z' = a' - y - \frac{1}{3}$.

We now use the fact that $\rho^{T_{B[1]}}$ is positive semidefinite (condition (26)). Using the submatrix of $\rho^{T_{B[1]}}$ indexed by $\{123, 213\}$ (in that order), we obtain

$$\begin{pmatrix} \rho_{123,123} & \rho_{113,223} \\ \rho_{223,113} & \rho_{213,213} \end{pmatrix} = \begin{pmatrix} y & x \\ x & y \end{pmatrix} \succeq 0,$$

implying $y \geq x = \frac{1}{3}$. Using the submatrix of $\rho^{T_{B[1]}}$ indexed by $\{111, 122, 133\}$ (in that order) gives

$$\begin{pmatrix} \rho_{111,111} & \rho_{121,112} & \rho_{131,113} \\ \rho_{112,121} & \rho_{122,122} & \rho_{132,123} \\ \rho_{113,131} & \rho_{123,132} & \rho_{133,133} \end{pmatrix} = \begin{pmatrix} x & x & x \\ x & z & y \\ x & y & z' \end{pmatrix}.$$

By taking the Schur complement w.r.t. the upper left corner and using the values of $z, z'$, we obtain

$$\begin{pmatrix} z-x & y-x \\ y-x & z'-x \end{pmatrix} = \begin{pmatrix} a-y-\frac{2}{3} & y-\frac{1}{3} \\ y-\frac{1}{3} & a'-y-\frac{2}{3} \end{pmatrix} \succeq 0.$$

In particular, $a-y-\frac{2}{3}, a'-y-\frac{2}{3} \geq 0$. Combining with $y \geq \frac{1}{3}$, we get that $a, a' \geq 1$, as desired.

Assume now $a, a' \geq 1$, we show that $\rho_{a,a'} \in \mathrm{SEP}_3$. For this, observe that the matrices $X, Y$ in Definition 3.16 satisfy $X = J_3 + X'$, $Y = J_3$, where $X' = X - J \geq 0$ since $a, a' \geq 1$. So, we have $\rho_{a,a'} = \rho_{(J_3,J_3)} + \rho_{(X',0)}$. The state $\rho_{(J_3,J_3)}$ is separable (e.g., since it is equal to $\Pi_{\mathrm{CLDUI}_3}(ee^* \otimes ee^*)$, with $e$ the all-ones vector). Also, the state $\rho_{(X',0)}$ is separable (using, e.g., (50)). Hence, the state $\rho_{a,a'}$ is the sum of two separable states and thus $\rho_{a,a'}$ is separable. This concludes the proof. $\square$

**Remark 3.21.** *In their recent work [GNS25] the authors consider LDOI states $\rho_{(X,Y,Z)}$, where $X, Y, Z$ are circulant matrices. In particular, when $Y = J_n$ is the all-ones matrix, they characterize membership in $\mathrm{SEP}_n$ and $\mathrm{DPS}_n^{(1)}$ (see Theorem VI.5). Note that the state $\rho_{a,a'}$ from Definition 3.16 has $X$ circulant and $Y = J_n$, so it falls within this class (for $n = 3$). In Theorem 3.20 we additionally characterize its membership in $\mathrm{DPS}_3^{(2)}$ and show equivalence with separability. Whether this property extends to more general states with circulant structure is left for future research.*

# 4 Dual of the symmetric DPS hierarchy and matrix copositivity

Given a matrix $A \in \mathcal{S}^n$, consider the matrix $M_{A,0} \in \mathrm{CLDUI}_n$ as defined in relation (49) and the associated polynomial

$$\langle M_{A,0}, xx^* \otimes xx^* \rangle = \langle A, (x \circ \overline{x})(x \circ \overline{x})^T \rangle = \sum_{i,j=1}^{n} A_{ij} |x_i|^2 |x_j|^2 = f_A(|x_1|^2, \ldots, |x_n|^2),$$

where $f_A$ is the polynomial from (34). Hence,

$$M_{A,0} \in (\mathrm{SEP}_n^{\mathrm{BS}})^* \iff A \in \mathrm{COP}_n.$$

Moreover, if $A_{ij} < 0$ for some $i < j$, then $\langle M_{A,0}, D_{ij} D_{ij}^* \rangle = A_{ij} < 0$; hence $M_{A,0}$ provides an entanglement witness that separates the entangled state $D_{ij} D_{ij}^*$ from $\mathrm{SEP}_n^{\mathrm{BS}}$. So, when restricting to matrices with diagonal unitary invariance, there is a tight connection between the dual cone $(\mathrm{SEP}_n^{\mathrm{BS}})^*$ and the copositive cone $\mathrm{COP}_n$, as shown in [MATS21, Theorem 2.1]. Recently, it is shown in [GNP25] that this connection extends to the hierarchies $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$ for $(\mathrm{SEP}_n^{\mathrm{BS}})^*$, and $\mathcal{K}_n^{(t)}$ for $\mathrm{COP}_n$. In this section we revisit this connection. First, we present a characterization of the dual cone $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$ that fully mirrors the result in Theorem 2.4 for $(\mathrm{DPS}_n^{(t)})^*$. Then, we use it to offer a simple argument for the connection between $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$ and $\mathcal{K}_n^{(t)}$, using only the basic correspondence (24) between real-sos Hermitian polynomials in complex variables and sos polynomials in real variables.

## 4.1 The dual of the symmetric DPS hierarchy

For $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$, recall the polynomial $F_M(x, \overline{x}, y, \overline{y}) \in \mathbb{C}[x, \overline{x}, y, \overline{y}]_{1,1,1,1}$ as defined in (37). By restricting to one set of variables, i.e., setting $y = x$, we obtain the polynomial

$$\widetilde{F}_M(x, \overline{x}) := F_M(x, \overline{x}, x, \overline{x}) = \langle M, xx^* \otimes xx^* \rangle \in \mathbb{C}[x, \overline{x}]_{2,2}, \tag{61}$$

with degree 2 in $x$ and degree 2 in $\overline{x}$. So, $M \in (\mathrm{SEP}_n^{\mathrm{BS}})^*$ means $F_M(x, \overline{x}, x, \overline{x}) \geq 0$ for all $x \in \mathbb{C}^n$ (equivalently, for all $x \in \mathbb{S}^{n-1}$). In the next result we characterize when $M$ belongs to the dual of the relaxation $\widetilde{\mathrm{DPS}}_n^{(t)}$, thus giving an analog of Theorem 2.4 for the symmetric setting.

**Theorem 4.1.** *Consider a matrix $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ and an integer $t \geq 1$. Set $\tau = \lfloor (t+1)/2 \rfloor$. The following assertions are equivalent.*

*(i)* $M \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$.

*(ii) The polynomial* $\|x\|^{2(t-1)} \widetilde{F}_M(x, \overline{x}) = \|x\|^{2t} \langle M, xx^* \otimes xx^* \rangle \in \mathbb{C}[x, \overline{x}]_{2(t+1),2(t+1)}$ *is r-sos.*

*(iii) There exist matrices* $B, W_0, W_1, \ldots, W_\tau \in \mathrm{Herm}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t})$ *such that*

$$M \otimes I_n^{\otimes (t-1)} = B + \sum_{s=0}^{\tau} W,$$

*where* $B \in \mathrm{Herm}(S^{t+1}(\mathbb{C}^n))^\perp$, $W_s \in \mathcal{W}_{n,s}^{(t)}$ *for* $s = 0, 1, \ldots, \tau$.

In comparison with Theorem 2.4, we are now asking in (iii) that the matrix $B$ belongs to the larger space $\mathrm{Herm}(S^{t+1}(\mathbb{C}^n))^\perp$, which contains the space $\mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))^\perp$ involved in Theorem 2.4(iii). In addition, we only need the subspaces $\mathcal{W}_{n,s}^{(t)}$ for $s \leq \tau = \lfloor (t+1)/2 \rfloor$.

**Remark 4.2.** *The set $\widetilde{\mathrm{DPS}}_n^{(t)}$ corresponds to the set $\mathrm{PPTBExt}_n^{(K_{t+1})}$ considered in [GNP25]. The characterization of the dual of $\mathrm{PPTBExt}_n^{(t)}$ given in [GNP25, Prop. 8.9] corresponds to the equivalence of items (i) and (iii) in Theorem 4.1. The additional characterization (ii) in terms of r-sos polynomials, which is present in Theorem 4.1 (as well as in Theorem 2.4), is not given in [GNP25]. Showing this characterization (ii) constitutes in fact the most technical part of the proof. On the other hand, it is especially relevant since it is directly comparable to the characterization (35) in terms of sums of squares for matrices $A \in \mathcal{K}_n^{(t)}$.*

Before giving the proof, note that, as in the general (non-symmetric) case, the LDUI projection preserves membership in $\widetilde{\mathrm{DPS}}_n^{(t)}$ and its dual cone, a property we will use in the next section.

**Lemma 4.3.** *Assume that $\rho_{AB}, M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$. Then, $\rho_{AB} \in \widetilde{\mathrm{DPS}}_n^{(t)}$ implies $\Pi_{\mathrm{LDUI}}(\rho_{AB}) \in \widetilde{\mathrm{DPS}}_n^{(t)}$, and $M \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$ implies $\Pi_{\mathrm{LDUI}}(M) \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$.*

*Proof.* It suffices to show the first claim, since it implies the second one using the fact that $\langle \Pi_{\mathrm{LDUI}}(M), \rho_{AB} \rangle = \langle M, \Pi_{\mathrm{LDUI}}(\rho_{AB} \rangle$. Assume $\rho_{AB} \in \widetilde{\mathrm{DPS}}_n^{(t)}$, and let $\rho_{AB[t]}$ be a $\widetilde{\mathrm{DPS}}^{(t)}$-certificate for it. Then, the projection of this certificate

$$\Pi_{\mathrm{LDUI}^{(t)}}(\rho_{AB[t]}) = \int_{\mathcal{DU}_n} U^{\otimes (t+1)} \rho_{AB[t]} (U^{\otimes (t+1)})^* dU$$

is a $\widetilde{\mathrm{DPS}}^{(t)}$-certificate for $\Pi_{\mathrm{LDUI}}(\rho_{AB})$, showing $\Pi_{\mathrm{LDUI}}(\rho_{AB}) \in \widetilde{\mathrm{DPS}}_n^{(t)}$. □

*of Theorem 4.1.* The proof is along the same lines as for Theorem 2.4 in [FF20]. There are, however, some differences since one needs to restrict to $s \leq \tau = \lfloor (t+1)/2 \rfloor$ in (iii), which adds some technicalities. Our argument is also more compact. Let $M \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ and let

$$p(x, \overline{x}) = \|x\|^{2(t-1)} \langle M, xx^* \otimes xx^* \rangle \in \mathbb{C}[x, \overline{x}]_{t+1,t+1}$$

denote the polynomial appearing in Theorem 4.1(ii). Recall the conditions involved in Theorem 4.1: (i) $M \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$; (ii) $p$ is r-sos; (iii) $M \otimes I_n^{(t-1)}$ belongs to $(\mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)})^\perp + \sum_{s=0}^{\tau} \mathcal{W}_{n,s}^{(t)}$; and the additional condition (iv) $M \otimes I_n^{(t-1)} \in \mathrm{cl}((\mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)})^\perp + \sum_{s=0}^{\tau} \mathcal{W}_{n,s}^{(t)})$ (where 'cl' denotes taking the closure). Recall the definition of $\widetilde{\mathrm{DPS}}_n^{(t)}$ in (31) and of $\mathcal{W}_{n,s}^{(t)}$ in (39), and $\tau = \lfloor (t+1)/2 \rfloor$.

The implication (iii) $\Longrightarrow$ (iv) is clear. The implication (iii) $\Longrightarrow$ (ii) follows by taking the inner product of $M \otimes I_n^{\otimes(t-1)}$ with $(xx^*)^{\otimes(t+1)}$ and using the fact that

$$\langle W_s, (xx^*)^{\otimes(t+1)} \rangle = \langle W_s^{T_B[s]}, xx^* \otimes (\overline{xx}^*)^{\otimes s} \otimes (xx^*)^{\otimes(t-s)} \rangle$$

is r-sos for any $W_s \in \mathcal{W}_{n,s}^{(t)}$ (since $W_s^{T_B[s]} \succeq 0$).

We now show (i) $\Longleftrightarrow$ (iv). By definition of the dual cone $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$,

$$\begin{aligned}
&M \in (\widetilde{\mathrm{DPS}}_n^{(t)})^* \Longleftrightarrow \langle M, \rho_{AB} \rangle \text{ for all } \rho_{AB} \in \widetilde{\mathrm{DPS}}_n^{(t)} \\
&\Longleftrightarrow \langle M \otimes I_n^{\otimes(t-1)}, \rho_{AB[t]} \rangle \text{ for all } \rho_{AB[t]} \in \mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)}) \cap \bigcap_{s=0}^{\tau} \mathcal{W}_{n,s}^{(t)} \\
&\Longleftrightarrow M \otimes I_n^{\otimes(t-1)} \in \Big( \mathrm{BS}(\mathbb{C}^n \otimes (\mathbb{C}^n)^{\otimes t}) \cap \bigcap_{s=0}^{\tau} \mathcal{W}_{n,s}^{(t)} \Big)^*
\end{aligned}$$

where the latter set is equal to $\mathrm{cl}\big((\mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)}))^\perp + \sum_{s=0}^{\tau} \mathcal{W}_{n,s}^{(t)}\big)$. Above, at the second line, we use the definition of the partial trace and of $\widetilde{\mathrm{DPS}}_n^{(t)}$ in (31). At the last line, we use the well-known convex geometry fact that the dual of an intersection of cones is the closure of the sum of the duals of the cones, combined with the fact that the cone $\mathcal{W}_{n,s}^{(t)}$ is self-dual.

We show (iv) $\Longrightarrow$ (ii). For this, assume $M \otimes I_n^{\otimes(t-1)} = \lim_{\ell\to\infty} A_\ell$, where $A_\ell = B_\ell + \sum_{s=0}^{\tau} W_{\ell,s}$ with $B_\ell \in (\mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)}))^\perp$ and $W_{\ell,s} \in \mathcal{W}_{n,s}^{(t)}$. Define the polynomial

$$\begin{aligned}
\sigma_\ell(x, \overline{x}) = \langle A_\ell, (xx^*)^{\otimes(t+1)} \rangle &= \Big\langle \sum_{s=0}^{\tau} W_{\ell,s}, (xx^*)^{\otimes(t+1)} \Big\rangle \\
&= \sum_{s=0}^{\tau} \langle W_{\ell,s}^{T_B[s]}, xx^* \otimes (\overline{xx}^*)^{\otimes s} \otimes (xx^*)^{\otimes(t-s)} \rangle.
\end{aligned}$$

Hence, $\sigma_\ell$ is r-sos since $W_{\ell,s}^{T_B[s]} \succeq 0$ for each $s$. As $p = \lim_{\ell\to\infty} \sigma_\ell$, it follows that $p$ is r-sos (using the fact that the cone of r-sos polynomials in $\mathbb{C}[x, \overline{x}]_{t+1,t+1}$ is a closed set). So, (ii) holds.

Finally, we show (ii) $\Longrightarrow$ (iii), which is the most technical part. Assume $p$ is r-sos. Then, $p = \sum_\ell q_\ell^2$ for some Hermitian polynomials $q_\ell \in \mathbb{C}[x, \overline{x}]$ with total degree $t+1$ in $x, \overline{x}$. We can write

$$q_\ell(x, \overline{x}) = \sum_{s=0}^{t} \langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)} \rangle \quad \text{ for some } a_{\ell,s} \in (\mathbb{C}^n)^{\otimes(t+1)}.$$

As $q_\ell$ is Hermitian, we have $q_\ell = \overline{q_\ell}$, which implies

$$\langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)} \rangle = \langle \overline{a_{\ell,t+1-s}}, x^{\otimes(t+1-s)} \otimes \overline{x}^{\otimes s} \rangle \text{ for } s = 0, 1, \ldots, t. \tag{62}$$

Then, $q_\ell^2 = \sum_{s,s'=0}^{t} \langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)}\rangle \cdot \langle a_{\ell,s'}, \overline{x}^{\otimes s'} \otimes x^{\otimes(t+1-s')}\rangle$. As $p = \sum_\ell q_\ell^2$ has degree $t+1$ in $\overline{x}$, it follows that the following sum is identically zero:

$$\sum_\ell \sum_{s,s'=0, s+s'\neq t+1}^{t} \langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)}\rangle \cdot \langle a_{\ell,s'}, \overline{x}^{\otimes s'} \otimes x^{\otimes(t+1-s')}\rangle = 0,$$

because any monomial occurring in it has degree in $\overline{x}$ distinct from $t+1$. Therefore, we obtain

$$\begin{aligned} p = \sum_\ell q_\ell^2 &= \sum_\ell \sum_{s=0}^{t} \underbrace{\langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)}\rangle \cdot \langle a_{\ell,t+1-s}, \overline{x}^{\otimes(t+1-s)} \otimes x^{\otimes s}\rangle}_{=T_{\ell,s}} \\ &= \sum_\ell \sum_{s=0}^{t} T_{\ell,s}. \end{aligned}$$

Observe that $T_{\ell,s} = T_{\ell,t+1-s}$. This implies that $\sum_{s=0}^{t} T_{\ell,s} = \sum_{s=0}^{\tau} c_s T_{\ell,s}$ with $c_s = 2$ for $0 \le s \le \tau - 1$, $c_\tau = 2$ for odd $t$, and $c_\tau = 1$ for even $t$. Consider the summand $\sum_\ell T_{\ell,s}$ for some given $s \le \tau$. Using (62), we obtain

$$\begin{aligned} \sum_\ell T_{\ell,s} &= \sum_\ell \langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)}\rangle \cdot \langle a_{\ell,t+1-s}, \overline{x}^{\otimes(t+1-s)} \otimes x^{\otimes s}\rangle \\ &= \sum_\ell \langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)}\rangle \cdot \overline{\langle a_{\ell,s}, \overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)}\rangle} \\ &= \sum_\ell (a_{\ell,s})^* (\overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)})(\overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)})^* a_{\ell,s} \\ &= \Big\langle \sum_\ell a_{\ell,s}(a_{\ell,s})^*, (\overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)})\ (\overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)})^* \Big\rangle \\ &= \langle A_s, (\overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)})\ (\overline{x}^{\otimes s} \otimes x^{\otimes(t+1-s)})^* \rangle \\ &= \langle A_s^{T_B[s]}, x^{\otimes(t+1)}(x^{\otimes(t+1)})^* \rangle. \end{aligned}$$

Above, at the last but one line, we set $A_s = \sum_\ell a_{\ell,s}(a_{\ell,s})^*$ and, at the last line, we take the partial transpose $T_{B[s]}$ at both arguments in the inner product. Putting things together we obtain

$$\begin{aligned} p = \sum_\ell q_\ell^2 = \sum_\ell \sum_{s=0}^{t} T_{\ell,s} &= \sum_\ell \sum_{s=0}^{\tau} c_s T_{\ell,s} \\ &= \sum_{s=0}^{\tau} c_s \sum_\ell T_{\ell,s} = \Big\langle \sum_{s=0}^{\tau} c_s A_s^{B[s]}, x^{\otimes(t+1)}(x^{\otimes(t+1)})^* \Big\rangle. \end{aligned}$$

So, we have shown the polynomial identity

$$p = \langle M \otimes I_n^{\otimes(t-1)}, (xx^*)^{\otimes(t+1)}\rangle = \Big\langle \sum_{s=0}^{\tau} c_s A_s^{T_{B[s]}}, (xx^*)^{\otimes(t+1)}\Big\rangle.$$

This implies $M \otimes I_n^{\otimes(t-1)} - \sum_{s=0}^{\tau} c_s A_s^{T_{B[s]}} \in (\mathrm{BS}((\mathbb{C}^n)^{\otimes(t+1)})^\perp$. This shows that (iii) holds, since $c_s A_s^{T_{B[s]}} \in \mathcal{W}_{n,s}^{(t)}$ (because $A_s \succeq 0$). This concludes the proof of Theorem 4.1. $\square$

### 4.2 Connections between the hierarchy $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$ and the hierarchy $\mathcal{K}_n^{(t)}$

Given a matrix $X \in \mathcal{S}^n$, consider the associated bipartite states $\rho_{(X,X)}$ and $\rho_{(X,X)}^{T_B} = \rho_{(X,\cdot,X)}$, which are, respectively, CLDUI and LDUI. We focus here on the state $\rho_{(X,X)}^{T_B}$ that has the additional property of being Bose symmetric. Recall from relation (13) that

$$\rho_{(X,X)} \in \mathrm{SEP}_n \Longleftrightarrow \rho_{(X,X)}^{T_B} \in \mathrm{SEP}_n \Longleftrightarrow X \in \mathrm{CP}_n.$$

Hence, to check separability of $\rho_{(X,X)}$, a first option is to use the DPS hierarchy. However, another, likely better, option is to use the stronger $\widetilde{\mathrm{DPS}}$ hierarchy, applied to the Bose symmetric state $\rho_{(X,X)}^{T_B}$. A third option is to use the hierarchy of cones $(\mathcal{K}_n^{(t)})^*$, applied to the matrix $X$. We will now show that these last two options are in fact equivalent (see Theorem 4.5).

For this, we first establish a link on the 'dual polynomial side'. In Theorem 4.4 we essentially[8] recover the result from [GNP25, Theorem 8.11]. Here, we give a direct proof for it, based on using Theorem 4.1(ii) combined with the correspondence (24) between Hermitian r-sos polynomials and their real couterparts.

Given a matrix pair $(S,T) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$, consider the matrix $M_{S,T}$ from (49), which is CLDUI by construction, so that its partial transpose is LDUI and reads

$$M_{S,T}^{T_B} = \sum_{i,j=1}^{n} S_{ij} e_i e_i^* \otimes e_j e_j^* + \sum_{i,j=1}^{n} T_{ij} e_j e_i^* \otimes e_i e_j^*. \tag{63}$$

**Theorem 4.4.** *For $(S,T) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$, consider the matrix $M_{S,T}$ and its partial transpose $M_{S,T}^{T_B}$ as in (63), and set $A = (S + S^T + T + T^T)/2 \in \mathcal{S}^n$. For any integer $t \geq 1$, we have*

$$M_{S,T}^{T_B} \in (\widetilde{\mathrm{DPS}}_n^{(t)})^* \iff A \in \mathcal{K}_n^{(t-1)}.$$

*In particular, for any $A \in \mathcal{S}^n$, $M_{A,0}^{T_B} \in (\widetilde{\mathrm{DPS}}_n^{(t)})^* \Longleftrightarrow A \in \mathcal{K}_n^{(t-1)}$.*

*Proof.* We only need to show the first equivalence since the second one follows as a direct application. Using (63), one can easily verify the following polynomial identity:

$$\begin{aligned} p(x,\overline{x}) &:= \|x\|^{2(t-1)} \langle M_{S,T}^{T_B}, xx^* \otimes xx^* \rangle \\ &= \|x \circ \overline{x}\|^{2(t-1)} \langle A, (x \circ \overline{x})(x \circ \overline{x})^T \rangle =: f(x \circ \overline{x}), \end{aligned} \tag{64}$$

where $A = (S + S^T + T + T^T)/2$. Then, the proof amounts to comparing the r-sos property for the polynomial $p$ (in complex variables $x, \overline{x}$) at the left-hand side, with the sos property for the polynomial $f$ (in real variables $x \circ \overline{x}$) at the right-hand side. For this, write $x = x_{\mathrm{Re}} + \mathbf{i} x_{\mathrm{Im}}$, where $x_{\mathrm{Re}} = (x_{k,\mathrm{Re}})_{k=1}^n, x_{\mathrm{Im}} = (x_{k,\mathrm{Im}})_{k=1}^n \in \mathbb{R}^n$ are the real and imaginary parts of $x$. Then, we have

[8] For a pair $(A,B) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n$ with $\mathrm{diag}(A) = \mathrm{diag}(B)$, [GNP25, Theorem 8.11] shows that $\rho_{(A,\cdot,B)}$ belongs to the dual of $\widetilde{\mathrm{DPS}}_n^{(t)}$ if and only if the matrix $A + A^T + 2\mathrm{Re}(B - D_B) \in \mathcal{K}_n^{(t-1)}$. In view of relation (53), we have $\rho_{(A,\cdot,B)} = \rho_{(A,B)}^{T_B} = M_{S,T}^{T_B}$ with $S = A$ and $T = B^T - D_B$, which makes the link to Theorem 4.4.

$x \circ \overline{x} = (|x_k|^2)_{k=1}^n = (x_{\mathrm{Re},k}^2 + x_{\mathrm{Im},k}^2)_{k=1}^n$ and thus the real part of the polynomial $p$ in (64) reads

$$\begin{aligned}
&p_{\mathrm{Re}}(x_{\mathrm{Re}}, x_{\mathrm{Im}}) \\
&= \Big(\sum_{h=1}^n (x_{h,\mathrm{Re}})^2 + (x_{h,\mathrm{Im}})^2\Big)^{t-1} \sum_{h,k=1}^n A_{hk}((x_{h,\mathrm{Re}})^2 + (x_{h,\mathrm{Im}})^2)((x_{k,\mathrm{Re}})^2 + (x_{k,\mathrm{Im}})^2) \\
&= \|(x_{\mathrm{Re}}, x_{\mathrm{Im}})\|^{2(t-1)} \begin{pmatrix} x_{\mathrm{Re}} \\ x_{\mathrm{Im}} \end{pmatrix}^T \begin{pmatrix} A & A \\ A & A \end{pmatrix} \begin{pmatrix} x_{\mathrm{Re}} \\ x_{\mathrm{Im}} \end{pmatrix} \\
&= \|(x_{\mathrm{Re}}, x_{\mathrm{Im}})\|^{2(t-1)} \begin{pmatrix} x_{\mathrm{Re}} \\ x_{\mathrm{Im}} \end{pmatrix}^T (J_2 \otimes A) \begin{pmatrix} x_{\mathrm{Re}} \\ x_{\mathrm{Im}} \end{pmatrix}.
\end{aligned}$$

Hence, the polynomial $p_{\mathrm{Re}}(x_{\mathrm{Re}}, x_{\mathrm{Im}})$ is a sum of squares if and only if the matrix $J_2 \otimes A$ belongs to $\mathcal{K}_{2n}^{(t-1)}$, which, using [GL07, Lemma 15], is equivalent to asking that $A$ belongs to $\mathcal{K}_n^{(t-1)}$.

We can now complete the proof: $M_{S,T}^{T_B}$ belongs to $\widetilde{\mathrm{DPS}}_n^{(t)}$ precisely when the polynomial $p(x, \overline{x})$ is r-sos. By relation (24), $p(x, \overline{x})$ is r-sos if and only if its real part $p_{\mathrm{Re}}(x_{\mathrm{Re}}, x_{\mathrm{Im}})$ is sos, which, as shown above, is equivalent to $A$ belonging to $\mathcal{K}_n^{(t-1)}$. □

Using duality arguments, one derives the following result, recovering [GNP25, Theorem 8.16].

**Theorem 4.5.** *For a matrix $X \in \mathcal{S}^n$ and an integer $t \geq 1$, we have*

$$\rho_{(X,X)}^{T_B} \in \widetilde{\mathrm{DPS}}_n^{(t)} \iff X \in (\mathcal{K}_n^{(t-1)})^*.$$

*Proof.* Assume $\rho_{(X,X)}^{T_B} \in \widetilde{\mathrm{DPS}}_n^{(t)}$, we show $X \in (\widetilde{\mathcal{K}}_n^{(t-1)})^*$. For this, we show that $\langle X, A\rangle \geq 0$ for any $A \in \mathcal{K}_n^{(t-1)}$. By Theorem 4.4, $A \in \mathcal{K}_n^{(t-1)}$ implies $M_{A,0}^{T_B} \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$. So, combining with (51) gives

$$0 \leq \langle M_{A,0}^{T_B}, \rho_{(X,X)}^{T_B}\rangle = \langle M_{A,0}, \rho_{X,X}\rangle = \langle A, X\rangle,$$

as desired. Conversely, assume $X \in (\mathcal{K}_n^{(t-1)})^*$, we show $\rho_{(X,X)}^{T_B} \in \widetilde{\mathrm{DPS}}_n^{(t)}$. For this, we show that $\langle \rho_{(X,X)}^{T_B}, M\rangle \geq 0$ for $M \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$. As $\rho_{(X,X)}^{T_B}$ is LDUI, equality $\langle \rho_{(X,X)}^{T_B}, M\rangle = \langle \rho_{(X,X)}^{T_B}, \Pi_{\mathrm{LDUI}}(M)\rangle$ holds. By Lemma 4.3, projecting onto $\mathrm{LDUI}_n$ preserves membership in the cone $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$. Hence, we may assume that $M$ is LDUI, i.e., of the form $M = M_{S,T}^{T_B}$ for some $S, T$. By Theorem 4.4, $M_{S,T}^{T_B} \in (\widetilde{\mathrm{DPS}}_n^{(t)})^*$ implies $S + S^T + T + T^T \in \mathcal{K}_n^{(t-1)}$. Then, we have

$$\langle M, \rho_{(X,X)}^{T_B}\rangle = \langle M_{S,T}^{T_B}, \rho_{(X,X)}^{T_B}\rangle = \langle M_{S,T}, \rho_{(X,X)}\rangle = \langle X, (S + S^T + T + T^T)/2\rangle \geq 0,$$

as desired. □

### 4.3 A class of Bose symmetric LDOI states

As an illustration we consider here a class of Bose symmetric states with LDOI structure. Given scalars $a, b \in \mathbb{R}$, consider the matrix $\rho(a,b) := \rho_{(X,Y,X)} \in \mathrm{Herm}(\mathbb{C}^3 \otimes \mathbb{C}^3)$, with

$$X = \begin{pmatrix} 1 & a & a \\ a & 1 & a \\ a & a & 1 \end{pmatrix}, Y = \begin{pmatrix} 1 & b & b \\ b & 1 & b \\ b & b & 1 \end{pmatrix},\ \rho(a,b) = \begin{pmatrix} 1 & b & b \\ b & 1 & b \\ b & b & 1 \end{pmatrix} \oplus \begin{pmatrix} a & a \\ a & a \end{pmatrix} \oplus \begin{pmatrix} a & a \\ a & a \end{pmatrix} \oplus \begin{pmatrix} a & a \\ a & a \end{pmatrix}, \quad (65)$$

where the first block is indexed by $\{11, 22, 33\}$ and the last three blocks are indexed, respectively, by $\{12, 21\}$, $\{23, 32\}$ and $\{31, 13\}$. Then, $\rho(a, b) \in \mathrm{LDOI}_3 \cap \mathrm{BS}(\mathbb{C}^3)$ (recall (15)) and thus any separable decomposition of it must be symmetric (Lemma 2.3).

In view of (65), $\rho(a, b)$ is a quantum state (i.e., $\rho(a, b) \succeq 0$) precisely when $a \geq 0$ and $-\frac{1}{2} \leq b \leq 1$. As we see in Lemma 4.6, separability of $\rho(a, b)$ is characterized already at the first level of the DPS hierarchy. This extends to the case when $X, Y$ are defined analogously with size $n \geq 3$, now requiring $-\frac{1}{n-1} \leq b$ instead of $-\frac{1}{2} \leq b$. More generally, equivalence of membership in $\mathrm{DPS}_n^{(1)}$ and $\mathrm{SEP}_n$ holds for LDOI states of the form $\rho_{(X,Y,Z)}$, where each of $X, Y, Z$ lies in the linear span of $I_n$ and the all-ones matrix $J_n$, see [PJPY24, Theorem 4.1] and [GNS25, Theorem III.3]. We yet give the (easy) details for the states $\rho(a, b)$ since this also provides examples of real-valued separable states that do not have real separable decompositions (Remark 4.7).

**Lemma 4.6.** *Given scalars $a, b \in \mathbb{R}$, we have*

$$\rho(a, b) \in \mathrm{SEP}_3 \Longleftrightarrow \rho(a, b) \in \mathrm{DPS}_3^{(1)} \Longleftrightarrow -\frac{1}{2} \leq b \text{ and } |b| \leq a \leq 1.$$

*Proof.* Only two implications need a proof. First, assume $\rho(a, b) \in \mathrm{DPS}_3^{(1)}$, we show that $-\frac{1}{2} \leq b$ and $|b| \leq a \leq 1$. Indeed, the first condition follows since $\rho(a, b) \succeq 0$ and the second one from the fact that $\rho(a, b)^{T_B} \succeq 0$, since

$$\rho(a, b)^{T_B} = \rho_{(X,X,Y)} = \begin{pmatrix} 1 & a & a \\ a & 1 & a \\ a & a & 1 \end{pmatrix} \oplus \begin{pmatrix} a & b \\ b & a \end{pmatrix} \oplus \begin{pmatrix} a & b \\ b & a \end{pmatrix} \oplus \begin{pmatrix} a & b \\ b & a \end{pmatrix}.$$

Assume now that $-\frac{1}{2} \leq b$ and $|b| \leq a \leq 1$, we show that $\rho(a, b) \in \mathrm{SEP}_3$. For this note that the set

$$\left\{(a, b) \in \mathbb{R}^2 : |b| \leq a \leq 1,\ -\frac{1}{2} \leq b\right\}$$

is convex bounded, and equals the convex hull of the four points $(0, 0)$, $(1, 1)$, $\left(\frac{1}{2}, -\frac{1}{2}\right)$, and $\left(1, -\frac{1}{2}\right)$. Hence, it suffices to show that $\rho(a, b)$ is separable for each of them. For $(a, b) = (0, 0)$ we have

$$\rho(0, 0) = (e_1 e_1^*)^{\otimes 2} + (e_2 e_2^*)^{\otimes 2} + (e_3 e_3^*)^{\otimes 2} \in \mathrm{SEP}_3.$$

The all-ones bipartite state $(ee^*)^{\otimes 2}$ (with $e = \sum_{i=1}^{3} e_i$) is separable, hence also its projection $\rho(1, 1) = \Pi_{\mathrm{LDOI}}((ee^*)^{\otimes 2})$ is separable. Next, one can verify that

$$\begin{gathered} \rho\Big(\frac{1}{2}, -\frac{1}{2}\Big) = \frac{1}{2} \Pi_{\mathrm{LDOI}}((xx^*)^{\otimes 2} + (yy^*)^{\otimes 2} + (zz^*)^{\otimes 2}), \\ \text{with } x = \begin{pmatrix} 0 \\ 1 \\ \mathbf{i} \end{pmatrix}, y = \begin{pmatrix} 1 \\ 0 \\ \mathbf{i} \end{pmatrix}, z = \begin{pmatrix} 1 \\ \mathbf{i} \\ 0 \end{pmatrix}, \end{gathered} \tag{66}$$

$$\begin{gathered} \rho\Big(1, -\frac{1}{2}\Big) = \Pi_{\mathrm{LDOI}}((uu^*)^{\otimes 2} + (vv^*)^{\otimes 2}), \\ \text{with } u = \begin{pmatrix} e^{\frac{\mathbf{i}\pi}{3}} \\ e^{\frac{-\mathbf{i}\pi}{3}} \\ 1 \end{pmatrix}, \quad v = \begin{pmatrix} e^{\frac{2\mathbf{i}\pi}{3}} \\ e^{\frac{-2\mathbf{i}\pi}{3}} \\ 1 \end{pmatrix}. \end{gathered} \tag{67}$$

Hence, $\rho(a, b) \in \mathrm{SEP}_3$ in both cases, again because the LDOI projection preserves separability. $\square$

**Remark 4.7.** *Observe that, if $a = b \in [0,1]$, then $\rho(a,b)$ has a separable decomposition that involves only real-valued rank one states (since this is the case for $\rho(0,0)$ and $\rho(1,1)$). However, if $b < a$, then no separable decomposition exists that uses only real-valued rank one states. To see this, observe that if $\rho(a,b) = \sum_\ell (x_\ell x_\ell^*)^{\otimes 2}$ for some $x_\ell \in \mathbb{R}^3$, then we have $b = \rho(a,b)_{11,22} = \sum_\ell (x_\ell)_1^2 (x_\ell)_2^2 = \rho(a,b)_{12,12} = a$. In particular, if $b = 0 < a \leq 1$, then $\rho(a,0) = \rho_{(X,\cdot,X)}$ (resp., $\rho(a,0)^{T_B} = \rho_{(X,X)}$) is LDUI (resp., CLDUI), separable, and has no real-valued separable decomposition.*

*In addition, observe that, for $b = -1/2$, any separable decomposition of the form $\rho(a,-1/2) = \sum_\ell (x_\ell x_\ell^*)^{\otimes 2}$ must satisfy the condition $\sum_\ell (x_\ell)_i^2 = 0$ for $i \in [3]$. Indeed, the vector $\sum_{i=1}^3 e_i \otimes e_i$ belongs to the kernel of $\rho(a,-1/2)$, and thus also to the kernel of each $(x_\ell x_\ell^*)^{\otimes 2}$, which implies the claimed fact. Hence, we again see that the $x_\ell$'s cannot be real-valued, and this also indicate how to come up with the separable decompositions from (66) and (67).*

# 5 Implementation

In this section we consider the question of how to implement the DPS hierarchy more efficiently in practice. For this, we reformulate it using the moment approach within the polynomial optimization framework. We do this first in the generic case and then we consider the CLDUI and LDOI cases. We conclude with a comparison of runtimes in the different regimes by showing how the developed sparsity reduction technique can be used to tackle a class of examples motivated by the PPT$^2$ conjecture from quantum information theory.

## 5.1 The DPS hierarchy in the moment formalism

Suppose one is given a bipartite quantum state $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)_+$ and one wants to test whether $\rho_{AB}$ lies in a given level $t$ of the DPS hierarchy, i.e., whether $\rho_{AB} \in \mathrm{DPS}_n^{(t)}$. The obvious way to do so is to implement the semidefinite program modeling definition (28), asking for the existence of an extended state $\rho_{AB[t]} \in \mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$ that is positive semidefinite under partial transposition of the $B$-registers and recovers the original state $\rho_{AB}$ by taking a partial trace. We refer to this original viewpoint as the 'tensor formalism'.

In the tensor formalism the resulting SDP inherits redundancies arising from the symmetries in the $t$ $B$-registers as required in (25): for any $\sigma \in \mathfrak{G}_t$ and $i_0\underline{i} \in [n]^{t+1}$, the columns (and rows) indexed by $i_0\underline{i}$ and $i_0\underline{i}^\sigma$ are identical, i.e., $(\rho_{AB[t]})_{\cdot, i_0\underline{i}^\sigma} = (\rho_{AB[t]})_{\cdot, i_0\underline{i}}$. Hence, one can set up an equivalent, reduced SDP that is obtained by keeping only one column out of the orbit consisting of the columns indexed by $i_0\underline{i}^\sigma$ for $\sigma \in \mathfrak{G}_t$. An example of this fact was seen in Lemma 3.18 (and its proof), where it was used to show that the block of a $\mathrm{DPS}^{(2)}$-certificate indexed, e.g., by $\{123, 132\}$, is a scalar multiple of the all-ones matrix.

A way to carry out this reduction more systematically is to consider the DPS hierarchy in the 'moment formalism', as has been developed in [GLS21]. For this, note that two elements $i_0\underline{i}, j_0\underline{j} \in [n]^{t+1}$ indexing the extended state $\rho_{AB[t]}$ lie in the same orbit of $\mathfrak{G}_t$ if and only if $i_0 = j_0$ and $\alpha(\underline{i}) = \alpha(\underline{j})$. Hence, roughly speaking, it suffices to index the extended state by elements $\alpha(i_0)\alpha(\underline{i}) \in \mathbb{N}^n \times \mathbb{N}^n$ (indexing monomials) instead of sequences $i_0\underline{i} \in [n]^{t+1}$.

More precisely, the moment approach works as follows. We consider Hermitian linear functionals $L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t})^*$, i.e., $L : \mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t} \to \mathbb{C}$ acting on bihomogenous polynomials of degree 2 in $x, \overline{x}$ and of degree $2t$ in $y, \overline{y}$. Being Hermitian means that $L(\overline{p}) = \overline{L(p)}$ for any polynomial $p \in \mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t}$. Then, the corresponding moment matrix of $L$, denoted here as $M_{1,t}(L)$, is indexed by elements $(\alpha,\alpha',\beta,\beta') \in (\mathbb{N}^n)^4$ such that $|\alpha+\alpha'| = 1$ and $|\beta+\beta'| = t$; its $(\alpha\alpha'\beta\beta', \tilde{\alpha}\tilde{\alpha}'\tilde{\beta}\tilde{\beta}')$-

entry is $M_{1,t}(L)_{\alpha\alpha'\beta\beta',\tilde\alpha\tilde\alpha'\tilde\beta\tilde\beta'}$ , defined as

$$L(x^{\alpha}\overline{x}^{\alpha'}y^{\beta}\overline{y}^{\beta'} \cdot \overline{x^{\tilde\alpha}\overline{x}^{\tilde\alpha'}y^{\tilde\beta}\overline{y}^{\tilde\beta'}}) = L(x^{\alpha+\tilde\alpha'}\overline{x}^{\alpha'+\tilde\alpha}y^{\beta+\tilde\beta'}\overline{y}^{\beta'+\tilde\beta}).$$

Hence, $M_{1,t}(L)$ is a Hermitian matrix since $L$ is Hermitian. Moreover, we have $M_{1,t}(L) \succeq 0$ if and only if $L(p\overline{p}) \geq 0$ for any $p \in \mathbb{C}[x,\overline{x},y,\overline{y}]_{=1,=t}$, which reflects the fact that the moment approach is dual to the sum of squares approach used earlier. The key connection between the 'tensor formalism' and the 'moment formalism' is then established by setting

$$L(xx^* \otimes (yy^*)^{\otimes t}) = \rho_{AB[t]}, \tag{68}$$

where $L$ is applied entrywise to the matrix $xx^* \otimes (yy^*)^{\otimes t}$. Indeed, any linear functional $L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t})^*$ defines via (68) an extended state lying in $\mathrm{Herm}(\mathbb{C}^n \otimes S^t(\mathbb{C}^n))$ that satisfies (25). Conversely, given such an extended state $\rho_{AB[t]}$, relation (68) permits to define a linear functional $L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t})^*$ as follows: For $(\gamma,\gamma',\delta,\delta') \in (\mathbb{N}^n)^4$ such that $|\gamma+\gamma'| = 2$ and $|\delta+\delta'| = 2t$, set

$$L(x^{\gamma}\overline{x}^{\gamma'}y^{\delta}\overline{y}^{\delta'}) = (\rho_{AB[t]})_{i_0\underline{i},j_0\underline{j}} \text{ if } |\gamma| = |\gamma'| = 1 \text{ and } |\delta| = |\delta'| = t, \tag{69}$$

where $\gamma = \alpha(i_0), \gamma' = \alpha(j_0), \delta = \alpha(\underline{i}), \delta' = \alpha(\underline{j})$ and, otherwise, set $L$ to 0, i.e.,

$$L(x^{\gamma}\overline{x}^{\gamma'}y^{\delta}\overline{y}^{\delta'}) = 0 \text{ if } |\gamma| \neq |\gamma'| \text{ or } |\delta| \neq |\delta'|. \tag{70}$$

For the moment matrix of $L$, property (70) implies that $M_{1,t}(L)_{\alpha\alpha'\beta\beta',\tilde\alpha\tilde\alpha'\tilde\beta\tilde\beta'} \neq 0$ only if $|\alpha+\tilde\alpha'| = |\alpha'+\tilde\alpha| = 1$ and $|\beta+\tilde\beta'| = |\beta'+\tilde\beta| = t$. As observed in [GLS21, Section 5.2], this permits to show that the matrix $M_{1,t}(L)$ is block-diagonal and that its blocks are indexed[9] by the following sets

$$I_{r,s'} = \{(\alpha,\alpha',\beta,\beta') \in (\mathbb{N}^n)^4 : |\alpha+\alpha'| = 1, |\beta+\beta'| = t, |\alpha|-|\alpha'| = r, |\beta|-|\beta'| = s'\}$$

for $r \in \{-1,1\}$ and $s' \in \{-t,-t+2,-t+4,\ldots,t-4,t-2,t\}$. As we see in the next lemma, it suffices to consider $r=1$, in which case any $(\alpha,\alpha',\beta,\beta') \in I_{1,s}$ has $\alpha' = 0$, so that the entry $\alpha'$ can be ignored.

**Lemma 5.1.** *[GLS21] Let $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$. Then, $\rho_{AB} \in \mathrm{DPS}_n^{(t)}$ if and only if there exists a Hermitian linear functional $L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t})^*$ satisfying conditions (70) and (i),(ii) below:*

*(i) $L(xx^* \otimes yy^*||y||^{2(t-1)}) = \rho_{AB}$,*

*(ii) $M_{1,t}(L) \succeq 0$ or, equivalently, $M_{1,t}(L)[I_{r,s'}] \succeq 0$ for $r=1$ and $s' \in [-t,t]$ with $s' \equiv t$ (mod 2).*

*Proof.* The lemma essentially follows[10] from results in [GLS21, Section 5], we give a sketch of proof. As mentioned above, the guiding fact for the proof is relation (68) stating $\rho_{AB[t]} = L(xx^*\otimes(yy^*)^{\otimes t})$, which indicates how to construct a $\mathrm{DPS}^{(t)}$-certificate from a linear functional and vice versa.

[9] As we see in the proof of Lemma 5.1, the principal submatrix of $M_{1,t}(L)$ indexed by $I_{1,s'}$ corresponds to applying the partial transpose $T_{B[s]}$ to $\rho_{AB[t]}$, when $s' = t-2s$. This explains why we use the letter $s'$ here.

[10] We refer in particular to [GLS21, Prop.23] (which considers the general case where also the $A$-register is extended). There, the statement is in terms of existence of a linear functional $\tilde L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{\leq 2,\leq 2t})^*$ satisfying the 'ideal' conditions $\tilde L(p(1-\|x\|^2) = \tilde L(p(1-\|y\|^2) = 0$ for all $p \in \mathbb{C}[x,\overline{x},y,\overline{y}]$ such that $p(1-\|x\|^2), p(1-\|y\|^2) \in \mathbb{C}[x,\overline{x},y,\overline{y}]_{\leq 2,\leq 2t}$. This non-homogeneous setting was used in [GLS21] to give an alternative, real-algebraic proof for the completeness of the DPS hierarchy. Note that one can easily navigate between the non-homogeneous and homogeneous settings: by restricting $\tilde L$ to $\mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t}$ and, conversely, one can extend $L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{2,2t})^*$ to $\tilde L \in (\mathbb{C}[x,\overline{x},y,\overline{y}]_{\leq 2,\leq 2t})^*$ using the above 'ideal' constraints combined with (70).

First, note that $L(xx^* \otimes (yy^*)^{\otimes t})$ clearly satisfies condition (25). Second, note that condition (i) precisely corresponds to condition (27), since

$$\mathrm{Tr}_{B[2:t]}(L(xx^* \otimes (yy^*)^{\otimes t})) = L(\mathrm{Tr}_{B[2:t]}(xx^* \otimes (yy^*)^{\otimes t})) = L(xx^* \otimes yy^* ||y||^{2(t-1)}).$$

There remains to relate condition (ii) to condition (26). As observed above, under condition (70), $M_{1,t}(L)$ is block-diagonal, with its blocks indexed by the sets $I_{r,s'}$ for $r = \pm 1$ and $-t \leq s' \leq t$ with $s' \equiv t \pmod 2$. Hence, $M_{1,t}(L) \succeq 0$ if and only if $M_t(L)[I_{r,s'}] \succeq 0$ for all $r \in \{-1, 1\}$ and $s' \in \{-t, -t+2, \ldots, t-2, t\}$. Moreover, one can restrict to $r = 1$, since $L$ being Hermitian implies

$$M_{1,t}(L)[I_{r,s'}] = \overline{M_{1,t}(L)[I_{-r,-s'}]}$$

(and positive semidefiniteness is preserved under taking the complex conjugate). For $\rho_{AB[t]} = L(xx^* \otimes (yy^*)^{\otimes t})$ and $s \in \{0, 1, \ldots, t\}$, we have $(\rho_{AB[t]})^{T_{B[s]}} = L(xx^* \otimes (\overline{yy}^*)^{\otimes s} \otimes (yy^*)^{\otimes(t-s)})$ and thus $(\rho_{AB[t]})^{T_{B[s]}} \succeq 0$ if and only if $\widetilde{\rho} := L(xx^* \otimes (yy^*)^{\otimes(t-s)} \otimes (\overline{yy}^*)^{\otimes s}) \succeq 0$. The final step now relies on the fact (see relation (67) in [GLS21]) that $M_{1,t}(L)[I_{1,t-2s}]$ is identical to the matrix obtained from $\widetilde{\rho}$, by removing its identical rows and columns (arising from the Bose symmetry of the $t$ B-registers, as explained above). Hence, condition (ii) is equivalent to (26), as desired. $\square$

### 5.2 The DPS hierarchy for CLDUI and LDOI states in the moment formalism

We now specialize the result of Lemma 5.1 for bipartite states with CLDUI or LDOI sparsity structure. For $\alpha \in \mathbb{N}^n$, $\alpha \equiv 0 \pmod 2$ means that $\alpha_i$ is even for all $i \in [n]$.

**Lemma 5.2.** *Let $\rho_{AB} \in \mathrm{CLDUI}_n$ (resp., $\rho_{AB} \in \mathrm{LDOI}_n$). Then, $\rho_{AB} \in \mathrm{DPS}_n^{(t)}$ if and only if there exists a Hermitian linear functional $L \in (\mathbb{C}[x, \overline{x}, y, \overline{y}]_{2,2t})^*$ satisfying (70), conditions (i),(ii) from Lemma 5.1, and, for any $\gamma, \gamma', \delta, \delta' \in \mathbb{N}^n$ such that $|\gamma| = |\gamma'| = 1$ and $|\delta| = |\delta'| = t$,*

$$L(x^\gamma \overline{x}^{\gamma'} y^\delta \overline{y}^{\delta'}) = 0 \quad \text{if } \gamma + \delta' \neq \gamma' + \delta \quad (\text{resp., if } \gamma + \gamma' + \delta + \delta' \not\equiv 0 \ (\mathrm{mod}\ 2)).$$

*Proof.* Consider a $\mathrm{DPS}^{(t)}$-certificate $\rho_{AB[t]}$ for $\rho_{AB}$ and the associated linear functional $L$ defined via (68) as in Lemma 5.1. In particular, relations (69) and (70) hold. Assume first $\rho_{AB[t]} \in \mathrm{CLDUI}_n^{(t)}$. Then, by Lemma 3.2 (iii) (and the definition of the sparsity pattern $\Omega_n^{(t)}$ in (55)), $(\rho_{AB[t]})_{i_0\underline{i}, j_0\underline{j}} = 0$ if $e_{i_0} + \alpha(\underline{j}) \neq e_{j_0} + \alpha(\underline{j})$, which implies $L(x^\gamma \overline{x}^{\gamma'} y^\delta \overline{y}^{\delta'}) = 0$ if $\gamma + \delta' \neq \gamma' + \delta$.

Assume now $\rho_{AB[t]} \in \mathrm{LDOI}^{(t)}$. Then, its sparsity pattern is provided by the set $\Psi_n^{(t)}$ from (59). Hence, $(\rho_{AB[t]})_{i_0\underline{i}, j_0\underline{j}} = 0$ if $\alpha(i_0\underline{i}j_0\underline{j}) \neq 0 \pmod 2$, which implies $L(x^\gamma \overline{x}^{\gamma'} y^\delta \overline{y}^{\delta'}) = 0$ if $\gamma + \gamma' + \delta + \delta' \not\equiv 0 \pmod 2$. $\square$

In Tables 4, 5 and 6 below, we display the block sizes that arise when reformulating the DPS hierarchy in the moment formalism, in the following three regimes: $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ (generic case), $\rho_{AB} \in \mathrm{LDOI}_n$ (LDOI case), $\rho_{AB} \in \mathrm{CLDUI}_n$ (CLDUI case), respectively, We display these block sizes for $t = 2, 3, 4, 5, 6, 7$ and $n = 3, 4, 5$, and the notation $m_k$ is used to indicate that there are $k$ blocks of size $m$. For instance, for $(t, n) = (2, 3)$, the entry '$27_1, 18_2$' in Table 4 indicates that the SDP implementing the $\mathrm{DPS}^{(2)}$-relaxation for generic states in $\mathrm{Herm}(\mathbb{C}^3 \otimes \mathbb{C}^3)$ involves one block of size 27 and two blocks of size 18. We next give some more details for the case $(t, n) = (2, 3)$.

**Example 5.3.** *We consider the case $(t, n) = (2, 3)$ and discuss the associated entries in Tables 4 and 6, which give the block sizes in the reduced SDP's modeling existence of a $\mathrm{DPS}^{(2)}$-certificate in the moment formulation, for a generic or CLDUI bipartite state $\rho_{AB} \in \mathrm{Herm}(\mathbb{C}^3 \otimes \mathbb{C}^3)$.*

*Consider first the generic case. In the tensor formulation, the SDP involves three blocks of size* $3^3 = 27$*, corresponding to* $\rho_{AB[2]}, \rho_{AB[2]}^{T_{B[1]}}$ *and* $\rho_{AB[2]}^{T_{B[2]}}$*. In the moment formulation, both* $\rho_{AB[2]}$ *and* $\rho_{AB[2]}^{T_{B[2]}}$ *reduce to blocks of size 18 and* $\rho_{AB[2]}^{T_{B[1]}}$ *remains of size 27, thus matching the entry '*$27_1, 18_2$*' in Table 4. We will now argue why these size reductions do occur.*

*First, let us see why* $\rho_{AB[2]}$ *reduces to a block of size 18. Consider two rows of* $\rho_{AB[2]}$ *indexed by distinct* $i_0i_1i_2, j_0j_1j_2 \in [3]^2$*. If* $i_0 = j_0$ *and* $\{i_1, i_2\} = \{j_1, j_2\}$ *then, by (25), these two rows are equal and they correspond to a single row of* $M_{1,2}(L)$ *indexed by* $(\alpha = e_{i_0}, \alpha' = 0, \beta = \alpha(i_1i_2), \beta' = 0)$*. All possible reductions of this form arise for* $(i_012, i_021)$*,* $(i_013, i_031)$*, and* $(i_023, i_032)$ *for* $i_0 \in [3]$*. Hence, one can remove 9 rows/columns from* $\rho_{AB[2]}$ *so that it reduces to a block of size* $27 - 9 = 18$*.*

*The same analysis applies to* $\rho_{AB[2]}^{T_{B[2]}}$ *since the partial conjugate is applied to both B-registers, and thus* $\rho_{AB[2]}^{T_{B[2]}}$ *also reduces to a block of size 18. Note that, as expected, the row of* $\rho_{AB[2]}^{T_{B[2]}}$ *indexed by* $i_0i_1i_2$ *corresponds to the row of* $M_{1,2}(L)$ *indexed by* $(\alpha = e_{i_0}, \alpha' = 0, \beta = 0, \beta' = \alpha(i_1i_2))$*.*

*Consider now* $\rho_{AB[2]}^{T_{B[1]}}$*. By the definition of the partial transpose, for* $i_0i_1i_2$*,* $j_0j_1j_2, k_0k_1k_2 \in [3]^3$*,* $(\rho_{AB[2]}^{T_{B[1]}})_{i_0i_1i_2,k_0k_1k_2} = (\rho_{AB[2]}^{T_{B[1]}})_{j_0j_1j_2,k_0k_1k_2}$ *if and only if* $(\rho_{AB[2]})_{i_0k_1i_2,k_0i_1k_2} = (\rho_{AB[2]})_{j_0k_1j_2,k_0j_1k_2}$*. The latter equality holds using condition (25) only if* $i_0 = j_0$*,* $\{k_1, i_2\} = \{k_1, j_2\}$*,* $\{i_1, k_2\} = \{j_1, k_2\}$*, which implies* $i_0i_1i_2 = j_0j_1j_2$*. Hence, no size reduction can occur. Note that the row of* $\rho_{AB[2]}^{T_{B[1]}}$ *indexed by* $i_0i_1i_2$ *corresponds to the row of* $M_{1,2}(L)$ *indexed by* $(\alpha = e_{i_0}, \alpha' = 0, \beta = e_{i_2}, \beta' = e_{i_1})$*.*

*Assume now* $\rho_{AB} \in \mathrm{CLDUI}_3$*. In the tensor formalism, the SDP modeling a* $\mathrm{DPS}^{(2)}$*-certificate* $\rho_{AB[2]} \in \mathrm{CLDUI}_3^{(2)}$ *involves* $5_3, 2_3, 1_6$ *blocks for* $\rho_{AB[2]}$ *(see Table 1),* $5_3, 2_3, 1_6$ *blocks for* $\rho_{AB[2]}^{T_{B[1]}}$ *(see Table 2), and* $6_1, 3_6, 1_3$ *blocks for* $\rho_{AB[2]}^{T_{B[2]}}$ *(see Table 3), leading to a total of* $6_1, 5_6, 3_6, 2_6, 1_{15}$ *blocks. In comparison, the SDP in the moment formulation involves a total of* $5_3, 3_4, 2_9, 1_{18}$ *blocks, as can be seen in Table 6. To see why this size reduction takes place, it suffices to check all the maximal cliques that are listed in Tables 1, 2, 3. For each such clique, one just checks whether it contains two distinct indices* $i_0i_1i_2$ *and* $j_0j_1j_2$ *such that* $i_0 = j_0$ *and* $\{i_1, i_2\} = \{j_1, j_2\}$*, in which case one of them is removed from the clique. So, in Table 1, each clique of size 5 (resp., size 2) reduces to size 3 (resp., size 1), yielding block sizes* $3_3, 1_9$ *after reduction. In Table 2, no size reduction applies, so one keeps* $5_3, 2_3, 1_6$ *as block sizes. Finally, in Table 3, the clique of size 6 reduces to size 3 and each clique of size 3 reduces to size 2, yielding block sizes* $3_1, 2_6, 1_3$*. Putting things together one indeed arrives at a total of* $5_3, 3_4, 2_9, 1_{18}$ *blocks as shown in Table 6.*

| $t \backslash n$ | 3 | 4 | 5 |
|---|---|---|---|
| 2 | $27_1$, $18_2$ | $64_1$, $40_2$ | $125_1$, $75_2$ |
| 3 | $54_2$, $30_2$ | $160_2$, $80_2$ | $375_2$, $175_2$ |
| 4 | $108_1$, $90_2$, $45_2$ | $400_1$, $320_2$, $140_2$ | $1125_1$, $875_2$, $350_2$ |
| 5 | $180_2$, $135_2$, $63_2$ | $800_2$, $560_2$, $224_2$ | $2625_2$, $1750_2$, $630_2$ |
| 6 | $300_1$, $270_2$, $189_2$, $84_2$ | $1600_1$, $1400_2$, $896_2$, $336_2$ | $6125_1$, $5250_2$, $3150_2$, $1050_2$ |
| 7 | $450_2$, $378_2$, $252_2$, $108_2$ | $2800_2$, $2240_2$, $1344_2$, $480_2$ | $12250_2$, $9450_2$, $5250_2$, $1650_2$ |

Table 4: Block sizes in the moment formulation of $\mathrm{DPS}^{(t)}$-certificates for generic states

We now want to give some insight on how the size of the biggest block involved in the SDP in the generic setting compares to the biggest block in the LDOI setting. We restrict ourselves to the LDOI case, since going from generic to LDOI yields a far greater reduction in size than going from LDOI to CLDUI. Furthermore, the analysis in the LDOI case is significantly easier because

| $t\backslash n$ | 3 | 4 | 5 |
|---|---|---|---|
| 2 | $7_3$, $6_1$, $5_6$, $3_2$ | $10_4$, $7_8$, $6_4$, $3_8$ | $13_5$, $9_{10}$, $6_{10}$, $3_{20}$ |
| 3 | $15_2$, $13_6$, $9_2$, $7_6$ | $28_2$, $20_{12}$, $16_2$, $12_2$, $10_{12}$, $4_2$ | $45_2$, $27_{20}$, $25_2$, $13_{20}$, $12_{10}$, $4_{10}$ |
| 4 | $28_3$, $24_1$, $23_6$,<br>$21_2$, $12_6$, $9_2$ | $58_4$, $46_8$, $42_4$,<br>$34_8$, $22_8$, $13_8$ | $99_5$, $77_{10}$, $60_{10}$, $47_{20}$, $35_{10}$,<br>$30_1$, $20_2$, $17_{20}$, $5_2$ |
| 5 | $48_2$, $44_6$, $36_2$,<br>$33_6$, $18_2$, $15_6$ | $124_2$, $100_{12}$, $88_2$, $76_2$, $70_{12}$,<br>$52_2$, $40_2$, $28_{12}$, $16_2$ | $255_2$, $180_{20}$, $175_2$, $121_{20}$, $114_{10}$,<br>$75_2$, $73_{10}$, $45_{20}$, $21_{10}$ |
| 6 | $76_3$, $72_1$, $69_6$, $63_2$,<br>$48_6$, $45_2$, $22_6$, $18_2$ | $218_4$, $193_8$, $182_4$, $157_8$,<br>$124_8$, $100_8$, $50_8$, $34_8$ | $479_5$, $417_{10}$, $350_{10}$, $297_{20}$, $255_{10}$, $230_1$,<br>$195_2$, $177_{20}$, $105_2$, $95_{10}$, $55_{20}$, $25_2$ |
| 7 | $117_2$, $111_6$, $99_2$,<br>$93_6$, $66_2$, $62_6$,<br>$30_2$, $26_6$ | $404_2$, $350_{12}$, $328_2$, $296_2$,<br>$280_{12}$, $232_2$, $200_2$, $168_{12}$,<br>$136_2$, $80_2$, $60_{12}$, $40_2$ | $1045_2$, $825_2$, $817_{20}$, $633_{20}$,<br>$607_{10}$, $475_2$, $459_{10}$, $355_{20}$,<br>$245_{10}$, $175_2$, $115_{20}$, $65_{10}$ |

Table 5: Block sizes in the moment formulation of $\mathrm{DPS}^{(t)}$-certificates for states in $\mathrm{LDOI}_n$

| $t\backslash n$ | 3 | 4 | 5 |
|---|---|---|---|
| 2 | $5_3$, $3_4$, $2_9$, $1_{18}$ | $7_4$, $4_4$, $3_4$, $2_{24}$, $1_{40}$ | $9_5$, $5_5$, $3_{10}$, $2_{50}$, $1_{75}$ |
| 3 | $9_1$, $7_3$, $5_9$,<br>$3_9$, $2_{18}$, $1_{30}$ | $16_1$, $10_6$, $7_{16}$, $4_{11}$,<br>$3_{16}$, $2_{60}$, $1_{80}$ | $25_1$, $13_{10}$, $9_{25}$, $5_{15}$,<br>$4_5$, $3_{50}$, $2_{150}$, $1_{175}$ |
| 4 | $12_3$, $9_4$, $7_9$, $5_{18}$,<br>$3_{16}$, $2_{30}$, $1_{45}$ | $22_4$, $16_4$, $13_4$, $10_{24}$, $7_{40}$,<br>$4_{24}$, $3_{40}$, $2_{120}$, $1_{140}$ | $35_5$, $25_5$, $17_{10}$, $13_{50}$, $9_{75}$,<br>$5_{36}$, $4_{25}$, $3_{150}$, $2_{350}$, $1_{350}$ |
| 5 | $18_1$, $15_3$, $12_9$,<br>$9_9$, $7_{18}$, $5_{30}$,<br>$3_{25}$, $2_{45}$, $1_{63}$ | $40_1$, $28_6$, $22_{16}$, $16_{11}$,<br>$13_{16}$, $10_{60}$, $7_{80}$, $4_{45}$,<br>$3_{80}$, $2_{210}$, $1_{224}$ | $75_1$, $45_{10}$, $35_{25}$, $25_{15}$, $21_5$,<br>$17_{50}$, $13_{150}$, $9_{175}$, $5_{75}$,<br>$4_{75}$, $3_{350}$, $2_{700}$, $1_{630}$ |
| 6 | $22_3$, $18_4$, $15_9$, $12_{18}$,<br>$9_{16}$, $7_{30}$, $5_{45}$,<br>$3_{36}$, $2_{63}$, $1_{84}$ | $50_4$, $40_4$, $34_4$, $28_{24}$, $22_{40}$,<br>$16_{24}$, $13_{40}$, $10_{120}$, $7_{140}$,<br>$4_{76}$, $3_{140}$, $2_{336}$, $1_{336}$ | $95_5$, $75_5$, $55_{10}$, $45_{50}$, $35_{75}$,<br>$25_{36}$, $21_{25}$, $17_{150}$, $13_{350}$, $9_{350}$,<br>$5_{141}$, $4_{175}$, $3_{700}$, $2_{1260}$, $1_{1050}$ |
| 7 | $30_1$, $26_3$, $22_9$, $18_9$,<br>$15_{18}$, $12_{30}$, $9_{25}$, $7_{45}$,<br>$5_{63}$, $3_{49}$, $2_{84}$, $1_{108}$ | $80_1$, $60_6$, $50_{16}$, $40_{11}$, $34_{16}$,<br>$28_{60}$, $22_{80}$, $16_{45}$, $13_{80}$, $10_{210}$,<br>$7_{224}$, $4_{119}$, $3_{224}$, $2_{504}$, $1_{480}$ | $175_1$, $115_{10}$, $95_{25}$, $75_{15}$, $65_5$, $55_{50}$,<br>$45_{150}$, $35_{175}$, $25_{75}$, $21_{75}$, $17_{350}$, $13_{700}$,<br>$9_{630}$, $5_{245}$, $4_{350}$, $3_{1260}$, $2_{2100}$, $1_{1650}$ |

Table 6: Block sizes in the moment formulation of $\mathrm{DPS}^{(t)}$-certificates for states in $\mathrm{CLDUI}_n$

the LDOI condition in Lemma 5.2 is 'global', in the same sense as explained before Lemma 3.10. We fix $n \in \mathbb{N}$, $t \geq 1$, $s' \in [-t, t]$ such that $s' \equiv t \pmod 2$. Define

$$N_{s',t} := \max_{(\tilde{\alpha},\tilde{\beta},\tilde{\beta}')\in I_{1,s'}} |\{(\alpha,\beta,\beta') \in I_{1,s'} : \alpha+\beta+\beta' \equiv \tilde{\alpha}+\tilde{\beta}+\tilde{\beta}' \pmod 2\}|.$$

**Lemma 5.4.** *Let $n, t \in \mathbb{N}$ and $s' \in \{-t, -t+2, \ldots, t-2, t\}$. Then, we have*

$$\frac{N_{s',t}}{|I_{1,s'}|} \leq \frac{(\frac{t+|s'|}{2})!}{n^{\lceil \frac{t+|s'|}{4} \rceil}}.$$

*Hence, the ratio of the largest block size in the LDOI regime to the largest block size in the generic regime is given by*

$$\max_{s'} \frac{N_{s',t}}{|I_{1,s'}|} \leq \max_{s'} \frac{(\frac{t+|s'|}{2})!}{n^{\lceil \frac{t+|s'|}{4} \rceil}} \leq \frac{t!}{n^{\lceil \frac{t}{4} \rceil}}.$$

*Proof.* Fix an arbitrary $(\tilde{\alpha},\tilde{\beta},\tilde{\beta}') \in I_{1,s'}$. Assume first $0 \leq s'$. We want to count how many $(\alpha,\beta,\beta') \in I_{1,s'}$ exist such that $\alpha+\beta+\beta' \equiv \tilde{\alpha}+\tilde{\beta}+\tilde{\beta}' \pmod 2$. Define the odd support of $\tilde{\alpha}+\tilde{\beta}+\tilde{\beta}'$ as the set $O \subseteq [n]$ consisting of the indices $i \in [n]$ for which the $i$th entry of the vector $\tilde{\alpha}+\tilde{\beta}+\tilde{\beta}'$ is odd. Note that $|O| \equiv |\tilde{\alpha}+\tilde{\beta}+\tilde{\beta}'| = t+1 \pmod 2$. Therefore, we need to count the sequences $(\alpha,\beta,\beta') \in I_{1,s'}$ whose odd support is $O$.

First, we pick $\alpha$ and $\beta'$ arbitrarily, for which there are $n \cdot \binom{n-1+\frac{t-s'}{2}}{n-1}$ options. Denote the odd support of $\alpha+\beta'$ as $O' \subseteq [n]$. Now we will select $\beta$. In order to fulfil the desired congruence condition, the odd support of $\beta$ must be equal to the symmetric difference $O\Delta O'$ of $O$ and $O'$. Note that $|O'| \equiv |\alpha+\beta'| = 1+(t-s')/2 \pmod 2$. So, one must have $\beta = 2\gamma + \chi^{O\triangle O'}$, where $\gamma \in \mathbb{N}^n$ and $\chi^{O\Delta O'}$ is the characteristic vector of $O\Delta O'$ (with $i$th entry 1 if $i \in O\Delta O'$ and 0 otherwise). Since $|\beta| = \frac{t+s'}{2}$, it follows that $|\gamma| = (\frac{t+s'}{2} - |O\triangle O'|)/2$. This is a valid weight because $|O\Delta O'| \equiv |O|+|O'| \equiv t+(t-s')/2 \equiv (t+s)/2 \pmod 2$. In total we get $\binom{n-1+(\frac{t+s'}{2}-|O\triangle O'|)/2}{n-1}$ options for $\gamma$, which also gives the number of options for $\beta$. This term is clearly maximized for $|O\triangle O'|$ minimal, which depends on the parity of $\frac{t+s'}{2}$. Set $a=0$ if $\frac{t+s'}{2}$ is even and set $a=1$ if $\frac{t+s'}{2}$ is odd. We can conclude that

$$\begin{aligned} N_{s',t} \leq\ & n\binom{n-1+\frac{t-s'}{2}}{n-1}\binom{n-1+(\frac{t+s'}{2}-a)/2}{n-1} \\ =\ & n\binom{n-1+\frac{t-s'}{2}}{n-1}\binom{n-1+\lfloor\frac{t+s'}{4}\rfloor}{n-1}. \end{aligned} \tag{71}$$

Since $|I_{1,s'}| = n\binom{n-1+(t-s')/2}{n-1}\binom{n-1+(t+s')/2}{2}$, we obtain that

$$\frac{N_{s',t}}{|I_{1,s'}|} \leq \frac{\binom{n-1+\lfloor\frac{t+s'}{4}\rfloor}{n-1}}{\binom{n-1+\frac{t+s'}{2}}{n-1}} \leq (\frac{t+s'}{2})! \cdot \frac{n^{\lfloor\frac{t+s'}{4}\rfloor}}{n^{\frac{t+s'}{2}}},$$

where we get the second inequality by applying the following (easy to check) inequality

$$\frac{n^t}{t!} \leq \binom{n-1+t}{n-1} \leq n^t \text{ for any integers } n,t \geq 1.$$

One can quickly see that this formula coincides with the formula given in the lemma. Consider now the case $s' \leq 0$. Then we can redo the same analysis, only altering the approach by switching the roles of $\beta,\beta'$, i.e., first selecting $\beta$ arbitrarily and after that selecting $\beta'$. This leads to replacing $\frac{t+s'}{2}$ with $\frac{t-s'}{2}$ in formula (71). This completes the proof. □

**Remark 5.5.** *In the case $s=t=1$ the formula of Lemma 5.4 gives an upper bound of $\frac{1}{n}$. This exactly coincides with the known sparsity ratio for the LDOI pattern (and the CLDUI/LDUI patterns) (recall relation (8)).*

### 5.3 Runtime comparison for a class of examples based on the PPT$^2$ conjecture

The goal of this section is to present a comparison of the runtimes for an implementation of the DPS hierarchy in the three regimes: for generic, CLDUI, LDOI bipartite states. We first give an overview of the setup for our benchmark examples, which is motivated by the PPT$^2$ conjecture in quantum information. The PPT$^2$ conjecture is usually formulated on the 'channel side'. We will state it here on the 'state side' and only explain the necessary steps for setting up our benchmark instances.

Further details can be found in Appendix A. The PPT$^2$ conjecture states that the composition of any two PPT linear maps from $\mathbb{C}^{n\times n}$ to $\mathbb{C}^{n\times n}$ is entanglement breaking (see Conjecture A.4). It has been shown to hold for $n \le 3$ [CMHW19, CYT19] and for the linear maps arising from one state in $\mathrm{CLDUI}_n \cup \mathrm{LDUI}_n$ and the other one in $\mathrm{LDOI}_n$ [SN22, NP25]. It is still open whether it also holds when both states lie in $\mathrm{LDOI}_n$. For this reason we next formulate the PPT$^2$ conjecture for LDOI states, posed in [SN22, Conjecture 5.1].

**Conjecture 5.6** (The PPT$^2$ conjecture for LDOI states)**.** *Let* $(X_k, Y_k, Z_k) \in \mathbb{R}^{n\times n}\times \mathrm{Herm}^n \times \mathrm{Herm}^n$ *such that* $\mathrm{diag}(X_k) = \mathrm{diag}(Y_k) = \mathrm{diag}(Z_k)$ *for* $k = 1, 2$*. Assume that the corresponding LDOI states are positive semidefinite and have positive partial transpose, i.e.,* $\rho_{(X_k,Y_k,Z_k)} \in \mathrm{DPS}_n^{(1)}$ *for* $k = 1, 2$*. Then,* $\rho_{(X_3,Y_3,Z_3)} \in \mathrm{SEP}_n$*, where we define*

$$\begin{aligned}(X_3, Y_3, Z_3) &= (X_1, Y_1, Z_1) \bullet (X_2, Y_2, Z_2)\\ &:= (X_1X_2, Y_1 \circ Y_2 + Z_1 \circ Z_2^T + DY_3, Y_1 \circ Z_2 + Z_1 \circ Y_2^T + DZ_3),\end{aligned}$$

$DY_3 := \mathrm{Diag}(X_1X_2 - Y_1 \circ Y_2 - Z_1 \circ Z_2^T)$, $DZ_3 := \mathrm{Diag}(X_1X_2 - Y_1 \circ Z_2 - Z_1 \circ Y_2^T)$*, so that* $\mathrm{diag}(X_3) = \mathrm{diag}(Y_3) = \mathrm{diag}(Z_3)$ *holds.*

Suppose we want to construct a counterexample to the above conjecture. As mentioned above, the PPT$^2$ conjecture holds for $n \le 3$ and for states in $\mathrm{CLDUI}_n \cup \mathrm{LDUI}_n$; in addition, it holds if either $\rho_{(X_1,Y_1,Z_1)} \in \mathrm{SEP}_n$, or $\rho_{(X_2,Y_2,Z_2)} \in \mathrm{SEP}_n$ (see Lemma A.6). Hence, the smallest case to investigate is $n = 4$. So, we want to construct matrix triplets $(X, Y, Z) \in \mathbb{R}^{4\times 4} \times \mathrm{Herm}^4 \times \mathrm{Herm}^4$, such that $\mathrm{diag}(X) = \mathrm{diag}(Y) = \mathrm{diag}(Z)$, $\rho_{(X,Y,Z)} \in \mathrm{DPS}_4^{(1)} \setminus \mathrm{SEP}_4$, and neither $Y$ nor $Z$ is a diagonal matrix. Then, we will use such triplets as arguments $(X_k, Y_k, Z_k)$ $(k = 1, 2)$ to build their compositions $(X_3, Y_3, Z_3)$ that we will then test for existence of a $\mathrm{DPS}^{(t)}$-certificate. In case of a negative answer, one would obtain a counterexample to the PPT$^2$ conjecture.

For this, we start by considering the states $\rho_{a,a'}$ as defined in Definition 3.16. We will restrict[11] to $(a, a') \in \{(2, 1/2), (3, 1/3), (4, 1/4)\}$, in which case $\rho_{a,a'} \in \mathrm{DPS}_3^{(1)} \setminus \mathrm{DPS}_3^{(2)}$ in view of Lemma 3.17 and Theorem 3.20. Then, $\rho_{a,a'} = \rho_{(\tilde{X}_a,\tilde{Y})} \notin \mathrm{SEP}_3$, after setting

$$\tilde{X}_a = \begin{pmatrix} 1 & a & 1/a\\ 1/a & 1 & a\\ a & 1/a & 1\end{pmatrix},\ \tilde{Y} = \begin{pmatrix} 1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{pmatrix}.$$

We extend the matrices $\tilde{X}_a, \tilde{Y}$ to the following $4 \times 4$ matrices $X_a, Y$:

$$X_a = \begin{pmatrix} 1 & a & 1/a & 1\\ 1/a & 1 & a & 1\\ a & 1/a & 1 & 1\\ 1 & 1 & 1 & 1\end{pmatrix},\ Y = \begin{pmatrix} 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\end{pmatrix}. \tag{72}$$

By construction, $\rho_{(X_a,Y)} \in \mathrm{DPS}_4^{(1)}$ (i.e., $\rho_{(X_a,Y)}, \rho_{(X_a,Y)}^{T_B} = \rho_{(X_a,\cdot,Y)} \succeq 0$, which is easy to check using (10), (11)) and $\rho_{(X_a,Y)} \notin \mathrm{SEP}_4$ (since, otherwise, this would imply $\rho_{(\tilde{X}_a,\tilde{Y})} \in \mathrm{SEP}_3$). Next, we generate matrices $Z$ by choosing random unit vectors $v_k \in \mathbb{R}^4$ for $k \in [4]$ and defining $Z = (v_h^T v_k)_{h,k=1}^4$ as their Gram matrix. Then, $\mathrm{diag}(Z) = \mathrm{diag}(X_a)$ (since the $v_k$'s are unit vectors) and $\rho_{(X_a,Y,Z)} \in \mathrm{DPS}_4^{(1)} \setminus \mathrm{SEP}_4$. Indeed, $\rho_{(X_a,Y,Z)} \in \mathrm{DPS}_4^{(1)}$, because $\rho_{(X_a,Y,Z)} \succeq 0$ and $\rho_{(X_a,Y,Z)}^{T_B} =$

[11] We choose $a' = 1/a$, which implies the largest violation of the conditions $a' \ge 1/a$ (to ensure $\rho_{a,a'} \in \mathrm{DPS}_3^{(1)}$) and $a' < 1$ (to ensure $\rho_{a,a'} \notin \mathrm{DPS}_3^{(2)}$).

$\rho_{(X_a,Z,Y)} \succeq 0$ (as $|Z_{i,j}|^2 \leq (X_a)_{i,j}(X_a)_{j,i} = 1$ for any $1 \leq i < j \leq 4$ and using (10), (11)). Moreover, if $\rho_{(X_a,Y,Z)}$ would be separable then, by Lemma 2.5, also its CLDUI projection $\rho_{(X_a,Y)}$ would be separable, yielding a contradiction.

We generate five such random matrices $Z$, denoted as $Z[i]$ for $i \in [5]$. So, we get 15 triplets $(X_a, Y, Z[i])$ such that $\rho_{(X_a,Y,Z[i])} \in \mathrm{DPS}_4^{(1)} \setminus \mathrm{SEP}_4$, where $X_a, Y$ are as in (72) for $a = 2, 3, 4$. Now, the goal is to test whether the composed states[12] $\rho_{(X_a,Y,Z[i])\bullet(X_a,Y,Z[j])}$ are separable or entangled. Note that both arguments commute, because $Y$ and all $Z[i]$'s are real symmetric. So, we consider only $1 \leq i \leq j \leq 5$, which leads to a total of $3 \times 15 = 45$ different composed states $\rho_{AB}$ for which membership in $\mathrm{DPS}_4^{(t)}$ can be tested.

By construction, these composed states $\rho_{AB}$ have a LDOI sparsity structure. We use them to test the behaviour of the SDP implementing existence of a $\mathrm{DPS}^{(t)}$-certificate in the three regimes: first, in the generic case (searching for a $\mathrm{DPS}^{(t)}$-certificate in $\mathrm{Herm}((\mathbb{C}^n)^{\otimes(t+1)}$, thus ignoring the sparsity structure of $\rho_{AB}$), second in the LDOI regime (searching for a $\mathrm{DPS}^{(t)}$-certificate in $\mathrm{LDOI}_n^{(t)}$), and third in the CLDUI regime (searching for a $\mathrm{DPS}^{(t)}$-certificate for $\Pi_{\mathrm{CLDUI}}(\rho_{AB})$ in $\mathrm{CLDUI}_n^{(t)}$). We note that on all tested examples, a $\mathrm{DPS}^{(t)}$-certificate could be found. So, no instance of an entangled state was found, so that the status of the $\mathrm{PPT}^2$ conjecture remains open for LDOI states.

The graphic in Figure 1 below displays the different runtimes (in seconds) for the three regimes (generic, LDOI, CLDUI) and relaxation levels from $t = 1$ to $t = 7$. The runtime consists only of the time needed for solving the SDP. It excludes the preprocessing phase, since the preprocessing time remains in the seconds for every regime and every level $t$ displayed in Figure 1. The experiments were carried out on a laptop running Windows 11 Home 64-bit with an AMD Ryzen 7 8845HS @ 3.8GHz, 8 cores, 16 threads and 16GB of Ram. We used the programming language Julia [BEKS17] utilizing the JuMP package [DHL17] for coding[13] the problem formulation, and Hypatia [CKV22] as the semidefinite programming solver.

As expected, the generic implementation is the slowest and the CLDUI implementation is the fastest. For instance, for $t = 3$, the runtimes are roughly 2.5 minutes, 10 seconds and 1 second in the generic, LDOI and CLDUI cases and, for $t = 5$, roughly 30 seconds and 21 minutes for the CLDUI and LDOI cases. Note that the faster runtimes in the CLDUI regime allow to test membership in $\mathrm{DPS}_4^{(t)}$ up to level $t = 7$, while one can only test up to level $t = 5$ in the LDOI regime, and up to level $t = 3$ in the generic regime. Hence, this also indicates that the CLDUI implementation can be used as a useful necessary condition for testing existence of a $\mathrm{DPS}^{(t)}$-certificate for generic $\rho_{AB}$, by applying it to its projection $\Pi_{\mathrm{CLDUI}}(\rho_{AB})$, since one can then go to higher levels $t$.

## 6 Concluding remarks

In this paper we explore how structural properties of quantum bipartite states can be exploited to design more efficient variations of the semidefinite hierarchy $\mathrm{DPS}_n^{(t)}$ for testing separability and detecting quantum entanglement. On the one hand, we consider bipartite (CLDUI, LDUI, LDOI) states with diagonal unitary invariance. These states admit a block diagonal sparsity pattern that can be transferred to any given level of the DPS hierarchy. By applying block diagonalization and, in addition, reformulating the DPS hierarchy in the moment formalism, one obtains substantial matrix size reduction in the SDP models, so that higher levels can be computed in practice.

[12] We also tested states of the form $\rho_{(X_a,Y,Z[i])\bullet(X_b,Y,Z[j])}$ with $a \neq b$. We do not include the runtimes for these states in Figure 1 since the results are similar to those in the setup ($a = b$) described in the text.

[13] Our code is available at https://github.com/JonasBritz/ImplementationsDPSHierarchy.git.

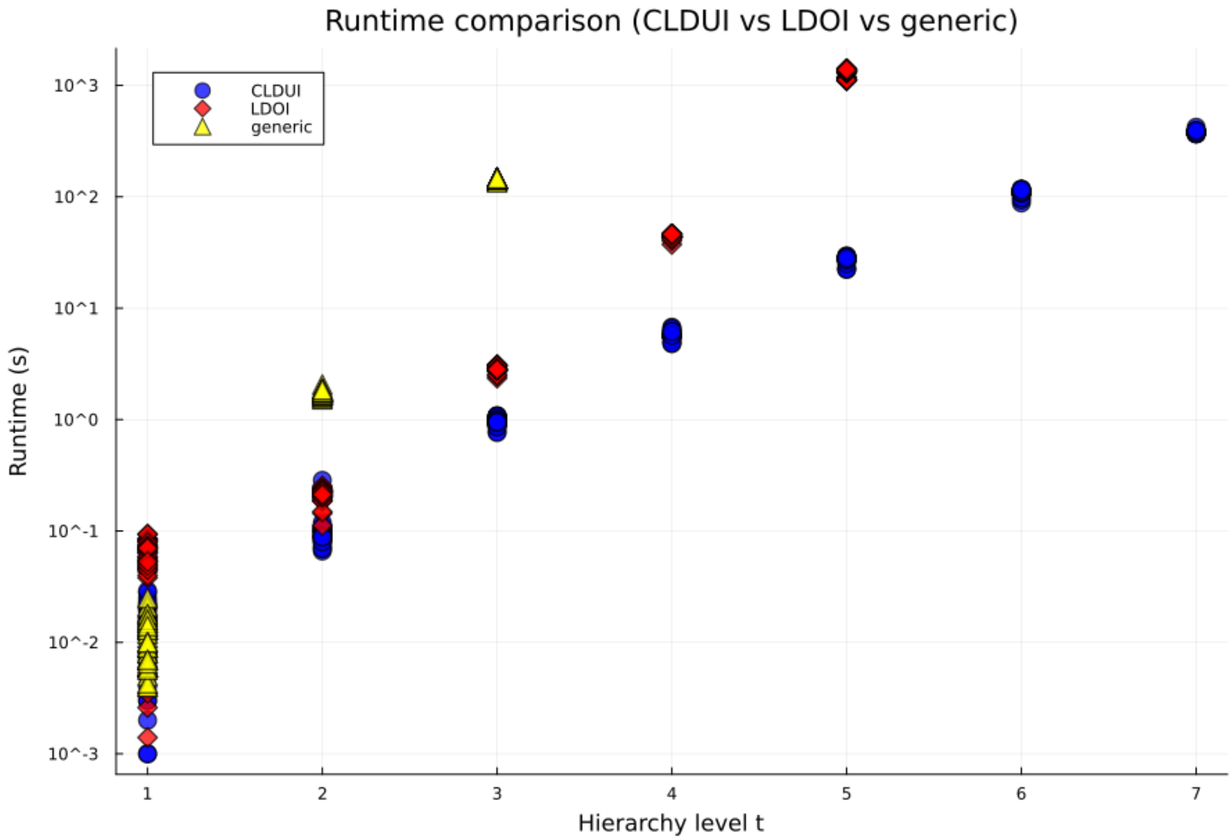


Figure 1: Graphic displaying the runtimes of the DPS hierarchy in three regimes: for CLDUI, LDOI and generic bipartite states

On the other hand, we consider Bose symmetric bipartite states, i.e., states that are symmetric in their two registers. This symmetry property can again be transferred to any given level of the DPS hierarchy. This leads to the stronger symmetry-adapted $\widetilde{\mathrm{DPS}}_n^{(t)}$ hierarchy. We characterize its dual, in terms of existence of a r-sum-of-squares representation for an associated complex polynomial. This characterization mirrors the known characterization of the dual of $\mathrm{DPS}_n^{(t)}$. In addition, it is closely related to the sum-of-squares characterization of the approximation cone $\mathcal{K}_n^{(t)}$ for $\mathrm{COP}_n$.

The completely positive cone $\mathrm{CP}_n$ and its dual $\mathrm{COP}_n$ play an important role within both settings. Indeed, separable bipartite states with CLDUI, LDUI (LDOI) sparsity structure can be captured by pairwise (triplewise) completely positive matrix pairs (triples), leading to the cones $\mathrm{PCP}_n, \mathrm{TCP}_n$ that generalize $\mathrm{CP}_n$. On the dual side, there is a close relationship between $\mathrm{COP}_n$ and the dual of the cone of Bose symmetric separable states, which extends to their respective conic approximations by $\mathcal{K}_n^{(t)}$ and $(\widetilde{\mathrm{DPS}}_n^{(t)})^*$.

Hence, there are interesting connections among several topics, ranging from quantum information to semidefinite optimization, matrix cones, and polynomial optimization. We now conclude with mentioning some open questions.

The symmetry-adapted DPS hierarchy applies to Bose symmetric states, so we have the inclusion $\widetilde{\mathrm{DPS}}_n^{(t)} \subseteq \mathrm{DPS}_n^{(t)} \cap \mathrm{BS}(\mathbb{C}^n \otimes \mathbb{C}^n)$ (the right most inclusion in (32)). Equality holds for $t = 1$ (since no state extension takes place). A natural question, already posed in [GNP25, Question 8.20], is whether equality holds for larger $t \geq 2$. We expect the answer to be negative, yet we could not find a counterexample. Let us briefly sketch our numerical approach for trying to find a counterexample.

Let $n = 5$ and $t = 2$. For $C \in \mathcal{K}_5^{(1)} \setminus \mathcal{K}_5^{(0)}$, consider the semidefinite program

$$p_C^* := \min\{\langle C, X\rangle : X \in \mathcal{S}^5,\ \rho_{(X,X)}^{T_B} \in \mathrm{DPS}_5^{(2)}\}$$

(which can be solved using the LDUI sparsity reduction). Note that, if we find a feasible $X$ such that $\langle C, X\rangle < 0$, then $X \notin (\mathcal{K}_5^{(1)})^*$ and thus, by Theorem 4.5, $\rho_{(X,X)}^{T_B} \in \mathrm{DPS}_5^{(2)} \setminus \widetilde{\mathrm{DPS}}_5^{(2)}$ while, by construction, $\rho_{(X,X)}^{T_B} \in \mathrm{BS}(\mathbb{C}^5 \otimes \mathbb{C}^5)$. Hence, $p_C^* < 0$ would imply strict inclusion $\widetilde{\mathrm{DPS}}_5^{(2)} \subset \mathrm{DPS}_5^{(2)} \cap \mathrm{BS}(\mathbb{C}^5 \otimes \mathbb{C}^5)$. The extreme rays of $\mathrm{COP}_5$ are fully characterized in [Hil12]: those that do not belong to $\mathcal{K}_5^{(0)}$ are the Horn matrix $H$ together with a class of parametrized matrices $T(\psi)$ (for $\psi \in \mathbb{R}^5$, $\psi > 0$ and $\sum_{i=1}^5 \psi_i < \pi$) and their positive diagonal scalings $DHD$, $DT(\psi)D$ for any positive diagonal matrix $D$. We computed the above SDP for the following matrices $C = H, T(\psi)$ for thousands of random choices of $\psi$, and for hundreds of diagonal scalings $DHD$ of the Horn matrix, making sure to select $D$ such that $DHD \in \mathcal{K}_5^{(1)}$ (following [LV23, Theorem 4]). The returned optimum value $p_C^*$ is (numerically) zero, so that no counterexample could be found.

Alternatively, one can try to show the following equality on the dual side: $(\widetilde{\mathrm{DPS}}_n^{(2)})^* = (\mathrm{DPS}_n^{(2)})^* + \mathrm{Herm}(S^2(\mathbb{C}^n))^\perp$. That is, if $M \in (\widetilde{\mathrm{DPS}}_n^{(2)})^*$ (meaning $M \otimes I_n = B + W_0 + W_1$ with $B \in \mathrm{Herm}(S^3(\mathbb{C}^n))^\perp$, $W_0 \succeq 0$, $W_1^{T_{B[1]}} \succeq 0$), does there exist $M' \in (\mathrm{DPS}_n^{(2)})^*$ (meaning $M' = B' + W_0' + W_1' + W_2'$ with $B' \in \mathrm{Herm}(\mathbb{C}^n \otimes S^2(\mathbb{C}^n))^\perp$, $W_0' \succeq 0$, $(W_1')^{T_{B[1]}} \succeq 0$, $(W_2')^{T_{B[2]}} \succeq 0$) such that $M - M' \in \mathrm{Herm}(S^2(\mathbb{C}^n))^\perp$? (Here, we have used Theorems 2.4 and 4.1.)

Consider now the inclusion $\mathrm{SEP}_n^{\mathrm{BS}} \subseteq \widetilde{\mathrm{DPS}}_n^{(t)}$ (the left most inclusion in (32)). By Theorem 4.5, if a matrix $X$ belongs $(\mathcal{K}_n^{(t)})^* \setminus \mathrm{CP}_n$, then the associated Bose symmetric (LDUI) state $\rho_{(X,X)}^{T_B}$ belongs to $\widetilde{\mathrm{DPS}}_n^{(t+1)} \setminus \mathrm{SEP}_n^{\mathrm{BS}}$ and thus the (CLDUI) state $\rho_{(X,X)}$ belongs to $\mathrm{DPS}_n^{(t+1)} \setminus \mathrm{SEP}_n$. Such matrices $X$ do exist for any $n \geq 5$ and $t \geq 0$; indeed, the inclusion $\mathcal{K}_n^{(t)} \subset \mathrm{COP}_n$ is shown to be strict in [DDGH13], which implies that also $\mathrm{CP}_n \subset (\mathcal{K}_n^{(t)})^*$ is a strict inclusion. This implies that both inclusions $\mathrm{SEP}_n^{\mathrm{BS}} \subset \widetilde{\mathrm{DPS}}_n^{(t)}$ and $\mathrm{SEP}_n \subset \mathrm{DPS}_n^{(t)}$ are strict for any $n \geq 5$ and $t \geq 1$, as observed in [GNP25]. In fact, Fawzi [Faw21] shows that the separable cone $\mathrm{SEP}_n$ is not semidefinite representable for any $n \geq 3$, which implies that the inclusion $\mathrm{SEP}_n \subset \mathrm{DPS}_n^{(t)}$ is strict for any $n \geq 3$ and $t \geq 1$. In contrast, recall that $\mathrm{SEP}_2 = \mathrm{DPS}_2^{(1)}$ (in fact this equality holds for bipartite states acting on $\mathbb{C}^3 \otimes \mathbb{C}^2$, see [Wor76]).

Examples of matrices $A \in \mathrm{COP}_n \setminus \cup_{t\geq 0}\mathcal{K}_n^{(t)}$ are constructed in [LV23] for any $n \geq 6$. Hence, in view of Theorem 4.4, any such matrix $A$ provides a LDUI instance $M_{A,0}^{T_B} \in (\mathrm{SEP}_n^{\mathrm{BS}})^* \setminus \cup_{t\geq 0}(\widetilde{\mathrm{DPS}}_n^{(t)})^*$. In addition, it is shown in [GNP25, Theorem 8.5] how to use such matrices $A$ to construct (C)LDUI matrices belonging to $\mathrm{SEP}_n^* \setminus \cup_{t\geq 0}(\mathrm{DPS}_n^{(t)})^*$.

As observed earlier, $\mathrm{COP}_4 = \mathcal{K}_4^{(0)}$, so that the hierarchy collapses: $\mathcal{K}_4^{(0)} = \mathcal{K}_4^{(t)}$ for all $t \geq 1$. In [GNP25, Question 8.21] the authors ask whether the inclusion $\mathcal{K}_n^{(t-1)} \subseteq \mathcal{K}_n^{(t)}$ is strict for $n \geq 5$ and $t \geq 1$. Note that, in view of Theorem 4.5, a positive answer would imply $\widetilde{\mathrm{DPS}}_n^{(t)} \neq \widetilde{\mathrm{DPS}}_n^{(t+1)}$. It is known that the inclusion $\mathcal{K}_5^{(0)} \subset \mathcal{K}_5^{(1)}$ is strict; for instance, the Horn matrix belongs to $\mathcal{K}_5^{(1)} \setminus \mathcal{K}_5^{(0)}$ [Par00]. We are not aware of explicit examples of matrices lying in $\mathcal{K}_n^{(t)} \setminus \mathcal{K}_n^{(t-1)}$ for $t \geq 2$ and $n \geq 5$.

Finally, let us mention again the $\mathrm{PPT}^2$ conjecture. It is expected that the conjecture fails in general. However, since it has been shown to hold when one state is LDOI and the other one is (C)LDUI [SN22, NP25], it remains intriguing to see whether it holds when both states are LDOI.

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# A The PPT$^2$ conjecture

We give here some background information about the PPT$^2$ conjecture. Set $M_n(\mathbb{C}) = \mathbb{C}^{n\times n}$ and let $\mathcal{T}_n(\mathbb{C})$ denote the set of linear maps $\Phi : M_n(\mathbb{C}) \to M_n(\mathbb{C})$. Let $I_n, \mathsf{T} \in \mathcal{T}_\mathsf{n}(\mathbb{C})$ denote, respectively, the identity map and the transpose map. Given two maps $\Phi_1, \Phi_2 \in \mathcal{T}_n(\mathbb{C})$, $\Phi_1 \circ \Phi_2 \in \mathcal{T}_n(\mathbb{C})$ denotes their composition, defined by $\Phi_1 \circ \Phi_2(X) = \Phi_1(\Phi_2(X))$ for $X \in M_n(\mathbb{C})$. We group some definitions about linear maps in $\mathcal{T}_n(\mathbb{C})$ and refer, e.g., to [SN21, SN22] and further references therein for a detailed treatment.

**Definition A.1.** *Consider a linear map $\Phi \in \mathcal{T}_n(\mathbb{C})$.*
• $\Phi$ *is called* positive *if* $\Phi(X) \succeq 0$ *for all* $X \in \mathrm{Herm}(\mathbb{C}^n)_+$.
• $\Phi$ *is called* completely positive *(CP)*[14] *if the map* $I_r \otimes \Phi : M_r(\mathbb{C}) \otimes M_n(\mathbb{C}) \to M_r(\mathbb{C}) \otimes M_n(\mathbb{C})$ *is positive for all* $r \in \mathbb{N}$.
• $\Phi$ *is called* PPT *if both* $\Phi$ *and* $\Phi \circ \mathsf{T}$ *are completely positive.*
• $\Phi$ *is called* entanglement breaking *if* $[I_n \otimes \Phi](Y) \in \mathrm{SEP}_n$ *for all* $Y \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)_+$.

Linear maps $\Phi \in \mathcal{T}_n(\mathbb{C})$ that are CP and preserve the trace (i.e., $\mathrm{Tr}(\Phi(X)) = \mathrm{Tr}(X)$ for all $X \in M_n(\mathbb{C})$) are known as *quantum channels*, they are used in quantum information to model the evolution of quantum systems. There is a well-known correspondence between maps $\Phi \in \mathcal{T}_n(\mathbb{C})$ and bipartite states in $M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ via their Choi (or Choi-Jamiołkowski) matrix $J(\Phi)$.

[14] This notion of CP linear map is classical in quantum information and should not be confused with the earlier notion of completely positive matrix.

**Definition A.2.** *For $\Phi \in \mathcal{T}_n(\mathbb{C}^n)$, its Choi state $J(\Phi) \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is defined by*

$$J(\Phi) = \sum_{r,s=1}^{n} \Phi(e_r e_s^*) \otimes e_r e_s^* \quad i.e., \quad (J(\Phi))_{ij,kl} = \Phi(e_j e_l^*)_{ik} \text{ for } i,j,k,l \in [n].$$

*Conversely, any state $\rho \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ corresponds to a linear map $\Phi_\rho \in \mathcal{T}_n(\mathbb{C})$ via the above relationship, given by $\Phi_\rho(e_j e_l^*)_{ik} = \rho_{ij,kl}$ for all $i,j,kl \in [n]$, so that $J(\Phi_\rho) = \rho$.*

Note that $J(\Phi)$ is Hermitian if and only if $\Phi$ preserves Hermitian matrices (i.e., $\Phi(X)$ is Hermitian whenever $X$ is Hermitian). Moreover, the following links can be shown (see, e.g., [SN21, SN22]).

**Lemma A.3.** *Let $\Phi \in \mathcal{T}_n(\mathbb{C})$ and $J(\Phi)$ its associated Choi state. Then,*

$$\begin{aligned} \Phi \text{ is CP} &\iff J(\Phi) \succeq 0, \\ \Phi \circ \mathsf{T} \text{ is CP} &\iff J(\Phi)^{T_B} \succeq 0, \\ \Phi \text{ is PPT} &\iff J(\Phi) \in \mathrm{DPS}_n^{(1)}, \\ \Phi \text{ is entanglement breaking} &\iff J(\Phi) \in \mathrm{SEP}_n. \end{aligned}$$

Hence, both $\Phi$ and $\Phi \circ \mathsf{T}$ are CP if and only if $J(\Phi) \in \mathrm{DPS}_n^{(1)}$. Another well-known fact is that any CP map $\Phi$ admits a Kraus decomposition: $\Phi(X) = \sum_{j=1}^{k} W_j X W_j^*$ for some $W_j \in M_n(\mathbb{C})$ (and $k \leq n^2$). Christandl posed the following conjecture in 2012, see also [CMHW19].

**Conjecture A.4** (PPT$^2$ conjecture)**.** *The composition $\Phi_1 \circ \Phi_2$ of two arbitrary PPT linear maps $\Phi_1, \Phi_2$ is entanglement breaking.*

**Conjecture A.5** (Restatement in state language)**.** *Let $\rho_1, \rho_2 \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)$ and let $\Phi_{\rho_1}, \Phi_{\rho_2}$ be the corresponding linear maps. If $\rho_1, \rho_2 \in \mathrm{DPS}_n^{(1)}$, then $J(\Phi_{\rho_1} \circ \Phi_{\rho_2}) \in \mathrm{SEP}_n$.*

As we now see, the conjecture holds if one of the two maps $\Phi_1, \Phi_2$ is entanglement breaking and the other one is CP.

**Lemma A.6.** *Assume $\Phi_1$ is CP and $\Phi_2$ is entanglement breaking, or vice versa, then their composition $\Phi_1 \circ \Phi_2$ is entanglement breaking.*

*Proof.* The proof relies on the following (easy to check) identity: For $\Psi_1, \Psi_2, \Gamma_1, \Gamma_2 \in \mathcal{T}_n(\mathbb{C})$,

$$(\Psi_1 \circ \Psi_2) \otimes (\Gamma_1 \circ \Gamma_2) = (\Psi_1 \otimes \Gamma_1) \circ (\Psi_2 \otimes \Gamma_2).$$

Therefore, since $I_n = I_n \circ I_n$, we get

$$I_n \otimes (\Phi_1 \circ \Phi_2) = (I_n \otimes \Phi_1) \circ (I_n \otimes \Phi_2).$$

Assume first that $\Phi_1$ is CP and $\Phi_2$ is entanglement breaking. By assumption, $I_n \otimes \Phi_2$ maps any $Y \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)_+$ to a separable state and separability is clearly preserved by $I_n \otimes \Phi_1$. Now, assume $\Phi_2$ is CP and $\Phi_1$ is entanglement breaking. Then, $I_n \otimes \Phi_2$ maps any $Y \in \mathrm{Herm}(\mathbb{C}^n \otimes \mathbb{C}^n)_+$ to a positive semidefinite state, which is thereafter mapped by $I_n \otimes \Phi_1$ to a separable state.

Linear maps $\Phi \in \mathcal{T}_n(\mathbb{C})$ whose Choi matrix $J(\Phi)$ has some diagonal unitary invariance are investigated in [SN21, SN22]. In particular, $J(\Phi) \in \mathrm{LDUI}_n$ (resp., $J(\Phi) \in \mathrm{CLDUI}_n$) if and only if $\Phi(UXU^*) = U^*\Phi(X)U$ (resp., $\Phi(UXU^*) = U\Phi(X)U^*$) for all $U \in \mathcal{DU}_n$ (in which case $\Phi$ is dubbed a DUC or CDUC map). The PPT$^2$ conjecture holds when restricting to such maps.

**Theorem A.7.** *[SN22, Theorem 4.5] The PPT² conjecture holds when restricting to DUC and CDUC linear maps $\Phi_1, \Phi_2$. That is, if $J(\Phi_1), J(\Phi_2)) \in \mathrm{CLDUI}_n \cup \mathrm{LDUI}_n$ and $\Phi_1, \Phi_2$ are PPT, then $\Phi_1 \circ \Phi_2$ is entanglement breaking.*

This motivates investigating (DOC) linear maps $\Phi$ whose Choi state $J(\Phi)$ belongs to $\mathrm{LDOI}_n$, in which case the conjecture has only been answered partially. The following results are shown in [NP25, Corollary 6.4, Theorem 6.5] and generalize the result from Theorem A.7.

**Theorem A.8.** *The PPT² conjecture holds when restricting to one DUC or CDUC linear map $\Phi_1$ and one DOC linear map $\Phi_2$. That is, if $J(\Phi_1)) \in \mathrm{CLDUI}_n \cup \mathrm{LDUI}_n$, $J(\Phi_2) \in \mathrm{LDOI}_n$ and $\Phi_1, \Phi_2$ are PPT, then $\Phi_1 \circ \Phi_2$ and $\Phi_2 \circ \Phi_1$ are entanglement breaking. Furthermore, the composition of two random DOC maps generically satisfies the PPT² conjecture.*

In what follows, for the convenience of the reader, we explain how to compute the DOC map of a LDOI state, i.e., the map $\Phi$ whose Choi matrix $J(\Phi)$ is a given LDOI state (see also [SN21, Lemma 9.3]). For a matrix $Y \in M_n(\mathbb{C})$, let $Y^0 := Y - \mathrm{Diag}(\mathrm{diag}(Y))$ denote the matrix obtained from $Y$ by setting to 0 its diagonal entries.

**Lemma A.9.** *Given $(X, Y, Z) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \times \mathrm{Herm}^n$ with $\mathrm{diag}(X) = \mathrm{diag}(Y) = \mathrm{diag}(Z)$, the linear map corresponding to $\rho_{(X,Y,Z)}$, denoted as $\Phi_{(X,Y,Z)} := \Phi_{\rho_{(X,Y,Z)}}$ for short, is defined by*

$$\Phi_{(X,Y,Z)}(M) = \mathrm{Diag}(X\mathrm{diag}(M)) + Y^0 \circ M + Z^0 \circ M^T \quad \textit{for } M \in M_n(\mathbb{C}).$$

*Proof.* We compute the Choi state $J(\Phi_{(X,Y,Z)}) = \sum_{i,j=1}^n \Phi_{(X,Y,Z)}(e_i e_j^*) \otimes e_i e_j^*$ and show that it coincides with

$$\rho_{(X,Y,Z)} = \sum_{i,j=1}^n X_{ij} e_i e_i^* \otimes e_j e_j^* + \sum_{i\neq j \in [n]} Y_{ij} e_i e_j^* \otimes e_i e_j^* + \sum_{i\neq j\in[n]} Z_{ij} e_i e_j^* \otimes e_j e_i^*.$$

For this we compute

$$\begin{aligned} \Phi_{(X,Y,Z)}(e_j e_j^*) &= \mathrm{Diag}(X e_j) = \mathrm{Diag}((X_{ij})_{i\in[n]}) = \sum_{i=1}^n X_{ij} e_i e_i^* && \text{for } j \in [n], \\ \Phi_{(X,Y,Z)}(e_i e_j^*) &= Y_{ij} e_i e_j^* + Z_{ji} e_j e_i^* && \text{for } i \neq j \in [n]. \end{aligned}$$

Putting both computations together yields $\sum_{i,j=1}^n \Phi_{(X,Y,Z)}(e_i e_j^*) \otimes e_i e_j^* = \rho_{(X,Y,Z)}$, as desired.

**Definition A.10.** *Let $(X_1, Y_2, Z_2), (X_2, Y_2, Z_2) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \times \mathrm{Herm}^n$ such that, for $k = 1, 2$, $\mathrm{diag}(X_k) = \mathrm{diag}(Y_k) = \mathrm{diag}(Z_k)$. We define their composition '$\bullet$' by*

$$(X_1, Y_2, Z_2) \bullet (X_2, Y_2, Z_2) = (X_1X_2, Y_1 \circ Y_2 + Z_1 \circ Z_2^T + DY_3, Y_1 \circ Z_2 + Z_1 \circ Y_2^T + DZ_3),$$

*setting $DY_3 := \mathrm{Diag}(X_1X_2 - Y_1 \circ Y_2 - Z_1 \circ Z_2^T)$ and $DZ_3 := \mathrm{Diag}(X_1X_2 - Y_1 \circ Z_2 - Z_1 \circ Y_2^T)$ (that are used to ensure that the three arguments in the resulting matrix triplet share the same diagonal).*

**Lemma A.11.** *Let $(X_1, Y_2, Z_2), (X_2, Y_2, Z_2) \in \mathbb{R}^{n\times n} \times \mathrm{Herm}^n \times \mathrm{Herm}^n$ such that, for $k = 1, 2$, $\mathrm{diag}(X_k) = \mathrm{diag}(Y_k) = \mathrm{diag}(Z_k)$, and $(X_3, Y_3, Z_3) := (X_1, Y_2, Z_2) \bullet (X_2, Y_2, Z_2)$ (as in Definition A.10). Then, we have*

$$\Phi_{\rho_{(X_3,Y_3,Z_3)}} = \Phi_{\rho_{(X_1,Y_1,Z_1)}} \circ \Phi_{\rho_{(X_2,Y_2,Z_2)}}.$$

*Proof.* Let $M \in M_n(\mathbb{C})$. By Lemma A.9, we have

$$\begin{aligned}
&\Phi_{(X_1,Y_1,Z_1)} \circ \Phi_{(X_2,Y_2,Z_2)}(M) = \Phi_{(X_1,Y_1,Z_1)}(\Phi_{(X_2,Y_2,Z_2)}(M)) \\
&= \underbrace{\mathrm{Diag}(X_1 \mathrm{diag}(\Phi_{(X_2,Y_2,Z_2)}(M)))}_{=A} + \underbrace{Y_1^0 \circ \Phi_{(X_2,Y_2,Z_2)}(M)}_{=B} + \underbrace{Z_1^0 \circ (\Phi_{(X_2,Y_2,Z_2)}(M))^T}_{=C}.
\end{aligned}$$

We compute each of the three summands $A, B, C$, using the fact (again, by Lemma A.9) that

$$\Phi_{(X_2,Y_2,Z_2)}(M) = \mathrm{Diag}(X_2 \mathrm{diag}(M)) + Y_2^0 \circ M + Z_2^0 \circ M^T.$$

As $Y_2^0$ and $Z_2^0$ are traceless, the same holds for $Y_2^0 \circ M + Z_2^0 \circ M^T$ and thus we have

$$A = \mathrm{Diag}(X_1 \mathrm{diag}(\mathrm{Diag}(X_2 \mathrm{diag}(M)))) = \mathrm{Diag}(X_1 X_2 \mathrm{diag}(M)).$$

As $Y_1^0$ and $Z_1^0$ are traceless, we obtain

$$\begin{aligned}
B &= Y_1^0 \circ (Y_2^0 \circ M + Z_2^0 \circ M^T) = Y_1^0 \circ Y_2^0 \circ M + Y_1^0 \circ Z_2^0 \circ M^T, \\
C &= Z_1^0 \circ (Y_2^0 \circ M + Z_2^0 \circ M^T)^T = Z_1^0 \circ (Y_2^0)^T \circ M^T + Z_1^0 \circ (Z_2^0)^T \circ M.
\end{aligned}$$

Putting everything together we obtain

$$A + B + C = \mathrm{Diag}(X_1 X_2 \mathrm{diag}(M)) + (Y_1^0 \circ Y_2^0 + Z_1^0 \circ (Z_2^0)^T) \circ M + (Y_1^0 \circ Z_2^0 + Z_1^0 \circ (Y_2^0)^T) \circ M^T,$$

which concludes the proof.

Using Lemma A.11 we now see that Conjecture 5.6 is indeed a reformulation of Conjecture A.5 for the case of LDOI states.