# Pairwise Completely Positive Matrices with Applications to Quantum Information Theory

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## Abstract

This thesis introduces a generalization of the set of completely positive matrices that we call "pairwise completely positive" (PCP) matrices. PCP matrix pairs are defined so that one matrix in the pair is necessarily positive semidefinite while the other is necessarily entrywise non-negative. After PCP matrices are defined we explore their basic properties and establish numerous necessary and sufficient conditions that can help test whether or not a pair meets our definition of PCP. We then relate these matrix pairs to the separability of conjugate local diagonal unitary invariant (CLDUI) quantum states. In particular, we show that determining whether or not a pair of matrices is pairwise completely positive is equivalent to determining whether or not a corresponding CLDUI state is separable.

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# Chapter 1

# Introduction

This thesis concerns itself with a generalization of completely positive matrices called *pairwise completely positive* (PCP) matrices. The characterization of this new set of matrix pairs is motivated by an existent result relating quantum separability and the membership problem in the set of completely positive matrices. In particular, in [1, 2] it was shown that for a natural family of quantum states called *mixed Dicke states*, checking separability is equivalent to determining whether or not a closely related matrix is completely positive. The contributions presented throughout this thesis include establishing the basic properties of PCP matrix pairs and their connection to the separability problem.

The organization of this thesis is as follows. The mathematical preliminaries required to discuss the generalization of completely positive matrices are presented in Chapter 2. Necessary background regarding quantum information theory is presented in Chapter 3, including a formal introduction to the separability problem and a brief overview of established separability criteria. Chapter 4 introduces and explores pairwise completely positive matrices, which are the main focus of this thesis. In particular, after a formal definition is presented, so too are necessary and sufficient conditions for testing pairwise complete positivity. The end of Chapter 4 focuses on establishing the connection between PCP matrices and quantum entanglement before closing in Chapter 5 with future directions arising from this work.

# Chapter 2

# Mathematical Preliminaries

## 2.1 Notation

Throughout this work bold letters like $\mathbf{v}, \mathbf{w} \in \mathbb{C}^n$ are used to denote vectors, non-bold uppercase letters like $A, B \in M_n(\mathbb{C})$ denote matrices, and non-bold lowercase letters like $c, d \in \mathbb{C}$ denote scalars. Subscripts on non-bold letters indicate particular entries of a vector or matrix (e.g., $v_1, v_2, v_3$ denote the first 3 coordinates of the vector $\mathbf{v}$), while subscripts of bold letters denote particular vectors (e.g., $\mathbf{v_1}, \mathbf{v_2}, \mathbf{v_3}$ are three vectors). Double subscripts are sometimes used to denote specific entries of vectors that are themselves denoted by subscripts (e.g., $v_{3,7}$ refers to the 7-th entry of the vector $\mathbf{v_3}$). At times it will be convenient to use square brackets to denote specific entries of a vector or a matrix—for example, $[\mathbf{v}]_j := v_j$. The $n \times n$ identity matrix is denoted by $I_n$, while $J_n$ denotes the $n \times n$ all ones matrix. Entrywise inequalities between matrices are denoted by standard inequality signs "$\geq$" and "$\leq$". The complex conjugate transpose of a matrix $X$ is denoted $X^*$. A matrix $X \in M_n$ is called *Hermitian* if $X^* = X$ and is called *unitary* if $X^*X = I_n$. Throughout this work unitary matrices are denoted by $U$. If a square complex matrix commutes with its conjugate transpose, i.e., if $X \in M_n$ satisfies $X^*X = XX^*$, then $X$ is called *normal*. Normal matrices are particularly important because these are the matrices for which the spectral decomposition can be applied. We note that it follows immediately from their definition that all Hermitian matrices and all unitary matrices are also normal.

## 2.2 Basic Results and Operations

The *tensor product* of two vectors $\mathbf{v} \in \mathbb{C}^m, \mathbf{w} \in \mathbb{C}^n$ or two matrices $A \in M_m, B \in M_n(\mathbb{C})$, denoted by $\mathbf{v} \otimes \mathbf{w} \in \mathbb{C}^m \otimes \mathbb{C}^n$ or $A \otimes B \in M_m \otimes M_n$, is defined in the following way:

$$\mathbf{v} \otimes \mathbf{w} = \begin{bmatrix} v_1\mathbf{w} \\ v_2\mathbf{w} \\ \vdots \\ v_m\mathbf{w} \end{bmatrix} \quad A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1m}B \\ a_{21}B & a_{22}B & \dots & a_{2m}B \\ \vdots & \vdots & & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mm}B \end{bmatrix}.$$

The *Hadamard product* of two vectors $\mathbf{v}, \mathbf{w} \in \mathbb{C}^n$ or two matrices $A, B \in M_{m,n}(\mathbb{C})$ (denoted by $\mathbf{v} \odot \mathbf{w}$ or $A \odot B$) is simply their entrywise product: $[\mathbf{v} \odot \mathbf{w}]_j := v_j w_j$ for all $j$ and $[A \odot B]_{i,j} := a_{i,j} b_{i,j}$ for all $i, j$.

The *trace* of a matrix $X$ is defined by $tr(X) = \sum_i^n x_{i,i}$. The following proposition states that if $X$ is a Hermitian matrix then the trace of X is the sum of its eigenvalues.

**Proposition 1.** *Let $X \in M_n(\mathbb{C})$, and $\lambda_1, \dots, \lambda_n$ be the eigenvalues of $X$. If $X = X^*$, then $tr(X) = \sum_{i=1}^n \lambda_i$*

*Proof.* If $X$ is Hermitian then it is normal, hence by the spectral decomposition $X$ can be written $X = UDU^*$, where $D$ is the diagonal matrix whose entries are the eigenvalues of $X$ and $U$ is the unitary matrix (i.e., $U^*U = UU^* = I_n$) whose columns are the corresponding eigenvectors. Then

$$tr(X) = tr(UDU^*) = tr(UU^*D^*) = tr(D^*) = \sum_{i=1}^n \lambda_i,$$

where the final inequality follows from the fact all Hermitian matrices have real eigenvalues. □

There are two matrix norms that will make frequent appearances throughout this work. The first of these is the *entrywise* 1-*norm* $\|\cdot\|_1$, defined simply via

$$\|X\|_1 \stackrel{\text{def}}{=} \sum_{i,j=1}^{n} |x_{i,j}|,$$

and the other one is the *trace norm* $\|\cdot\|_{\text{tr}}$, which is the sum of the singular values of the matrix:

$$\|X\|_{\text{tr}} \stackrel{\text{def}}{=} \sum_{k=1}^{n} \sigma_k(A).$$

The trace norm and the entrywise 1-norm are related by the following inequality [3]

$$\|X\|_{\text{tr}} \leq \|X\|_1. \tag{2.1}$$

## 2.3 Important Matrices

The following subsection focuses on exploring a particular family of normal matrices that are called positive semidefinite, however, we first require the introduction of yet another special kind of matrix, called the Gram matrix. If $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ is a set of vectors in $\mathbb{C}^n$, then the *Gram Matrix* $A = Gram(\mathbf{v_1}, \ldots, \mathbf{v_n})$ is defined by $[A]_{i,j} := \langle \mathbf{v_i}, \mathbf{v_j} \rangle$ [4]. We note that a Gram matrix is symmetric, and if the angle between any two vectors from the set $\{\mathbf{v_n}\}$ is less than or equal to 90 degrees then the Gram matrix is also entrywise non-negative.

### 2.3.1 PSD Matrices

A Hermitian matrix $X$ is called *positive semidefinite*, or PSD, if $\mathbf{v}^* X \mathbf{v} \geq 0$ for all $\mathbf{v} \in \mathbb{C}^n/0$. A few equivalent characterizations of PSD matrices that will arise throughout the remainder of this thesis are now stated, with particular emphasis on the representation given in (c).

**Proposition 2.** *Let $X \in M_n$ be a symmetric matrix with $rank(X) = m$. Then the following are equivalent:*

*a) $X$ is positive semidefinite.*

b) *All eigenvalues of $X$ are non-negative.*

c) *There exists an $n \times m$ matrix $V$ such that $X = VV^T$.*

d) *There exist $m$ vectors $\mathbf{v_1}, \ldots, \mathbf{v_m} \in \mathbb{R}^n$ such that $X = \sum_{i=1}^{m} \mathbf{v_i}\mathbf{v_i}^T$.*

e) *There exists an $m$-dimensional vector subspace $W$ and vectors $\mathbf{w_1}, \ldots, \mathbf{w_n} \in W$ such that $X = Gram(\mathbf{w_1}, \ldots, \mathbf{w_n})$.*

One way to test if certain matrices are PSD requires introducing a special type of matrix which will be referenced several times throughout this thesis, called a diagonally dominant matrix. A square matrix $X \in M_n$ is called *diagonally dominant* if for each of its rows, the sum of its off-diagonal entries is no more than the magnitude of its corresponding diagonal element. That is, $X \in M_n$ is diagonally dominant if $\sum\limits_{i \neq j} |x_{i,j}| \leq |x_{i,i}|$ for all $i$. The following proposition states the relationship between diagonally dominant and PSD matrices.

**Proposition 3.** *Let $X \in M_n$ be a Hermitian matrix with non-negative diagonal entries. If $X$ is diagonally dominant then it is positive semidefinite.*

The next proposition states that if $X$ is PSD, then computing the trace norm simply amounts to computing the trace.

**Proposition 4.** *Let $X \in M_n$ be a positive semidefinite matrix. Then $\|X\|_{\text{tr}} = tr(X)$*

*Proof.* If $X$ is PSD then the spectral decomposition can be applied to write $X = U\Lambda U^*$, where $U$ is a unitary matrix whose columns are the eigenvectors of $X$ and $\Lambda$ is the diagonal matrix whose entries are the eigenvalues $\lambda_k$ of $X$ (which are real and non-negative, since $X$ is PSD). By the singular value decomposition, the singular values $\{\sigma_k(X)\}$ of $X$ are the square roots of the eigenvalues of $XX^*$. Then $XX^* = (U\Lambda U^*)(U\Lambda U^*)^* = (U\Lambda U^*)(U\Lambda U^*) = UDU^*$, where $D$ is the diagonal matrix with diagonal entries $|\lambda_k|^2$. Since the entries $|\lambda_k|^2$ of $D$ are also the eigenvalues of $XX^*$, it follows that $\|X\|_{\text{tr}} = \sum\limits_{k=1}^{n} \sigma_k(X) = \sum\limits_{k=1}^{n} |\lambda_k| = tr(X)$. □

The following proposition states two well known properties satisfied by the entries of PSD matrices.

**Proposition 5.** *If $X \in M_n$ is a positive semidefinite matrix, then:*

*a)* $|x_{i,j}| \leq \frac{1}{2}(x_{i,i} + x_{j,j})$ *for* $i = 1, \dots, n-1, \quad j = 1, \dots, n$.

*b)* $|x_{i,j}| \leq \sqrt{x_{i,i} x_{j,j}}$ *for* $i = 1, \dots, n-1, \quad j = 1, \dots, n$.

### 2.3.2 Completely Positive Matrices

A matrix $A \in M_n(\mathbb{R})$ is called *completely positive* if there exists a matrix $B \in M_{nxm}(\mathbb{R})$, with $b_{i,j} \geq 0 \quad \forall i, j$ such that

$$A = BB^T.$$

We will refer to such a decomposition as a completely positive decomposition, and the matrix $B$ as the decomposition matrix of $A$. A straightforward implication of the above definition is that $A$ is (by construction) both PSD and entrywise nonnegative. We call matrices with these two properties *doubly non-negative* matrices, hence all completely positive matrices are also doubly non-negative. As an example of a completely positive matrix and its corresponding decomposition, consider:

$$X = \begin{bmatrix} 3 & 2 & 1 \\ 1 & 3 & 2 \\ 7 & 2 & 1 \end{bmatrix} \begin{bmatrix} 3 & 1 & 7 \\ 2 & 3 & 2 \\ 1 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 14 & 11 & 26 \\ 11 & 14 & 15 \\ 26 & 15 & 54 \end{bmatrix}.$$

An equivalent definition of complete positivity says that a matrix $A$ is completely positive if there exist entrywise non-negative vectors $\{\mathbf{b_1}, \cdots, \mathbf{b_m}\} \subseteq \mathbb{C}^n$ (which we choose to be the columns of $B$ in $A = BB^T$), such that:

$$A = \sum_{k=1}^{m} \mathbf{b_k b_k}^T = \mathbf{b_1 b_1^T} + \mathbf{b_2 b_2^T} + \cdots + \mathbf{b_m b_m^T} = BB^T$$

Since each term in the sum is a rank one matrix, this decomposition is sometimes called the rank one decomposition of a completely positive matrix. Yet another way of representing completely positive matrices comes from recalling the Gram matrix of a set of vectors. If we partition the decomposition matrix $B$ of a completely positive matrix into rows instead of columns by letting $\mathbf{v_i}^T$ be the $i-th$ row of B for $i = 1, \ldots, n$, then $A$ can be written:

$$A = BB^T = \begin{bmatrix} \mathbf{v_1}^T \\ \vdots \\ \mathbf{v_n}^T \end{bmatrix} \begin{bmatrix} \mathbf{v_1} & \cdots & \mathbf{v_n} \end{bmatrix} = \begin{bmatrix} \langle \mathbf{v_1}, \mathbf{v_1} \rangle & \cdots & \langle \mathbf{v_1}, \mathbf{v_n} \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{v_n}, \mathbf{v_1} \rangle & \cdots & \langle \mathbf{v_n}, \mathbf{v_1} \rangle \end{bmatrix} = Gram(\mathbf{v_1}, \ldots, \mathbf{v_n}).$$

A connection can be made between completely positive matrices and the question that asks under which conditions a set of vectors can be embedded into the non-negative orthant of some vector space. In particular, a matrix $A = Gram(\mathbf{x}_1, \ldots, \mathbf{x}_n)$ with $\mathbf{x}_i \in \mathbb{R}^n$ is completely positive if and only if there exists an isometry $T : \mathbb{R}^n \to \mathbb{R}^m$ for which $T\mathbf{x}_i$ lies in the non-negative orthant of $\mathbb{R}^m$ for all $i$ [4]. That is to say, $A$ is completely positive if it is the Gram matrix of vectors that can be rotated into the non-negative orthant of some vector space, without altering the length of those vectors.

Because of their applicability to problem solving methods in areas such as mathematical optimization and quantum information theory [5], characterizing the set of completely positive matrices is a question of particular interest in recent linear algebra research [6, 7]. The main question surrounding this set of matrices is one that asks how to determine if a given matrix is completely positive. It has been shown that this problem is NP-hard [8], but there have been extensive efforts to characterize these matrices. It will be useful to state some known results (without proof), which will be referenced later in the thesis. The first provides a characterization of completely positive matrices in small dimensions [4].

**Proposition 6.** *If $n \leq 4$, then $A \in M_n$ is doubly non-negative matrix if and only if it is completely positive.*

The next result holds for arbitrarily large $n$, and states that a doubly non-negative matrix is completely positive if it is diagonally dominant [9].

**Proposition 7.** *If a doubly non-negative matrix $A \in M_n$ is diagonally dominant, then $A$ is completely positive.*

# Chapter 3

# Quantum Information

## 3.1 State Vectors and Density Operators

The information contained in a quantum system is called a quantum state. This thesis concerns itself with mixed quantum states, which will be denoted by the Greek letter $\rho$. A mixed quantum state is represented by a *density matrix*, a matrix $\rho := \sum_j p_j \mathbf{v_j}\mathbf{v_j}^*$, where $\{p_j\}$ forms a set of real numbers such that $0 \leq p_j \leq 1$ and $\sum_j p_j = 1$. That is to say, the set is normalized, and since each element is positive, each element is between 0 and 1. Any matrix of this form is Hermitian, positive semidefinite and has trace equal to one. On the other hand, by the spectral decomposition every positive semidefinite matrix with trace one can be written as $\rho := \sum_j p_j \mathbf{v_j}\mathbf{v_j}^*$, with $\sum_j p_j = 1$, and thus represents a mixed quantum state.

## 3.2 The Separability Problem

As we saw in Section 3.1, a *quantum state* is a positive semidefinite matrix $\rho \in M_n(\mathbb{C})$ with trace 1. A mixed quantum state is separable if it can be written as a combination of quantum states. Put more precisely, we say a mixed quantum state $\rho \in M_m \otimes M_n$ is separable if it can be written:

$$\rho = \sum_{k=1}^{m} p_k \mathbf{v}_k \mathbf{v}_k^* \otimes \mathbf{w}_k \mathbf{w}_k^* \tag{3.1}$$

with $\sum_{k=1}^{m} p_k = 1$ and for some $\{\mathbf{v}_k\}, \{\mathbf{w}_k\} \subseteq \mathbb{C}^n$. If $\rho$ can't be written in this way, $\rho$ is called entangled [10]. We note that the set of separable states is closed and convex.

One way to think about separability is that statistical correlations of systems in separable states do not violate Bell's inequality [11]. Alternatively, a system of states is separable if it can be produced using only local operations and classical communications [12], which amounts to the restriction that any quantum operations act only on the individual subsystems and not on both at once. Entangled states can not be made in this way and require an exchange of quantum information between subsystems. As a result, these states violate a Bell inequality [13].

An important question in quantum information theory asks how to determine whether or not a given quantum state $\rho \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is separable. This problem is called *The Separability Problem*.

## 3.3 Positive Partial Transpose

In 2003, it was shown by Gurvits that the separability problem is NP-hard [14], indicating to mathematicians that an efficient solution to the separability problem in complete generality should not be expected. Since then, there have been many efforts to establish one sided tests. A *one-sided test* is a procedure that takes in a quantum state $\rho$ and outputs *one* of the following:

- $\rho$ is entangled (a *necessary* test)
- $\rho$ is separable (a *sufficient* test).

That is, a one sided test is able to prove either separability or entanglement for particular subsets of states. The most important separability criterion this thesis concerns itself with is based on something called the partial transposition. The *partial transposition* is a linear map $\Gamma$ on $M_m \otimes M_n$, defined by $\Gamma(A \otimes B) = A \otimes B^T$. If we write a matrix in its block form, its partial transposition is the matrix that results from taking the transpose of each block. For example,

$$\Gamma\left(\begin{bmatrix} X_{1,1} & X_{1,2} & \cdots & X_{1,n} \\ X_{2,1} & X_{2,2} & \cdots & X_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ X_{n,1} & X_{n,2} & \cdots & X_{n,n} \end{bmatrix}\right) = \begin{bmatrix} X_{1,1}^T & X_{1,2}^T & \cdots & X_{1,n}^T \\ X_{2,1}^T & X_{2,2}^T & \cdots & X_{2,n}^T \\ \vdots & \vdots & \ddots & \vdots \\ X_{n,1}^T & X_{n,2}^T & \cdots & X_{n,n}^T \end{bmatrix}.$$

The following theorem shows that the partial transposition criterion can be used to detect entanglement in certain quantum states and is referred to as the PPT criterion [15, 1].

**Proposition 8.** *(PPT criterion) Let $\rho \in M_m \otimes M_n$ be a quantum state. If $\rho$ is separable then $\Gamma(\rho)$ is PSD.*

*Proof.* If $\rho$ is separable, then it can be written $\rho = \sum_{k=1}^{m} p_k \mathbf{v}_k \mathbf{v}_k^* \otimes \mathbf{w}_k \mathbf{w}_k^*$. The partial transposition of $\rho$ is then $\Gamma(\rho) = \sum_{k=1}^{m} p_k \mathbf{v_k} \mathbf{v_k^*} \otimes (\mathbf{w}_k \mathbf{w}_k^*)^T$. Since $\mathbf{v_k}\mathbf{v_k}^*$ and $(\mathbf{w_k}\mathbf{w_k}^*)^T$ are positive semidefinite, we have that $\Gamma(\rho)$ is also positive semidefinite. □

If the partial transpose of $\rho$ is PSD, $\rho$ is said to have *positive partial transpose*. In most cases the usefulness of the PPT criterion arises from the contrapositive: if $\Gamma(\rho)$ is not positive semidefinite, then $\rho$ is entangled. For example, the matrix $\rho \in M_2 \otimes M_2$ given by

$$\rho = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

has eigenvalues $\{0, 0, 0, 1\}$ (hence $\rho$ is indeed a valid quantum state). Taking the partial transposition yields the matrix

$$\Gamma(\rho) = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

which has eigenvalues $\{-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$. Since $\Gamma(\rho)$ has a negative eigenvalue, it is not PSD, hence by Proposition 8 we conclude $\rho$ is entangled.

In general, if we just have that $\Gamma(\rho)$ is positive semidefinite, we can't actually conclude whether $\rho$ is separable or entangled. However, we can in certain special cases. The following proposition shows that in small dimensions, $\Gamma(\rho)$ being positive semidefinite is enough to conclude that $\rho$ is separable.

**Proposition 9.** *Let $\rho \in M_m \otimes M_n$ with $mn \leq 6$. Then $\rho$ is separable if and only if $\Gamma(\rho)$ is positive semidefinite.*

The proof of Proposition 9 is rather involved and is thus omitted, however, the interested reader is referred to [1].

A state $\rho \in M_m \otimes M_n$ is called *absolutely* PPT (APPT) if $(U\rho U^*)$ has positive partial transpose for all unitary $U \in M_m(\mathbb{C}) \otimes M_n(\mathbb{C})$. That is, $\rho \in M_m \otimes M_n$ is APPT if $\Gamma(U\rho U^*)$ is positive semidefinite for all unitary matrices $U \in M_m(\mathbb{C}) \otimes M_n(\mathbb{C})$ [16].

## 3.4 The Absolute Separability Problem

A quantum state $\rho \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is called *absolutely separable* if $U\rho U^*$ is separable for all unitary $U \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ [17]. The question of characterizing absolutely separable states remains an open problem [18]. On the other hand, the set of absolutely PPT states have been fully characterized [16], so one approach to the absolute separability problem is to investigate the correspondence between the set of absolutely separable states and the set of absolutely PPT states.

In the $n = 2$ case, the set of absolutely separable and absolutely PPT states have been completely characterized [16], and they both equal the set of states with eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0$ such that

$$\begin{bmatrix} 2\lambda_4 & \lambda_3 - \lambda_1 \\ \lambda_3 - \lambda_1 & 2\lambda_2 \end{bmatrix}$$

is positive semidefinite. An equivalent characterization of absolutely PPT states in the $n = 2$ case reduces the problem of checking separability of $U\rho U^*$ for all unitary $U \in M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$ to the problem of checking separability of $U_1\rho U_1^*$ for one particular $U_1 \in M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$. The test says that if $\Lambda$ is the diagonal matrix with diagonal entries $\lambda_1, \ldots, \lambda_4$, and $U_1$ is the unitary matrix

$$\begin{bmatrix} \cdot & \cdot & \cdot & 1 \\ 1/\sqrt{2} & \cdot & 1/\sqrt{2} & \cdot \\ -1/\sqrt{2} & \cdot & 1/\sqrt{2} & \cdot \\ \cdot & 1 & \cdot & \cdot \end{bmatrix}$$

then $\rho$ is absolutely separable if and only if $U_1 \Lambda U_1^*$ is separable. Before moving on we note that in the case of absolutely PPT states $\rho \in M_n \otimes M_n$, $n \geq 3$, there exist characterizations which reduce the problem of checking whether $U\rho U^*$ has positive partial transpose for all unitary $U$ to that of checking if it has positive partial transpose for a certain finite number of unitaries [16]. We will return to the question of whether the set of absolutely separable states coincides with the set of APPT states in Section 4.3.

# Chapter 4

# Pairwise Completely Positive Matrices

This chapter introduces the formal definition of what we called Pairwise Complete Positive matrices, documents the relevant results we obtained, and relates them to the absolute separability problem in quantum mechanics.

## 4.1 Definition and Basic Properties

Recall from Section 2.3.2 that a completely positive matrix is a matrix whose decomposition ensures it has both the positive semidefinite property and the entrywise non-negative property. Pairwise Complete Positivity is a generalization of such matrices. The idea is that each matrix in a PCP pair has one of the properties of complete positivity, so that "together" they capture the essence of a completely positive matrix. This is done by defining matrices that make up a PCP pair by their decompositions, so that these properties are simply a result of their construction.

**Definition 1.** *Suppose $X, Y \in M_n(\mathbb{C})$. We say that the pair $(X, Y)$ is* pairwise completely positive *(*PCP*) if there exist matrices $V, W \in M_{n,m}(\mathbb{C})$ (with $m$ arbitrary) such that*

$$X = (V \odot W)(V \odot W)^* \qquad \textit{and} \qquad Y = (V \odot \overline{V})(W \odot \overline{W})^*.$$

*Equivalently, $(X, Y)$ is PCP if there exist families of vectors $\{\mathbf{v_k}\}, \{\mathbf{w_k}\} \subseteq \mathbb{C}^n$ (which are the columns of $V$ and $W$, respectively) such that*

$$X = \sum_{k=1}^{m} (\mathbf{v_k} \odot \mathbf{w_k})(\mathbf{v_k} \odot \mathbf{w_k})^* \qquad \textit{and} \qquad Y = \sum_{k=1}^{m} (\mathbf{v_k} \odot \overline{\mathbf{v_k}})(\mathbf{w_k} \odot \overline{\mathbf{w_k}})^*. \tag{4.1}$$

An immediate consequence of the definition is that $X$ is positive semidefinite, since it can be written $X = AA^T$ where $A = V \odot W$. While $X$ being PSD is required by its construction, the definition does not require it be entrywise non-negative. This can be seen by directly computing the entries of $X$ in terms of the entries of $\{\mathbf{v_k}\}$ and $\{\mathbf{w_k}\}$ :

$$x_{i,j} = \sum_k \left[(\mathbf{v_k} \odot \mathbf{w_k})(\mathbf{v_k} \odot \mathbf{w_k})^*\right]_{i,j} = \sum_k v_{k,i} w_{k,i} \overline{v_{k,j} w_{k,j}}.$$

Similarly $Y$ is entrywise non-negative but is not necessarily positive semidefinite. In fact, the definition does not even require it be symmetric:

$$y_{i,j} = \sum_k \left[(\mathbf{v_k} \odot \overline{\mathbf{v_k}})(\mathbf{w_k} \odot \overline{\mathbf{w_k}})^*\right]_{i,j} = \sum_k |v_{k,i}|^2 |w_{k,j}|^2.$$

Beyond the PSD and entrywise nonnegative properties, there are a few other quick ways of checking whether a pair $(X, Y)$ could potentially meet the definition of pairwise complete positivity. These conditions are summarized in the following theorem. Recall that the entrywise 1- norm: $\|\cdot\|_1$ is the sum of the magnitude of each matrix element, while the trace norm of a matrix: $\|\cdot\|_{\text{tr}}$, is the sum of its singular values.

**Theorem 1.** *Suppose $X, Y \in M_n(\mathbb{C})$ are such that $(X, Y)$ is pairwise completely positive. Then each of the following conditions hold:*

*a) $X$ is (Hermitian) positive semidefinite.*

*b) $Y$ is real and entrywise non-negative.*

*c) $X$ and $Y$ have the same diagonal entries: $x_{i,i} = y_{i,i}$ for all $1 \leq i \leq n$.*

*d) $Y$ is "almost" entrywise larger than X: $|x_{i,j}|^2 \leq y_{i,j} y_{j,i}$ for all $1 \leq i, j \leq n$.*

*e) $X$ is "more diagonal" than $Y$: $\|X\|_1 - \|X\|_{\text{tr}} \leq \|Y\|_1 - \|Y\|_{\text{tr}}$.*

*Proof.* We already noted properties (a) and (b), which follow straightforwardly from the definition of PCP matrices.

For property (c), note that if $(X,Y)$ is PCP then we can compute the diagonal entries of $X$ and $Y$ in terms of the entries of the vectors $\{\mathbf{v_k}\}$ and $\{\mathbf{w_k}\}$:

$$x_{i,i} = \sum_k \left[(\mathbf{v_k} \odot \mathbf{w_k})(\mathbf{v_k} \odot \mathbf{w_k})^*\right]_{i,i} = \sum_k |v_{k,i}|^2 |w_{k,i}|^2 \quad \text{and}$$
$$y_{i,i} = \sum_k \left[(\mathbf{v_k} \odot \overline{\mathbf{v_k}})(\mathbf{w_k} \odot \overline{\mathbf{w_k}})^*\right]_{i,i} = \sum_k |v_{k,i}|^2 |w_{k,i}|^2,$$

which are equal to each other.

For property (d), we again directly compute the relevant entries of $X$ and $Y$ in terms of the entries of $\{\mathbf{v_k}\}$ and $\{\mathbf{w_k}\}$:

$$x_{i,j} = \sum_k \left[(\mathbf{v_k} \odot \mathbf{w_k})(\mathbf{v_k} \odot \mathbf{w_k})^*\right]_{i,j} = \sum_k v_{k,i} w_{k,i} \overline{v_{k,j} w_{k,j}} \quad \text{and}$$
$$y_{i,j} = \sum_k \left[(\mathbf{v_k} \odot \overline{\mathbf{v_k}})(\mathbf{w_k} \odot \overline{\mathbf{w_k}})^*\right]_{i,j} = \sum_k |v_{k,i}|^2 |w_{k,j}|^2.$$

Then the fact that $|x_{i,j}|^2 \leq y_{i,j} y_{j,i}$ is then simply a result of applying the Cauchy–Schwarz inequality to the vectors

$$(v_{1,i}\overline{w_{1,j}}, v_{2,i}\overline{w_{2,j}}, v_{3,i}\overline{w_{3,j}}, \ldots) \quad \text{and} \quad (w_{1,i}\overline{v_{1,j}}, w_{2,i}\overline{v_{2,j}}, w_{3,i}\overline{v_{3,j}}, \ldots).$$

The proof of property (e) is provided in [3].

□

There are a few important remarks worth mentioning. First, if $Y$ is symmetric then part (d) of the theorem implies that $Y$ is entrywise larger than $X$: $y_{i,j} \geq |x_{i,j}|$ for all $1 \leq i,j \leq n$. Also, by Inequality 2.1 the quantities $\|X\|_1 - \|X\|_{\text{tr}}$ and $\|Y\|_1 - \|Y\|_{\text{tr}}$ in part (e) of the theorem are both non-negative. Another important remark is that since $X$ is necessarily positive semidefinite, by Proposition 4 we have $\|X\|_{\text{tr}} = \text{Tr}(X)$ (but no similar simplification can be made for $\|Y\|_{\text{tr}}$ in general).

The next example demonstrates how Theorem 1 can be used to determine a matrix is *not* PCP:

if a pair fails to satisfy properties (a)-(e) of Theorem 1 we may conclude that the pair is not PCP, however satisfying these properties is not enough to conclude $X$ and $Y$ are pairwise completely positive without explicit decompositions satisfying definition 1.

**Example 1.** *Let $a > 0$ be a real number and consider the pair of matrices*

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad \text{and} \quad Y = \begin{bmatrix} 1 & a \\ a & 1 \end{bmatrix}.$$

*It is straightforward to check that $(X, Y)$ satisfies properties (a), (b), (c) of Theorem 1 regardless of the value of $a > 0$. However, $|x_{1,2}|^2 = 1$ while $y_{1,2}y_{2,1} = a^2$, thus for $a < 1$ property (d) of Theorem 1 is violated and we may conclude that $(X, Y)$ is not PCP. On the other hand, when $a = 1$ we have the decomposition of $(X, Y)$: $\mathbf{v_1} = \mathbf{w_1} = (1, 1)^T$, therefore we may conclude the pair* is *PCP.*

In the previous example $(X, Y)$ was pairwise completely positive when $X = Y$ was completely positive. The following theorem shows that this fact holds in general, and thus pairwise completely positive matrices are indeed a generalization of completely positive matrices.

**Theorem 2.** *Suppose $X \in M_n(\mathbb{C})$. Then $X$ is completely positive if and only if $(X, X)$ is pairwise completely positive.*

The proof of Theorem 2 is omitted but is stated in [3]. If we recall from Section 2.3.2 that checking complete positivity of a given matrix is NP-hard, a straightforward implication of Theorem 2 says that determining whether or not the pair $(X, Y)$ is pairwise completely positive is also NP-hard, thus we don't expect to find results for checking pairwise complete positivity that are both necessary and sufficient.

It is worth noting that we can combine PCP matrix pairs via addition while preserving pairwise complete positivity. That is, if $(X_1, Y_1)$ and $(X_2, Y_2)$ are PCP then so is $(X_1 + X_2, Y_1 + Y_2)$. This follows straightforwardly from considering how the PCP decomposition of $(X, Y)$ changes as a result of the sum. Below we present some other cases of pairs $(X,Y)$ for which the PCP property can be easily confirmed.

**Lemma 1.** *Suppose $X,Y \in M_n(\mathbb{C})$ satisfy conditions (a)–(c) of Theorem1. If $X$ is diagonal then $(X,Y)$ is pairwise completely positive.*

*Proof.* Define families of vectors $\{\mathbf{v_{i,j}}\}$ and $\{\mathbf{w_{i,j}}\}$ by $\mathbf{v_{i,j}} = \mathbf{e_i}$ and $\mathbf{w_{i,j}} = \sqrt{y_{i,j}}\mathbf{e_j}$ for all $1 \leq i,j, \leq n$. It is then straightforward to verify that

$$\sum_{i,j=1}^{n} (\mathbf{v_{i,j}} \odot \mathbf{w_{i,j}})(\mathbf{v_{i,j}} \odot \mathbf{w_{i,j}})^* = \sum_{j=1}^{n} (\sqrt{y_{j,j}}\mathbf{e_j})(\sqrt{y_{j,j}}\mathbf{e_j})^* = X \quad \text{and}$$
$$\sum_{i,j=1}^{n} (\mathbf{v_{i,j}} \odot \overline{\mathbf{v_{i,j}}})(\mathbf{w_{i,j}} \odot \overline{\mathbf{w_{i,j}}})^* = \sum_{i,j=1}^{n} \mathbf{e_i}(y_{i,j}\mathbf{e_j})^* = Y,$$

which is a PCP decomposition of $(X,Y)$. □

The above lemma shows that if the off-diagonal entries of $X$ are a minimum (i.e., equal to zero) and conditions (a)–(c) of Theorem1 are satisfied, then the off-diagonal entries of $Y$ can be arbitrarily large. This idea is closely related to properties (d) and (e) of Theorem 1, which basically say that if $(X,Y)$ is PCP then the off-diagonal portion of $Y$ must be larger than that of $X$. The following lemma is another way of formalizing the relationship between the off diagonal elements of a PCP pair $(X,Y)$. It says that if the off-diagonal entries of a matrix $Y$ in a PCP pair $(X,Y)$ are as small as possible, the off-diagonal entries of $X$ must be as small as possible.

**Lemma 2.** *Suppose $X,Y \in M_n(\mathbb{C})$ satisfy conditions (a)–(c) of Theorem 1 and furthermore that $Y$ is diagonal. Then $(X,Y)$ is pairwise completely positive if and only if $X$ is diagonal.*

*Proof.* The “if” direction of this result follows immediately from Lemma 1. For the “only if” direction, suppose $(X,Y)$ is PCP. Then Theorem 1(d) tells us that $|x_{i,j}|^2 \leq y_{i,j}y_{j,i}$ for all $1 \leq i,j \leq n$. Since $Y$ is diagonal, we know that $y_{i,j} = 0$ whenever $i \neq j$, so $x_{i,j} = 0$ when $i \neq j$ as well (i.e., $X$ is also diagonal). □

The following lemma presents another extension of the idea that the off-diagonal entries of $Y$ in a PCP pair should be large relative to the off-diagonal entries of $X$. The idea of the following lemma is that given a PCP pair $(X,Y)$, the off-diagonal entries of $Y$ can be increased by any amount and the pair will maintain pairwise complete positivity. We're also able to increase the diagonal entries of both matrices by the same amount while preserving the PCP property.

**Lemma 3.** *Suppose $X, Y, P \in M_n(\mathbb{C})$ are such that $(X,Y)$ is pairwise completely positive and $P$ is entrywise non-negative. Then $(X + \mathrm{diag}(P), Y + P)$ is also pairwise completely positive.*

*Proof.* We just note that $(\mathrm{diag}(P), P)$ is PCP by Lemma 1, and the sum of two PCP pairs is again PCP, so $(X,Y) + (\mathrm{diag}(P), P) = (X + \mathrm{diag}(P), Y + P)$ is PCP as well. □

As an immediately corollary, we get the following slight strengthening of Theorem 2:

**Corollary 1.** *Suppose $X, Y \in M_n(\mathbb{C})$ have the same diagonal entries and are such that $X$ is completely positive and $Y \geq X$ (where this inequality is meant entrywise). Then $(X,Y)$ is pairwise completely positive.*

*Proof.* Follows immediately from combining Lemma 3 with Theorem 2. □

## 4.2 Sufficient Conditions

Recall the characterization of completely positive matrices in small dimensions given in Proposition 6: when $n \leq 4$, $X$ is CP if and only if it is doubly non-negative [4]. Akin to the result for CP matrices, the first non trivial sufficient condition characterizes pairwise completely positive matrices for $n = 2$.

**Theorem 3.** *Suppose $X, Y \in M_2(\mathbb{C})$. Then $(X,Y)$ is pairwise completely positive if and only if conditions (a)–(d) of Theorem 1 hold.*

*Proof.* Theorem 1 already establishes the "only if" direction, so we only need to prove the "if" direction. With this in mind, suppose properties (a)–(d) of Theorem 1 hold and write

$$X = \begin{bmatrix} x_{1,1} & \overline{x_{2,1}} \\ x_{2,1} & x_{2,2} \end{bmatrix}, \quad Y = \begin{bmatrix} x_{1,1} & y_{1,2} \\ y_{2,1} & x_{2,2} \end{bmatrix}.$$

If $x_{1,1} = 0$ then $x_{1,2} = x_{2,1} = 0$ by positive semidefiniteness of $X$, so $X$ is diagonal and thus Lemma 1 shows that $(X, Y)$ is PCP. Similarly, if $y_{1,2} = 0$ then property (d) of Theorem 1 tells us that $x_{1,2} = x_{2,1} = 0$, so again $X$ is diagonal and $(X, Y)$ is PCP. We thus assume from now on that $x_{1,1} \neq 0$ and $y_{1,2} \neq 0$, and our goal is to show that there exist families of vectors $\{\mathbf{v_j}\}, \{\mathbf{w_j}\} \subseteq \mathbb{C}^2$ such that

$$X = \sum_j (\mathbf{v_j} \odot \mathbf{w_j})(\mathbf{v_j} \odot \mathbf{w_j})^* \quad \text{and} \quad Y = \sum_j (\mathbf{v_j} \odot \overline{\mathbf{v_j}})(\mathbf{w_j} \odot \overline{\mathbf{w_j}})^*.$$

To this end, define vectors $\mathbf{v_1}, \mathbf{v_2}, \mathbf{w_1}, \mathbf{w_2}$ in terms of the entries of $X$ and $Y$ as follows:

$$\mathbf{v_1} = \begin{bmatrix} 1 \\ \frac{x_{2,1}}{\sqrt{x_{1,1}y_{1,2}}} \end{bmatrix}, \quad \mathbf{v_2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \mathbf{w_1} = \begin{bmatrix} \sqrt{x_{1,1}} \\ \sqrt{y_{1,2}} \end{bmatrix}, \quad \text{and} \quad \mathbf{w_2} = \begin{bmatrix} \sqrt{y_{2,1} - \frac{|x_{2,1}|^2}{y_{1,2}}} \\ \sqrt{x_{2,2} - \frac{|x_{2,1}|^2}{x_{1,1}}} \end{bmatrix},$$

where we note that positive semidefiniteness of $X$ ensures that $x_{2,2} - \frac{|x_{2,1}|^2}{x_{1,1}} \geq 0$ (recall Proposition 5), and property (d) of Theorem 1 ensures that $y_{2,1} - \frac{|x_{2,1}|^2}{y_{1,2}} \geq 0$.

Then direct computation shows that

$$\sum_{j=1}^{2} (\mathbf{v_j} \odot \mathbf{w_j})(\mathbf{v_j} \odot \mathbf{w_j})^* = \begin{bmatrix} x_{1,1} & \overline{x_{2,1}} \\ x_{2,1} & \frac{|x_{2,1}|^2}{x_{1,1}} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & x_{2,2} - \frac{|x_{2,1}|^2}{x_{1,1}} \end{bmatrix} = X, \quad \text{and}$$

$$\sum_{j=1}^{2} (\mathbf{v_j} \odot \overline{\mathbf{v_j}})(\mathbf{w_j} \odot \overline{\mathbf{w_j}})^* = \begin{bmatrix} x_{1,1} & y_{1,2} \\ \frac{|x_{2,1}|^2}{y_{1,2}} & \frac{|x_{2,1}|^2}{x_{1,1}} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ y_{2,1} - \frac{|x_{2,1}|^2}{y_{1,2}} & x_{2,2} - \frac{|x_{2,1}|^2}{x_{1,1}} \end{bmatrix} = Y,$$

as desired. □

The theorem presented above provides a simple characterization of PCP matrices in the case where $n = 2$. We now consider a short example that uses Theorem 3 to show that a pair of matrices is PCP.

**Example 2.** *Consider the pair of matrices:*

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad \text{and} \quad Y = \begin{bmatrix} 1 & 3 \\ 1/3 & 1 \end{bmatrix}.$$

*It is straightforward to check that $(X, Y)$ satisfies properties (a), (b), (c) of Theorem 1. In particular, $X$ is PSD since we can write $X = \mathbf{v}\mathbf{v}^*$ where $\mathbf{v} = (1, 1)^T$. Properties (b) and (c) can be verified upon inspection, so the only condition left to check is that $|x_{i,j}|^2 \leq y_{i,j}y_{j,i}$ for all $1 \leq i, j \leq n$. Well, $|x_{1,2}|^2 = 1 = y_{1,2}y_{2,1}$ hence property (d) of Theorem 1 holds, and by Theorem 3, the pair $(X, Y)$ is PCP. The proof of Theorem 3 suggests the following PCP decomposition of the pair:*

$$\mathbf{v_1} = \begin{bmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{bmatrix}, \quad \mathbf{w_1} = \begin{bmatrix} 1 \\ \sqrt{3} \end{bmatrix}, \quad (\mathbf{v_1} \odot \mathbf{w_1}) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \mathbf{v_1} \odot \overline{\mathbf{v}}_\mathbf{1} = \begin{bmatrix} 1 \\ \frac{1}{3} \end{bmatrix}, \quad \mathbf{w_1} \odot \overline{\mathbf{w}}_\mathbf{1} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

*Which yields the desired pair $(X, Y)$:*

$$X = (\mathbf{v_1} \odot \mathbf{w_1})(\mathbf{v_1} \odot \mathbf{w_1})^* = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \text{and} \quad Y = (\mathbf{v_1} \odot \overline{\mathbf{v}}_\mathbf{1})(\mathbf{w_1} \odot \overline{\mathbf{w}}_\mathbf{1})^* = \begin{bmatrix} 1 & 3 \\ 1/3 & 1 \end{bmatrix}.$$

The next Example contrasts the result for the $2 \times 2$ matrix pair presented in Example 2, and shows that the result stated in Theorem 3 can't be extended to matrices $X, Y \in M_3(\mathbb{C})$.

**Example 3.** *Consider the pair of matrices*

$$X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad Y = \begin{bmatrix} 1 & 3 & 1/3 \\ 1/3 & 1 & 3 \\ 3 & 1/3 & 1 \end{bmatrix}.$$

*It is straightforward to show that $(X, Y)$ satisfies properties (a), (b), (c), and (d) of Theorem 1. However, direct calculation shows that*

$$\|X\|_1 = 9, \ \|X\|_{\text{tr}} = 3, \ \|Y\|_1 = 13, \quad \text{and} \quad \|Y\|_{\text{tr}} = \frac{13 + 4\sqrt{13}}{3}.$$

*Thus $\|X\|_1 - \|X\|_{\text{tr}} = 9 - 3 = 6$, whereas*

$$\|Y\|_1 - \|Y\|_{\text{tr}} = 13 - \frac{13 + 4\sqrt{13}}{3} \approx 3.86,$$

*So we find that $\|X\|_1 - \|X\|_{\text{tr}}$ is strictly greater than $\|Y\|_1 - \|Y\|_{\text{tr}}$, hence by Theorem 1(e) we conclude $(X, Y)$ is not PCP.*

We are not able to get a complete necessary and sufficient condition in dimension 3 or larger, but we can prove the following sufficient condition that reduces to that of the above theorem when $n = 2$.

**Theorem 4.** *Suppose $X, Y \in M_n(\mathbb{C})$ satisfy properties (a)–(c) of Theorem 1. For each $k = 1, 2, \ldots, n$ define the vectors $\mathbf{v_k}, \mathbf{w_k} \in \mathbb{C}^n$ recursively via the following formulas for their entries:*

$$v_{k,j} = \begin{cases} 0 & \text{if } 1 \leq j < k \\ \dfrac{x_{j,k} - \sum_{i=1}^{k-1} v_{i,j} w_{i,j} \overline{v_{i,k} w_{i,k}}}{\sqrt{y_{k,j} - \sum_{i=1}^{k-1} |v_{i,k}|^2 |w_{i,j}|^2}} & \text{if } k \leq j \leq n \end{cases} \qquad \text{and} \qquad w_{k,j} = \frac{\sqrt{y_{k,j} - \sum_{i=1}^{k-1} |v_{i,k}|^2 |w_{i,j}|^2}}{v_{k,k}}.$$

*As long as all of the quantities under square roots above are non-negative and quantities in* *denominators are non-zero, the pair $(X,Y)$ is pairwise completely positive via the decomposition*

$$X = \sum_{k=1}^{n} (\mathbf{v_k} \odot \mathbf{w_k})(\mathbf{v_k} \odot \mathbf{w_k})^* \qquad \textit{and} \qquad Y = \sum_{k=1}^{n} (\mathbf{v_k} \odot \overline{\mathbf{v_k}})(\mathbf{w_k} \odot \overline{\mathbf{w_k}})^*.$$

*Proof.* We just need to show that that claimed decompositions do indeed give us $X$ and $Y$, which just amounts to some somewhat tedious computations. For simplicity of notation, we start by defining the quantities

$$c_{j,k} = \sum_{i=1}^{k-1} v_{i,j} w_{i,j} \overline{v_{i,k} w_{i,k}} \quad \text{and} \quad d_{k,j} = \sum_{i=1}^{k-1} |v_{i,k}|^2 |w_{i,j}|^2,$$

so what we can express $x_{k,j}$ and $y_{k,j}$ more simply as

$$v_{k,j} = \begin{cases} 0 & \text{if } 1 \leq j < k \\ \dfrac{x_{j,k} - c_{j,k}}{\sqrt{y_{k,j} - d_{k,j}}} & \text{if } k \leq j \leq n \end{cases} \qquad \text{and} \qquad w_{k,j} = \frac{\sqrt{y_{k,j} - d_{k,j}}}{v_{k,k}}. \tag{4.2}$$

Let's start by computing the $(j,k)$-entry of the claimed decomposition of $Y$:

$$\begin{aligned}\left[\sum_{i=1}^{n} (\mathbf{v_i} \odot \overline{\mathbf{v_i}})(\mathbf{w_i} \odot \overline{\mathbf{w_i}})^*\right]_{j,k} &= \sum_{i=1}^{n} |v_{i,j}|^2 |w_{i,k}|^2 = \sum_{i=1}^{j} |v_{i,j}|^2 |w_{i,k}|^2 = \left(\sum_{i=1}^{j-1} |v_{i,j}|^2 |w_{i,k}|^2\right) + |v_{j,j}|^2 |w_{j,k}|^2 \\ &= d_{j,k} + |v_{j,j}|^2 |w_{j,k}|^2 = d_{j,k} + |v_{j,j}|^2 \left(\frac{y_{j,k} - d_{j,k}}{|v_{j,j}|^2}\right) = y_{j,k},\end{aligned}$$

where the second equality follows from the fact $v_{i,j} = 0$ whenever $i > j$ and the second-to-last equality follows from plugging in the formula 4.2 for $w_{j,k}$.

Thus this is indeed a valid PCP decomposition of $Y$. Similarly, to see that the theorem gives the correct $X$, we compute the $(j,k)$-entry of the claimed decomposition of $X$:

$$\begin{aligned}\left[\sum_{i=1}^{n}(\mathbf{v_i}\odot\mathbf{w_i})(\mathbf{v_i}\odot\mathbf{w_i})^*\right]_{j,k} &= \sum_{i=1}^{n} v_{i,j}w_{i,j}\overline{v_{i,k}w_{i,k}} = \sum_{i=1}^{k} v_{i,j}w_{i,j}\overline{v_{i,k}w_{i,k}} \\ &= \left(\sum_{i=1}^{k-1} v_{i,j}w_{i,j}\overline{v_{i,k}w_{i,k}}\right) + v_{k,j}w_{k,j}\overline{v_{k,k}w_{k,k}} = c_{j,k} + v_{k,j}w_{k,j}\overline{v_{k,k}w_{k,k}},\end{aligned} \tag{4.3}$$

where the second equality again follows from the fact that $v_{i,k} = 0$ whenever $i > k$. Let's now compute the final term above (i.e., the term that we pulled out of the sum) by plugging in the formulas 4.2 for $v_{k,j}$, $w_{k,j}$, and $w_{k,k}$:

$$v_{k,j}w_{k,j}\overline{v_{k,k}w_{k,k}} = \frac{x_{j,k}-c_{j,k}}{\sqrt{y_{k,j}-d_{k,j}}}\left(\frac{\sqrt{y_{k,j}-d_{k,j}}}{v_{k,k}}\right)(\overline{v_{k,k}})\left(\frac{\sqrt{y_{k,k}-d_{k,k}}}{\overline{v_{k,k}}}\right) = \frac{\sqrt{y_{k,k}-d_{k,k}}}{v_{k,k}}(x_{j,k}-c_{j,k}),$$

where the second equality just follows from canceling terms where possible. If we now plug in the formula 4.2 for $v_{k,k}$ then we see that this quantity equals

$$v_{k,j}w_{k,j}\overline{v_{k,k}w_{k,k}} = (y_{k,k}-d_{k,k})\left(\frac{x_{j,k}-c_{j,k}}{x_{k,k}-c_{k,k}}\right) = x_{j,k}-c_{j,k},$$

where the final equality follows from the facts that $y_{k,k} = x_{k,k}$ and $d_{k,k} = c_{k,k}$. Finally, plugging this equation into Equation

$$\left[\sum_{i=1}^{n}(\mathbf{v_i}\odot\mathbf{w_i})(\mathbf{v_i}\odot\mathbf{w_i})^*\right]_{j,k} = c_{j,k} + v_{k,j}w_{k,j}\overline{v_{k,k}w_{k,k}} = c_{j,k} + (x_{j,k}-c_{j,k}) = x_{j,k}.$$

It follows that this PCP decomposition gives the correct $X$ matrix as well, completing the proof.

□

The idea behind the decomposition presented in Theorem 4 is to construct $X$ and $Y$ "from top to bottom" one row at a time by exploiting the symmetry in $X$. The vectors $\mathbf{v_1}$ and $\mathbf{w_1}$ are chosen to give the correct first row and column of $X$ and the first row of $Y$. Then adding $\mathbf{v_2}$ and $\mathbf{w_2}$ give the second row and column of $X$ and the second row of $Y$ (without affecting the entries in their first row/column), and the decomposition continues in this way until we get $(X, Y)$, as long as the defined vectors have non negative quantities under all square roots. As a result of the decomposition's "top down" approach and the fact that it specifies there be $n$ terms, there are cases for which Theorem 4 fails due to a negative quantity under a square root. Nevertheless, the proposed decomposition provides a sufficient condition under certain restraints on the entries of pairs $(X, Y)$.

**Example 4.** *Consider the pair of matrices*

$$X = \begin{bmatrix} 3 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad \textit{and} \quad Y = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 2 & 4 \\ 2 & 2 & 1 \end{bmatrix}.$$

*We will apply Theorem 4 and try to find a PCP decomposition of $(X, Y)$. It is straightforward to show that $(X, Y)$ satisfies properties (a), (b), (c) of Theorem 1. The decomposition defines the following vectors:*

$$\mathbf{v_1} = \begin{bmatrix} \sqrt{3} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \quad \mathbf{w_1} = \begin{bmatrix} 1 \\ \sqrt{\frac{2}{3}} \\ \sqrt{\frac{2}{3}} \end{bmatrix}, \quad \mathbf{v_2} = \begin{bmatrix} 0 \\ \frac{\sqrt{5}}{\sqrt{3}} \\ \frac{2}{\sqrt{33}} \end{bmatrix}, \quad \mathbf{w_2} = \begin{bmatrix} \frac{3}{\sqrt{10}} \\ 1 \\ \sqrt{\frac{11}{5}} \end{bmatrix}, \quad \mathbf{v_3} = \begin{bmatrix} 0 \\ 0 \\ \sqrt{\frac{2}{5}} \end{bmatrix}, \quad \mathbf{w_3} = \begin{bmatrix} \frac{3\sqrt{17}}{2\sqrt{11}} \\ \sqrt{\frac{85}{22}} \\ 1 \end{bmatrix}.$$

*Then direct computation yields:*

$$\begin{aligned} \sum_i (\mathbf{v_i} \odot \mathbf{w_i})(\mathbf{v_i} \odot \mathbf{w_i})^* &= \begin{bmatrix} 3 & 1 & 1 \\ 1 & 1/3 & 1/3 \\ 1 & 1/3 & 1/3 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 5/3 & 2/3 \\ 0 & 2/3 & 4/15 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2/5 \end{bmatrix} \\ &= \begin{bmatrix} 3 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} = X \\ \sum_i (\mathbf{v_i} \odot \overline{\mathbf{v_i}})(\mathbf{w_i} \odot \overline{\mathbf{w_i}})^* &= \begin{bmatrix} 3 & 2 & 2 \\ 1/2 & 1/3 & 1/3 \\ 1/2 & 1/3 & 1/3 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 3/2 & 5/3 & 11/3 \\ 6/55 & 4/33 & 4/15 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 153/110 & 17/11 & 2/5 \end{bmatrix} \\ &= \begin{bmatrix} 3 & 2 & 2 \\ 2 & 2 & 4 \\ 2 & 2 & 1 \end{bmatrix} = Y. \end{aligned}$$

Recall that a matrix $X$ is diagonally dominant if $\sum_{i\neq j}|x_{i,j}| \leq |x_{i,i}|$ for all $i$. The next sufficient condition is motivated by Proposition 7, which states that if a doubly nonnegative matrix is diagonally dominant, then it is completely positive. The following theorem is the natural generalization of this result to pairwise completely positive matrices.

**Theorem 5.** *Suppose $X, Y \in M_n(\mathbb{C})$ satisfy conditions (a)–(d) of Theorem 1. If $X$ is diagonally dominant then $(X,Y)$ is pairwise completely positive.*

*Proof.* Suppose that conditions (a)–(d) of Theorem 1 hold and $X$ is diagonally dominant. First, we note that we can assume without loss of generality that $x_{i,i} = \sum_{j\neq i}|x_{i,j}|$ for all $1 \leq i \leq n$ and $y_{i,j}y_{j,i} = |x_{i,j}|^2$ for all $1 \leq i \neq j \leq n$, since the more general case where the quantities on the left are larger than the quantities on the right then follows from Lemma 3.

Using an approach motivated by [!], we construct matrices $V, W, \in M_{n,m}(\mathbb{C})$ with $m = n(n-1)/2$ such that $X = (V \odot W)(V \odot W)^*$ and $Y = (V \odot \overline{V})(W \odot \overline{W})^*$. We index the $n$ rows of $V$ and $W$ in the usual way (by a number $1 \leq j \leq n$), but we index their $n(n-1)/2$ columns by sets $\{k,\ell\}$ for which $k \neq \ell$ (we will think of these columns as corresponding to the $n(n-1)/2$ entries in the strictly upper-triangular portion of $X$ and $Y$).

We define $V$ and $W$ entrywise as follows (we use the convention that $k < \ell$ throughout this definition):

$$v_{j,\{k,\ell\}} = \begin{cases} \mathrm{sign}(x_{k,\ell})y_{k,\ell}^{1/4} & \text{if } j = k \\ y_{\ell,k}^{1/4} & \text{if } j = \ell \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad w_{j,\{k,\ell\}} = \begin{cases} y_{\ell,k}^{1/4} & \text{if } j = k \\ y_{k,\ell}^{1/4} & \text{if } j = \ell \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathrm{sign}(x_{k,\ell})$ is the (complex) sign of $x_{k,\ell}$: the number on the unit circle in the complex plane with the property that $x_{k,\ell} = \mathrm{sign}(x_{k,\ell})|x_{k,\ell}|$. Then

$$\big[(V \odot \overline{V})(W \odot \overline{W})^*\big]_{i,j} = \sum_{k<\ell} |v_{i,\{k,\ell\}}|^2 |w_{j,\{k,\ell\}}|^2.$$

When $i \neq j$, the only nonzero term in this sum arises when $\{k, \ell\} = \{i, j\}$, so it simplifies considerably to

$$\left[(V \odot \overline{V})(W \odot \overline{W})^*\right]_{i,j} = |v_{i,\{i,j\}}|^2 |w_{j,\{i,j\}}|^2 = (y_{i,j}^{1/4})^2 (y_{i,j}^{1/4})^2 = y_{i,j},$$

as desired. Similarly, if $i < j$ then the $(i, j)$-entry of $X$ is given by

$$\left[(V \odot W)(V \odot W)^*\right]_{i,j} = v_{i,\{i,j\}} w_{i,\{i,j\}} \overline{v_{j,\{i,j\}} w_{j,\{i,j\}}} = \text{sign}(x_{i,j}) y_{i,j}^{1/4} y_{j,i}^{1/4} y_{j,i}^{1/4} y_{i,j}^{1/4} = x_{i,j},$$

with the computation when $i > j$ being analogous.

Finally, we show the given factorization yields the correct diagonal entries $y_{i,i} = x_{i,i} = \sum_{k \neq i} |x_{i,k}|$:

$$\left[(V \odot \overline{V})(W \odot \overline{W})^*\right]_{i,i} = \sum_{k<\ell} |v_{i,\{k,\ell\}}|^2 |w_{i,\{k,\ell\}}|^2 = \sum_{k \neq i} y_{i,k}^{1/2} y_{k,i}^{1/2} = \sum_{k \neq i} |x_{i,k}| = x_{k,k},$$

which completes the proof .

□

We note that the above theorem does *not* follow directly from combining the known result that diagonal dominance implies complete positivity stated in Proposition 7 with Theorem 2, since the result for completely positive matrices only applies to matrices $X$ with non-negative entries. Our result, however, applies even if $X$ has negative (or complex) entries.

**Example 5.** *Consider the pair of matrices*

$$X = \begin{bmatrix} 2 & 1 & -1 \\ 1 & 3 & 2i \\ -1 & -2i & 3 \end{bmatrix} \quad \textit{and} \quad Y = \begin{bmatrix} 2 & 1 & 2 \\ 1 & 3 & 4 \\ 1/2 & 1 & 3 \end{bmatrix}.$$

*Since this pair satisfies conditions (a)–(d) of Theorem 1 and X is diagonally dominant, Theorem*

*5 tells us that $(X, Y)$ is pairwise completely positive. To construct an explicit PCP decomposition of it, we compute the matrices $V, W \in M_{n,m}(\mathbb{C})$ by following along through the proof of that theorem. Since $n = 3$, these matrices have three rows indexed by $1 \leq j \leq 3$, and $m = n(n-1)/2 = 3$ columns indexed by the sets $\{k, \ell\}$ with $1 \leq k < \ell \leq 3$. The only non-zero entries of $V$ and $W$ are the ones for which $j$ equals either $k$ or $\ell$, so we know there are two entries to be computed for each of the three pairs, resulting in six non-zero entries in each of these matrices. For example, if $\{k, \ell\} = \{1, 2\}$ then we have*

$$v_{1,\{1,2\}} = \text{sign}(x_{1,2})y_{1,2}^{1/4} = 1^{1/4} = 1 \qquad w_{1,\{1,2\}} = y_{2,1}^{1/4} = 1^{1/4} = 1$$
$$v_{2,\{1,2\}} = y_{2,1}^{1/4} = 1^{1/4} = 1 \qquad w_{2,\{1,2\}} = y_{1,2}^{1/4} = 1^{1/4} = 1.$$

*Similar computations show that*

$$v_{1,\{1,3\}} = \text{sign}(x_{1,3})y_{1,3}^{1/4} = -2^{1/4} \qquad w_{1,\{1,3\}} = y_{3,1}^{1/4} = (1/2)^{1/4} = 2^{-1/4}$$
$$v_{3,\{1,3\}} = y_{3,1}^{1/4} = (1/2)^{1/4} = 2^{-1/4} \qquad w_{3,\{1,3\}} = y_{1,3}^{1/4} = 2^{1/4},$$
$$v_{2,\{2,3\}} = \text{sign}(x_{2,3})y_{2,3}^{1/4} = i\sqrt{2} \qquad w_{2,\{2,3\}} = y_{3,2}^{1/4} = 1^{1/4} = 1$$
$$v_{3,\{2,3\}} = y_{3,2}^{1/4} = 1^{1/4} = 1 \qquad w_{3,\{2,3\}} = y_{2,3}^{1/4} = 4^{1/4} = \sqrt{2}.$$

*With all of the non-zero entries computed, we can now construct the matrices $V$ and $W$ that make up the PCP decomposition of $(X, Y)$:*

$$V = \begin{bmatrix} v_{1,\{1,2\}} & v_{1,\{1,3\}} & v_{1,\{2,3\}} \\ v_{2,\{1,2\}} & v_{2,\{1,3\}} & v_{2,\{2,3\}} \\ v_{3,\{1,2\}} & v_{3,\{1,3\}} & v_{3,\{2,3\}} \end{bmatrix} = \begin{bmatrix} 1 & -2^{1/4} & 0 \\ 1 & 0 & i\sqrt{2} \\ 0 & 2^{-1/4} & 1 \end{bmatrix} \quad \textit{and} \quad W = \begin{bmatrix} 1 & 2^{-1/4} & 0 \\ 1 & 0 & 1 \\ 0 & 2^{1/4} & \sqrt{2} \end{bmatrix}.$$

An extension of the result that diagonal dominance implies completely positivity was provided in [19], and states that if $X$ is doubly non-negative and its *comparison matrix*,

$$M(X) \stackrel{\text{def}}{=} \begin{bmatrix} |x_{1,1}| & -|x_{1,2}| & \cdots & -|x_{1,n}| \\ -|x_{2,1}| & |x_{2,2}| & \cdots & -|x_{2,n}| \\ \vdots & \vdots & \ddots & \vdots \\ -|x_{n,1}| & -|x_{n,2}| & \cdots & |x_{n,n}| \end{bmatrix}.$$

is positive semidefinite, then $X$ is completely positive. The following theorem states the generalization of this result to pairwise completely positive matrices. The proof of Theorem 6, given in [3].

**Theorem 6.** *Suppose $X, Y \in M_n(\mathbb{C})$ satisfy conditions (a)–(d) of Theorem 1. If $M(X)$ is positive semidefinite then $(X, Y)$ is pairwise completely positive.*

## 4.3 Applications to Quantum Entanglement

As stated in Section 2.3.2, determining separability of a given quantum state is NP-hard [14], thus mathematicians have made several efforts to establish necessary or sufficient conditions as tests. One of the results that motivated the development of PCP matrices applies to a particular family of quantum states called *mixed Dicke States*, and states that the separability of a mixed Dicke State is characterized by the complete positivity of an associated matrix[2, 20]. In this section we will show that an analogous result holds for pairwise completely positive matrices and a more general set of quantum states. In particular, we show that members of this more general set are separable if and only if a matrix pair associated with the state is pairwise completely positive. We now introduce the elusive “more general quantum state” .

**Definition 2.** *A mixed state $\rho \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is called a* conjugate local diagonal unitary invariant (CLDUI) state *if*

$$(U \otimes \overline{U})\rho(U \otimes \overline{U})^* = \rho$$

*for all diagonal unitary matrices $U \in M_n(\mathbb{C})$.*

It turns out that in order for a matrix $\rho$ to satisfy the above definition, it must have a very particular pattern of zeroes as well as symmetry in the non zero terms. We claim that CLDUI states are exactly those that can be written in the form

$$\rho = \sum_{i,j=1}^{n} x_{i,j}\mathbf{e_i}\mathbf{e_j}^* \otimes \mathbf{e_i}\mathbf{e_j}^* + \sum_{i\neq j=1}^{n} y_{i,j}\mathbf{e_i}\mathbf{e_i}^* \otimes \mathbf{e_j}\mathbf{e_j}^*, \tag{4.4}$$

where the $\{\mathbf{e_j}\}$ are the standard basis vectors. To verify that CLDUI states do indeed have the claimed form, simply observe that if we use $[\rho]_{i,j,k,\ell} = \rho_{i,j,k,\ell}$ to denote the coefficient of the basis matrix $\mathbf{e_i}\mathbf{e_j}^* \otimes \mathbf{e_k}\mathbf{e}_\ell^*$ in $\rho$, then

$$[(U\otimes\overline{U})\rho(U\otimes\overline{U})^*]_{i,j,k,\ell} = u_i\overline{u_j}\overline{u_k}u_\ell\rho_{i,j,k,\ell},$$

which equals $\rho_{i,j,k,\ell}$ for all diagonal $U$ if and only if $(i,\ell) = (j,k)$, $(i,\ell) = (k,j)$, or $\rho_{i,j,k,\ell} = 0$. For example, in the $(3\otimes 3)$-dimensional case, every CLDUI state $\rho$ can be written in the standard basis in the following form, where we use $\cdot$ to denote entries equal to $0$:

$$\rho = \left[\begin{array}{ccc|ccc|ccc}
x_{1,1} & \cdot & \cdot & \cdot & x_{1,2} & \cdot & \cdot & \cdot & x_{1,3} \\
\cdot & y_{1,2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & y_{1,3} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\hline
\cdot & \cdot & \cdot & y_{2,1} & \cdot & \cdot & \cdot & \cdot & \cdot \\
x_{2,1} & \cdot & \cdot & \cdot & x_{2,2} & \cdot & \cdot & \cdot & x_{2,3} \\
\cdot & \cdot & \cdot & \cdot & \cdot & y_{2,3} & \cdot & \cdot & \cdot \\
\hline
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & y_{3,1} & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & y_{3,2} & \cdot \\
x_{3,1} & \cdot & \cdot & \cdot & x_{3,2} & \cdot & \cdot & \cdot & x_{3,3}
\end{array}\right].$$

In order to establish a correspondence between CLDUI states $\rho$ and matrix pairs $(X,Y)$, we collect the coefficients $\{x_{i,j}\}$ and $\{y_{i,j}\}$ into smaller matrices $X$ and $Y$, and define $y_{i,i} = x_{i,i}$ for all $i$. Since the submatrix $Y$ is constructed from the diagonal entries of $\rho$ it follows that Y is entrywise nonnegative, that is, $Y \geq 0$. Another implication of this correspondence is that $X$ is PSD, since $X$ is a principal submatrix of the quantum state $\rho$. We thus note that as a consequence of their construction, the matrix pair $(X, Y)$ immediately satisfies properties (a)–(c) of Theorem 1. For a pair of matrices $(X, Y)$ constructed in this way, we use $\rho_{X,Y}$ to denote their associated CLDUI state.

The following result states that determining separability of a CLDUI state $\rho_{X,Y}$ is equivalent to the question of whether or not the associated pair of coefficient matrices $(X, Y)$ is pairwise completely positive. It also states how the other necessary conditions of Theorem 1 relate to the PPT separability criterion.

**Theorem 7.** *Suppose $X, Y \in M_n(\mathbb{C})$. Then the pair of matrices $(X, Y)$ has the following relationship with properties of the CLDUI state $\rho_{X,Y}$:*

*a) $\rho_{X,Y}$ is a positive semidefinite if and only if $X$ is positive semidefinite, $Y$ is entrywise nonnegative, and $X$ and $Y$ have the same diagonal entries.*

*b) $\rho_{X,Y}$ is furthermore a valid quantum state (i.e., $\mathrm{Tr}(\rho_{X,Y}) = 1$) if and only if $\|Y\|_1 = 1$.*

*c) $\rho_{X,Y}$ is separable if and only if $(X, Y)$ is pairwise completely positive.*

*d) $\rho_{X,Y}$ has positive partial transpose if and only if $(X, Y)$ satisfies property (d) of Theorem 1.*

We omit the proof of the above theorem, noting it is presented in [3], and focus instead on how it can be used. Recall that several special cases of CLDUI states correspond to well known quantum states. One special case of CLDUI states are the isotropic states [21]. These states can be written

$$\rho_{X,Y} = a(I_n \otimes I_n) + b\left(\sum_{i=1}^{n} \mathbf{e_i} \otimes \mathbf{e_i}\right)\left(\sum_{i=1}^{n} \mathbf{e_i} \otimes \mathbf{e_i}\right)^*,$$

and correspond to the matrix pair defined by $X = aI_n + bJ_n$ and $Y = bI_n + aJ_n$. The next example uses Theorem 7 to show separability of a particular isotropic state $\rho_{X,Y}$ in the$(3 \otimes 3)$-dimensional case.

**Example 6.** *Consider the isotropic quantum state described by the following matrix, where $\cdot$ denotes entries equal to zero:*

$$\rho = \frac{1}{24}\left[\begin{array}{ccc|ccc|ccc} 2 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & -1 \\ \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & \cdot & \cdot & \cdot & 2 & \cdot & \cdot & \cdot & -1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot \\ -1 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & 2 \end{array}\right].$$

*The associated coefficient matrices $(X, Y)$ are:*

$$X = \frac{1}{24}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix} \quad \textit{and} \quad Y = \frac{1}{24}\begin{bmatrix} 2 & 3 & 3 \\ 3 & 2 & 3 \\ 3 & 3 & 2 \end{bmatrix}.$$

*Note that $X$ is diagonally dominant and $(X, Y)$ satisfy properties (a)–(d) of Theorem 1. Then by Theorem 5 we have that the pair $(X, Y)$ is PCP. Since isotropic states are CLDUI states, by Theorem 7(c), we have that $\rho_{X,Y}$ is separable.*

Although the conditions from Theorem 1 are consequences of well-known separability criteria, to the best of our knowledge the tests from Theorems 4 and 6 provide novel methods of showing that CLDUI states are separable. Of particular note is the following result:

**Corollary 2.** *Suppose $\rho \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is a CLDUI state. If $\rho$ has positive partial transpose and $M(\rho)$ is positive semidefinite then $\rho$ is separable.*

*Proof.* The proof is a direct consequence of combining Theorems 6 and 7. □

In the next section this result is used to answer a question about absolutely separable states. The question of whether or not it is possible to extend Corollary 2 to arbitrary states is left as an open question.

## 4.4 Applications to Absolute Separability

Recall from Section 3.4 that absolutely separable quantum states are not fully characterized when $n \geq 3$. In particular, it is unknown whether or not the set of absolutely separable states equals the set of absolutely PPT states [16]. We now remark that the findings presented in Section 4.3 may support the equivalence, since they imply that whenever the states $\Gamma(U_j \Lambda U_j^*)$ are PPT they are also separable. This follows from the following fact, which we state without proof: if $U_j$ is one of the special unitaries characterizing PPT states, then $\Gamma(U_j \Lambda U_j^*)$ is necessarily a CLDUI state with non-positive off-diagonal entries. A direct implication of this is that $\Gamma(U_j \Lambda U_j^*)$ is equal to its comparison matrix, hence its comparison matrix is PSD. It then follows from Corollary 2 that $U_j \Lambda U_j^*$ is separable if it is PPT. Since it is unknown whether or not separability of each $U_j \Lambda U_j^*$ necessitates separability of $U \Lambda U^*$ for *all* unitary matrices $U$, this fact isn't enough to show that the set of absolutely separable states equals the set of APPT states. However, the fact that the matrices $U_j \Lambda U_j^*$ are separable in all dimensions does indicate supportive evidence, and warns against the approach to finding a gap between the two sets by searching for entanglement in the states constructed from the special unitaries: $U_j \Lambda U_j^*$.

# Chapter 5

# Conclusion

This thesis presented a generalization of completely positive matrices called *pairwise completely positive* matrices. Their connection to the quantum separability problem was established by showing PCP matrix pairs are in one-to-one correspondence with conjugate local diagonal unitary invariant quantum states, meaning a PCP matrix pair corresponds to a separable CLDUI quantum state. Such a correspondence shows that the problem of determining separability for CLDUI states can be translated into a matrix analysis question that asks under what conditions is the matrix pair $(X, Y)$ guaranteed to meet the definition of pairwise complete positivity. Motivated by this question, several necessary as well as sufficient conditions to determine whether a given matrix pair meets the definition of PCP were presented. The results regarding PCP matrices have been accepted for publishing in the Electronic Journal of Linear Algebra in a paper titled Pairwise Completely Positive Matrices and Conjugate Local Diagonal Unitary Invariant Quantum States [3].

One possible future direction is a generalization of pairwise completely positive matrices that involves exploring a matrix *triple* which arises by considering the quantum states that are invariant under all *real* diagonal unitary matrices. Such states have a slightly more general form than CLDUI states given by

$$\rho = \sum_{i,j=1}^{n} x_{i,j}\mathbf{e_i}\mathbf{e_j}^* \otimes \mathbf{e_i}\mathbf{e_j}^* + \sum_{i\neq j=1}^{n} y_{i,j}\mathbf{e_i}\mathbf{e_i}^* \otimes \mathbf{e_j}\mathbf{e_j}^* + \sum_{i\neq j=1}^{n} z_{i,j}\mathbf{e_i}\mathbf{e_j}^* \otimes \mathbf{e_j}\mathbf{e_i}^*,$$

which are CLDUI states if and only if $z_{i,j} = 0$ for all $i, j$. As mentioned in [3], checking separability of these states in a manner analogous to that of Theorem 7 leads to a triple of matrices $(X, Y, Z)$ with the property that $\rho$ is separable if and only if there exist matrices

$V, W \in M_{n,m}(\mathbb{C})$ such that

$$X = (V \odot W)(V \odot W)^*, \qquad Y = (V \odot \overline{V})(W \odot \overline{W})^*, \quad \text{and} \quad Z = (V \odot \overline{W})(V \odot \overline{W})^*.$$

Such a construction maintains that the matrices have the same diagonal entries, and also implies that both $X$ and the additional matrix $Z$ are positive semidefinite, while $Y$ is entrywise non-negative. The details of this generalization are left as an open question since Dr. Johnston's interest in pairwise completely positive matrices was motivated mainly by connections to the absolute separability problem, in which the relevant states are CLDUI.

# Glossary

| | |
|---|---|
| PSD | Positive Semidefinite: |
| CP | Completely Positive: |
| PCP | Pairwise Completely Positive: |
| PPT | Positive Partial Transpose: The mean distance from the sun to the earth. Approximately 1.49 x $10^{11}$ m. |
| APPT | Absolutely Positive Partial Transpose: |
| CLDUI | Conjugate Local Diagonal Unitary Invariant: |
| $\rho$ | Denotes a quantum state. |

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