Description of rank four PPT entangled states of two qutrits

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It is known that some two qutrit entangled states of rank 4 with positive partial transpose (PPT) can be built from the unextendible product bases (UPB) [Phys. Rev. Lett. \textbf{82}, 5385 (1999)]. We show that this fact is indeed universal, namely all such states can be constructed from UPB as conjectured recently by Leinaas, Myrheim and Sollid. We also classify the 5-dimensional subspaces of two qutrits which contain only finitely many product states (up to scalar multiple), and in particular those spanned by a UPB.

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I. INTRODUCTION

The positive-partial-transpose entangled states (PPTES) are of particular importance and interest in quantum information (for a review see [29]). For a state $\rho$ acting on the Hilbert space $\mathcal{H} := \mathcal{H}_A \otimes \mathcal{H}_B$, the partial transpose computed in an orthonormal (o.n.) basis $\{|a_i\rangle\}$ of system A, is defined by $\rho^\Gamma := \sum_{ij} \langle a_i | \rho | a_j \rangle | a_j \rangle \langle a_i |$. We say that $\rho$
is a PPT \([NPT]\) state if \(\rho^T \geq 0 \implies \rho^T \neq 0\), i.e., \(\rho^T\) has at least one negative eigenvalue]. The most intriguing feature of PPTES is their non-distillability under local operations and classical communications (LOCC) \([24]\). This means that a PPTES, say \(\rho\), cannot be locally converted (asymptotically) into a pure entangled state even if infinitely many copies of \(\rho\) are provided. Since most quantum-information tasks require pure entangled states, a PPTES is a quantum resource which cannot be directly used in practice \([4]\). Nevertheless in the past few years the PPTES have been extensively studied in connection with the phenomena of entanglement activation and universal usefulness \([23, 32]\), the distillable key \([22]\), the symmetry permutations \([38]\) and entanglement witnesses \([32]\), both in theory and experiment.

For many applications, it is an important and basic problem to decide whether a given PPT state is entangled or separable, i.e., the convex sum of product states \(\sum_i |a_i, b_i\rangle \langle a_i, b_i|\) \([39]\). The separability problem has an extensive application in quantum information, metrology, computing, quantum non-locality, and mathematics (like positive maps and \(C^*\)-algebras). Moreover, the problem has been proved to be \(NP\)-hard and hence it attracted a lot of attention from computer scientists \([18]\). In 1996, the first necessary condition was given by Peres \([34]\), saying that the separable states are always PPT. So to solve the problem it suffices to consider only the PPT states. Next in 1999, the Horodeckis \([25]\) showed that this is necessary and sufficient for \(2 \otimes 2\) and \(2 \otimes 3\) states. However both of these cases lack the PPTES. Actually since the first PPTES was constructed \([27]\), researchers lacked for a long time the analytical characterization of PPTES in any bipartite systems of given rank and local dimensions. For example, it was surprisingly difficult to decide whether a given state of rank 4 in \(3 \otimes 3\) space is a PPTES, which is also the smallest space in which PPTES may exist \([25]\). A well-known method \([3]\) for construction of PPTES proposed in 1999 was based on the unextendible product bases (UPB). It is applicable to arbitrary bipartite and multipartite quantum systems. Another systematic method for two-qutrit systems was provided by Chen and Doković who proved in 2010 that a PPT state of rank 4 is entangled if and only if there is no product state in its range \([31]\).

Our main result (see Theorem \([25]\)) shows that any two-qutrit PPTES \(\rho\) of rank 4 can be constructed from an unextendible product basis (UPB) \([25]\) by using the method proposed by Leinaas, Myrheim and Sollid in \([51]\). We state their conjecture formally as Conjecture \([15]\). Explicitly, we prove that (up to normalization) \(\rho = A \otimes B \Pi \{\psi\} A^\dagger \otimes B^\dagger\), where \(\Pi \{\psi\}\) is a UPB, \(\Pi\) is the projector on the subspace orthogonal to \(\{\psi\}\), and \(A, B \in GL_3\), the group of invertible complex matrices of order 3. Let us point out that the papers \([20, 37]\) provided strong numerical evidence for the validity of this result and motivated us to pursue this study. Moreover, the authors of these papers suggest that the higher dimensional PPTES may have similar properties, although some of them have to be modified. This may be of interest for further research in this direction.

It is well-known that the set \(\mathcal{S}_{SEP}\) of separable states and the set \(\mathcal{S}_{PPT}\) of PPT states are both compact and convex, and that \(\mathcal{S}_{SEP} \subseteq \mathcal{S}_{PPT}\). A basic task is then to characterize their extreme points. The latter are the states which are not convex sums of other states in the convex set. It is also a well-known fact that we can generate any state in such a set by taking the convex sum of extreme points. Though it is known that the extreme points of \(\mathcal{S}_{SEP}\) are exactly the pure product states \([39]\), we know quite little about the extreme points of \(\mathcal{S}_{PPT}\) \([39]\). Only in the case of \(2 \otimes 4\) systems, the PPTES have been partially classified by the ranks of both the state and its partial transpose \([1]\). Here, we will show that all two-qutrit PPTES of rank 4 are such extreme points (and also edge PPTES).

We also show that no PPTES of rank 4 exist in the symmetric subspace of the two-qutrit system. Furthermore, it is known that the UPB basis states are not distinguishable under LOCC \([22]\). Thus we exhibit the essential connection between the LOCC-indistinguishability and PPTES.

The content of our paper is as follows. In Sec. \([\text{III}]\) we define the notion of general position for \(m\)-tuples of product vectors (or points on the Segre variety \(\mathcal{P}^2 \times \mathcal{P}^2\)), see Definitions \([\text{I}]\) and \([\text{II}]\). We also define and study the properties of the biprojective (BP) equivalence of such \(m\)-tuples, and in particular for quintuples. To a quintuple of product vectors in general position we assign six \(GL_3 \times GL_3\) invariants \((J^A_i, J^B_i)\), \(i = 1, 2, 3\), and show that two quintuples are BP-equivalent if and only if they share the same invariants. These invariants are subject to the relations \(J^A_1J^A_2J^A_3 = 1\) and \(J^B_1J^B_2J^B_3 = 1\), and can take any complex values except 0 and 1. We then investigate the product states contained in the 5-dimensional subspace spanned by a quintuple of product states in general position. In particular, it follows form the part(a) of Proposition \([\text{I}]\) that if \(\rho\) is a two-qutrit PPT state of rank 4 then its kernel contains only finitely many product vectors (up to scalar multiple). This fact is used later to prove Theorem \([22]\).

In Sec. \([\text{III}]\) we consider the \(8\)-dimensional complex projective space associated to the \(3 \otimes 3\) Hilbert space \(\mathcal{H}\). We consider the case where a \(4\)-dimensional projective subspace, \(\mathcal{P}^4\), and the Segre variety \(\Sigma_{2,2}\) intersect only at finitely many points. Then there are at most 6 points of intersection and to each of them one assigns (in Algebraic Geometry) a positive integer known as the intersection multiplicity. The sum of these integers is necessarily equal to 6. We refer to the corresponding partition of 6 as the intersection pattern of \(\mathcal{P}^4\) and \(\Sigma_{2,2}\). We show that all feasible patterns, i.e., all partitions of 6, occur. For instance, there exists a 5-dimensional vector subspace of \(\mathcal{H}\) which contains only one product state (up to a scalar multiple).

In Sec. \([\text{IV}]\) we study the invariants of quintuples of product states in general position which arise from UPB. These invariants are real and take values in one of the open intervals \(N := (-\infty, 0)\), \(p := (0, 1)\) and \(P := (1, +\infty)\). By
replacing the values of the 6 invariants by the letter designating the interval to which the invariant belongs, we obtain the 6-letter symbol attached to the quintuple. We show that among the 120 permutations of the 5 product states of a UPB, there are exactly 12 different symbols that arise in this way. We say that these 12 symbols are UPB symbols. The same assertion is valid if we use all 6 product states contained in the 5-dimensional subspace spanned by a UPB and construct from them all 720 possible quintuples. Their symbols are also UPB symbols. This is the key tool in the proof of our main result.

In Sec. [VI] we prove that the kernel of any PPTES \( \rho \) of rank 4 contains exactly 6 product states (up to scalar multiple) and that these 6 states are in general position. Next we show that there exist \( A, B \in \text{GL}_3 \) such that the transformed state \( \sigma := A \otimes B \rho A^\dagger \otimes B^\dagger \) is invariant under partial transpose, i.e., \( \sigma^T = \sigma \). We also show that if two normalized PPTES of rank 4 have the same range (or kernel) then they are equal. Finally, by making use of the UPB symbols we prove our main result, Theorem [25]. We conclude that (Sec. V) is isomorphic to the product of two copies of the complex projective plane \( \mathbb{C}P^8 \) associated to the 9-dimensional Hilbert space \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). Then the product vectors form the so called Segre variety \( \Sigma_{2,2} = \mathbb{P}^2 \times \mathbb{P}^2 \subseteq \mathbb{P}^8 \), isomorphic to the product of two copies of the complex projective plane \( \mathbb{P}^2 \).

II. PRODUCT STATES OF TWO QUTRITS

For convenience, we shall represent any product vector \( |x,y\rangle \) as a \( 3 \times 3 \) matrix \( [x_iy_j] \) where \( i, j \in \{1,2,3\} \). In this notation, product vectors correspond to matrices of rank 1. We shall often work with these vectors only up to scalar multiple, in which case we consider them as points in the 8-dimensional complex projective space \( \mathbb{P}^8 \).

A. Projective invariants \( J_1, J_2, J_3 \)

The complex general linear group in dimension 3, that is the group of invertible complex matrices of order 3, will be denoted by \( \text{GL}_3 \). We shall also use the group \( \text{GL} := \text{GL}_3 \times \text{GL}_3 \), the direct product of two copies of \( \text{GL}_3 \). It acts naturally on \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \) via invertible linear operators (ILO) \( A \otimes B \). The points of the complex projective plane \( \mathbb{P}^2 \) will be identified with the 1-dimensional subspaces of \( \mathcal{H}_A \) (or \( \mathcal{H}_B \)). As \( \text{GL}_3 \) permutes the 1-dimensional subspaces of \( \mathcal{H}_A \), it induces an action on \( \mathbb{P}^2 \). The subgroup \( \text{C}^* \), consisting of nonzero scalar matrices of \( \text{GL}_3 \), acts trivially on \( \mathbb{P}^2 \). Thus we obtain an action of the quotient group \( \text{PGL}_3 := \text{GL}_3 / \text{C}^* \) on \( \mathbb{P}^2 \). This group is known as the complex projective general linear group (in dimension 3) and the transformations that it induces on \( \mathbb{P}^2 \) are known as projective transformations. The direct product \( \text{PGL} := \text{PGL}_3 \times \text{PGL}_3 \) acts on the Segre variety \( \mathbb{P}^2 \times \mathbb{P}^2 \), and we refer to it as the group of biprojective transformations of \( \Sigma_{2,2} \).

We say that two \( n \)-partite states \( \rho \) and \( \sigma \) are equivalent under stochastic LOCC (or SLOCC-equivalent) if \( \rho = \bigotimes_{i=1}^n A_i \sigma \bigotimes_{i=1}^n A_i^\dagger \) for some ILO \( A_1, \ldots, A_n \). They are LU-equivalent if \( A_i \) can be chosen to be unitary. In most cases of the present work, we will have \( n = 2 \). Both LOCC and SLOCC are referred to as physical operations in quantum information [29]. The essential difference between them is that LOCC can be implemented with certainty while SLOCC succeeds only with some nonzero probability.

Definition 1 We say that an \( m \)-tuple of pure states \( (|\phi_k\rangle)_{k=0}^{m-1} \) in \( \mathcal{H}_A \) (or \( \mathcal{H}_B \)) is in general position if any two or three of them are linearly independent. If \( (|\phi_k\rangle)_{k=0}^{m-1} \) and \( (|\phi'_k\rangle)_{k=0}^{m-1} \) are two \( m \)-tuples in \( \mathcal{H}_A \) such that \( A|\phi_k\rangle \propto |\phi'_k\rangle \) for some invertible matrix \( A \), then we say that they are projectively equivalent or P-equivalent.

Let us recall the following elementary fact from Linear Algebra also known as the Four Point Lemma (see e.g. [14, Lemma 11.2]):

Lemma 2 If \( (|\phi_k\rangle)_{k=0}^3 \) and \( (|\phi'_k\rangle)_{k=0}^3 \) are quadruples of pure states in general position in \( \mathcal{H}_A \), then there exists an invertible matrix \( A \), unique up to a scalar factor, such that \( A|\phi_k\rangle \propto |\phi'_k\rangle \) for each \( k \).
In particular, for any quadruple \( (|\phi_k\rangle)_{k=0}^4 \) in general position there exists an invertible matrix \( A \) such that \( A|\phi_k\rangle \propto |k\rangle \) for \( k = 0, 1 \) and \( A|\phi_3\rangle = |0\rangle + |1\rangle + |2\rangle \). For convenience, we say that \( A \) transforms the quadruple \( (|\phi_k\rangle)_{k=0}^3 \) into the canonical form. One can construct \( A \) explicitly as follows. Let \( X = \{ |\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle \} \) and let \( D \) be the diagonal matrix whose diagonal entries are the components of the vector \( X^{-1}|\phi_3\rangle \). Then we have \( A = D^{-1}X^{-1} \).

In the language of Projective Geometry the above lemma can be restated as follows. If \( (P_k)_{k=0}^3 \) and \( (P'_k)_{k=0}^3 \) are two quadruples of points in the complex projective plane \( \mathcal{P}^2 \) in general position (i.e., they are distinct and no three points \( P_k \) are collinear, and similarly for the points \( P'_k \)) then there is a projective transformation \( T = T(P_k) = P'_k \) for each \( k \).

However, the action of \( \text{GL}_3 \) on quintuples of points in general position in \( \mathcal{P}^2 \) is not transitive. Indeed let \( (P_k = |\phi_k\rangle)_{k=0}^4 \) be such a quintuple. Then all determinants
\[
\Delta_{i,j,k} = \det[|\phi_i\rangle \langle \phi_j| |\phi_k\rangle], \quad (i, j, k \text{ distinct}),
\]
are nonzero. The rational functions
\[
J_1 = \frac{\Delta_{0,1,2,3}}{\Delta_{0,1,4}}, \quad J_2 = \frac{\Delta_{0,1,4,2,3}}{\Delta_{0,1,3}}, \quad J_3 = \frac{\Delta_{0,1,3,4,2}}{\Delta_{0,1,2}}
\]
are projective \( \text{GL}_3 \)-invariants of quintuples in general position. These invariants may take arbitrary complex values, except 0 and 1, subject to the relation \( J_1J_2J_3 = 1 \). The following result follows easily from the Four Point Lemma and the fact that the quadruple \( (P_k)_{k=0}^3 \) and the values of the invariants \( J_i \).

**Proposition 3** Two quintuples of points \( (P_k = |\phi_k\rangle)_{k=0}^4 \) and \( (P'_k = |\phi'_k\rangle)_{k=0}^4 \) in general position are \( P \)-equivalent if and only if they share the same values of the three invariants \( J_i \).

This means that if the two quintuples satisfy the invariance conditions, then there exists \( A \in \text{GL}_3 \) such that \( A|\phi_k\rangle = c_k|\phi'_k\rangle \) for some scalars \( c_k \), which may be all different.

**Definition 4** We say that an \( m \)-tuple \( (|\psi_k\rangle = |\phi_k\rangle \otimes |\chi_k\rangle)_{k=0}^m \) of non-normalized product states in a \( 3 \times 3 \) system is in general position if each of the \( m \)-tuples \( (|\phi_k\rangle)_{k=0}^m \) and \( (|\chi_k\rangle)_{k=0}^m \) is in general position. In that case we also say that the corresponding \( m \)-tuple of points \( (P_k = |\psi_k\rangle)_{k=0}^m \) on \( \Sigma_2,2 \) is in general position. We also say that two \( m \)-tuples of product states \( (|\psi_k\rangle = |\phi_k\rangle \otimes |\chi_k\rangle)_{k=0}^m \) and \( (|\psi'_k\rangle = |\phi'_k\rangle \otimes |\chi'_k\rangle)_{k=0}^m \) are biprojectively equivalent or \( \text{BP} \)-equivalent if there exists \( A \otimes B \in \text{GL}_3 \) such that \( (A \otimes B)|\psi_k\rangle \propto |\psi'_k\rangle \) for each \( k \).

We shall use the same terminology for the \( m \)-tuples of points lying on \( \Sigma_2,2 \).

In the important case \( m = 5 \), we have two sets of invariants, one for \( (|\phi_k\rangle)_{k=0}^4 \) and the other for \( (|\chi_k\rangle)_{k=0}^4 \). We shall denote the former by \( J_i^A \) and the latter by \( J_i^B \).

The following proposition is an immediate consequence of the definitions and results stated above.

**Proposition 5** The group \( \text{GL}_3 \) acts transitively on the quadruplets of points in general position in \( \Sigma_2,2 \). Two quintuples of points \( (P_k = |\phi_k\rangle \otimes |\chi_k\rangle)_{k=0}^4 \) and \( (P'_k = |\phi'_k\rangle \otimes |\chi'_k\rangle)_{k=0}^4 \) in \( \Sigma_2,2 \), both in general position, are \( \text{BP} \)-equivalent if and only if the quintuplets of points \( (|\phi_k\rangle)_{k=0}^4 \) and \( (|\phi'_k\rangle)_{k=0}^4 \) in \( \mathcal{P}^2 \) are \( P \)-equivalent and the same is true for the quintuplets of points \( (|\chi_k\rangle)_{k=0}^4 \) and \( (|\chi'_k\rangle)_{k=0}^4 \).

We apply our results to the manipulation of families of quantum states. That is, we consider the condition on which two sets of quantum states \( \{\rho_1, \ldots, \rho_n\} \) and \( \{\sigma_1, \ldots, \sigma_n\} \) can be (probabilistically) simultaneously convertible via a physical operation \( \epsilon \), i.e., \( \epsilon(\rho_i) := \sum_j A_j(\rho_i) A_j^\dagger = \sigma_i \), for all \( i \). The problem is in general difficult even for the case of single-party and \( n = 2 \), which has been studied in terms of single-party states for distinguishing quantum operations [12]. In present work, \( \rho_i \) and \( \sigma_j \) are single-party pure states in general position. To realize the conversion, the Kraus operators \( A_i \) have to be pairwise proportional. So the Four Point Lemma and Proposition 4 can be used to decide the simultaneous conversion between two sets of 4 and 5 qutrit states in general position, respectively. Moreover, Proposition 5 works for the conversion between two sets of bipartite product states. Hence we have produced some new manipulable families of states. Further, we have

**Lemma 6** If \( (|\psi_k\rangle)_{k=0}^5 \) is a quadruple of product states in general position, then the subspace that they span contains no other product state.
Proof. Let $|\psi_k\rangle = |\phi_k\rangle \otimes |\chi_k\rangle$, $k = 0, \ldots, 3$. By applying the Four Point Lemma in $H_A$ and $H_B$, we may assume that the quadruples $\langle (|\psi_k\rangle)_{k=0}^3 \rangle$ are in the canonical form

$$|\psi_k\rangle \propto |kk\rangle, \ (k = 0, 1, 2), \ |\psi_3\rangle \propto \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}. \tag{3}$$

Note that the space of $3 \times 3$ diagonal matrices contains only 3 product vectors (up to a scalar multiple). Hence the assertion of the lemma follows from the fact that a non-diagonal matrix

$$\begin{bmatrix} \alpha & \delta & \delta \\ \delta & \beta & \delta \\ \delta & \delta & \gamma \end{bmatrix} \tag{4}$$

has rank 1 if and only if $\alpha = \beta = \gamma = \delta$. \qed

B. Intersection of $P^4$ and $\Sigma_{2,2}$

Projective geometry has quite different properties from those of the affine geometry. For instance, in the complex affine plane, $C^2$, there exist distinct straight lines which are parallel (and so do not meet). However, in the complex projective plane, $P^2$, any two distinct lines meet at exactly one point. More generally, any two projective varieties $X$ and $Y$ in $P^n$ must meet if $\dim X + \dim Y \geq n$.

Let $V$ be a 5-dimensional subspace of the $3 \times 3$ system $H = H_A \otimes H_B$ and $P^4$ the projective 4-dimensional subspace associated to $V$. Since the complex dimensions of $P^4$ and $\Sigma_{2,2}$, namely 4 and 4, add up to the dimension 8 of the ambient projective space $P^8$, these two varieties must have nonempty intersection, i.e., $V$ always contains at least one product state, see e.g. [21, Proposition 11.4]. On the other hand $V$ may contain infinitely many product states, i.e., the intersection of this $P^4$ and the Segre variety $\Sigma_{2,2}$, may have positive dimension. Let us assume that $V$ contains only finitely many product states which we treat as points in the ambient projective space $P^8$, these two varieties must have nonempty intersection, i.e., $V$ always contains at least one product state, see e.g. [21, Proposition 11.4]. Bézout Theorem tells us that $1 \leq k \leq 6$. More precisely, we have $\mu_1 + \cdots + \mu_k = 6$ where $\mu_i$, a positive integer, is the intersection multiplicity of the point $P_i$. See e.g. [14, 21] for more details about these multiplicities and the Bézout Theorem.

We next consider an arbitrary quintuple $\langle (|\psi_k\rangle)_{k=0}^4 \rangle$ of product vectors in general position and the 5-dimensional subspace $V$ that they span. We would like to determine whether $V$ contains any additional product states. The following proposition gives the answer. Since the invariants determine uniquely (up to BP-equivalence) the quintuple of points on $\Sigma_{2,2}$ in general position, it is possible to analyze and answer the above question solely in terms of the invariants.

Proposition 7 Let $(P_k = |\psi_k\rangle = |\phi_k\rangle \otimes |\chi_k\rangle)_{k=0}^4$ be a quintuple of product states in general position, and let $J_i^A$ and $J_i^B$ ($i = 1, 2, 3$) be its invariants. Denote by $V$ the subspace spanned by the $|\psi_k\rangle$ and by $P^4$ the associated projective space. We consider the five equations:

$$J_i^A = J_i^B, \quad (i = 1, 2, 3), \tag{5}$$

$$J_2^A(1 - J_4^A)(1 - J_2^B) = J_2^B(1 - J_4^B)(1 - J_2^A), \tag{6}$$

$$J_1^A(1 - J_3^A)(1 - J_1^B) = J_1^B(1 - J_3^B)(1 - J_1^A). \tag{7}$$

(a) If any two of these equations hold, then all of them do. In that case $V$ contains infinitely many product states. Moreover, any state $\rho$ with $\ker \rho = V$ must be NPT.

(b) If exactly one of the above equations holds, then $V$ contains no additional product states.

(c) If none of the above five equations holds, then $V$ contains exactly one additional product state, say $|\psi\rangle = |c, z\rangle = [c|z]\rangle$. The vectors $|c\rangle$ and $|z\rangle$ are given (up to a scalar factor) by the formulae

$$|c\rangle = A^{-1} \begin{bmatrix} (1 - J_1^B)/(J_1^B - J_1^A) \\ J_2^A(1 - J_2^B)/(J_2^B - J_2^A) \\ (1 - J_2^B)/(J_2^B - J_2^A) \end{bmatrix}, \tag{8}$$

$$|z\rangle = B^{-1} \begin{bmatrix} (1 - J_1^A)/(J_1^B - J_1^A) \\ J_2^B(1 - J_2^B)/(J_2^B - J_2^A) \\ (1 - J_2^B)/(J_2^B - J_2^A) \end{bmatrix}, \tag{9}$$
where $A$ and $B$ are the matrices which transform the quadruples $(|\psi_k\rangle)_{k=0}^3$ and $(|\chi_k\rangle)_{k=0}^3$ to the canonical form, respectively. Moreover the six product states $|\psi_k\rangle$, $k = 0, \ldots, 4$ and $|\psi\rangle$ are in general position.

**Proof.** We begin by transforming the quintuples $(|\psi_k\rangle)_{k=0}^4$ and $(|\chi_k\rangle)_{k=0}^4$ by matrices $A$ and $B$, respectively. Thus we may assume that the quadruples $(|\psi_k\rangle)_{k=0}^3$ and $(|\chi_k\rangle)_{k=0}^3$ are in the canonical form, i.e.,

$$
|\psi_k\rangle \propto |kk\rangle \quad (k = 0, 1, 2),
$$

$$
|\psi_3\rangle = \sum_{i,j=0}^2 |ij\rangle,
$$

$$
|\psi_4\rangle = [b, y] = [b_i y_j].
$$

Since the $P_k$ are in general position, all components $b_i$ and $y_i$ are nonzero, and $b_i \neq b_j$ and $y_i \neq y_j$ for $i \neq j$. A computation shows that

$$
J_1^A = b_2/b_3, \quad J_2^A = b_3/b_1, \quad J_3^A = b_1/b_2;
$$

$$
J_1^B = y_2/y_3, \quad J_2^B = y_3/y_1, \quad J_3^B = y_1/y_2.
$$

Thus we have $J_i^A \neq 1$ and $J_i^B \neq 1$ for $i = 1, 2, 3$, and the equations (6) and (7) can be written as

$$
b_1 y_2 + b_2 y_3 + b_3 y_1 = b_1 y_3 + b_2 y_1 + b_3 y_2,
$$

$$
\frac{1}{b_1 y_2} + \frac{1}{b_2 y_3} + \frac{1}{b_3 y_1} = \frac{1}{b_1 y_3} + \frac{1}{b_2 y_1} + \frac{1}{b_3 y_2},
$$

respectively.

We consider first the case (a). If two of the equations (10) hold, so does the third because of the identity $J_1 J_2 J_3 = 1$. Clearly, the remaining two equations also hold. The other cases can be treated similarly. Let us just consider the hardest case where the two equations displayed above hold. By solving the first for $y_3$ and substituting into the second, we obtain that

$$
\frac{(y_1 - y_2)(b_1 - b_3)(b_2 - b_3)(b_1 y_2 - b_2 y_1)}{b_1 b_2 b_3 y_2 (b_1 y_2 - b_2 y_1 + b_3 y_1 - b_3 y_2)} = 0.
$$

Note that $b_1 y_2 - b_2 y_1 + b_3 y_1 - b_3 y_2 \neq 0$ because $y_3 \neq 0$. Hence we conclude that $b_1 y_2 - b_2 y_1 = 0$, i.e., $J_3^A = J_3^B$. This means that this case reduces to one of the other cases, and the first assertion of (a) is proved.

We now assume that all five equations hold. We can further assume that $b_1 = y_1 = 1$ and, consequently, $b_2 = y_2$ and $b_3 = y_3$. Thus $V$ consists of all symmetric matrices

$$
\begin{bmatrix}
  u & \alpha + \beta b_2 & \alpha + \beta b_1 \\
  \alpha + \beta b_2 & v & \alpha + \beta b_2 b_3 \\
  \alpha + \beta b_1 & \alpha + \beta b_2 b_3 & w
\end{bmatrix}, \quad u, v, w, \alpha, \beta \in \mathbb{C}.
$$

By specializing the diagonal entries

$$
u = \frac{(\alpha + \beta b_2)(\alpha + \beta b_1)}{\alpha + \beta b_2 b_3}, \quad v = \frac{(\alpha + \beta b_2)(\alpha + \beta b_2 b_3)}{\alpha + \beta b_3}, \quad w = \frac{(\alpha + \beta b_3)(\alpha + \beta b_2 b_3)}{\alpha + \beta b_2}
$$

in the above matrix (18), we obtain a family of non-normalized product states depending on two complex parameters $\alpha$ and $\beta$. Since it is contained in $V$, the second assertion of (a) is proved.

Let $\rho$ be a non-normalized state with $\ker \rho = V$. Its range, $V^\perp$, is spanned by $|01\rangle - |10\rangle$, $|12\rangle - |21\rangle$, $|20\rangle - |02\rangle$ and $|\varphi\rangle := b(|01\rangle + |10\rangle) - (1 + b)(|12\rangle + |21\rangle) + (|20\rangle + |02\rangle)$, where $b^* = -b_3(1 - b_2)/b_2(1 - b_3)$. Without loss of generality, we can write $\rho = \sum_{i=0}^3 |\theta_i\rangle \langle \theta_i|$, where $|\theta_i\rangle$ are linearly independent non-normalized pure states

$$
|\theta_0\rangle = |01\rangle - |10\rangle,
$$

$$
|\theta_1\rangle = a_0(|01\rangle - |10\rangle) + a_1(|12\rangle - |21\rangle),
$$

$$
|\theta_2\rangle = a_2(|01\rangle - |10\rangle) + a_3(|12\rangle - |21\rangle) + a_4(|20\rangle - |02\rangle),
$$

$$
|\theta_3\rangle = a_5(|01\rangle - |10\rangle) + a_6(|12\rangle - |21\rangle) + a_7(|20\rangle - |02\rangle) + x|\varphi\rangle,
$$

where $a_i \in \mathbb{C}$ and $x = \frac{\alpha + \beta b_2}{\alpha + \beta b_3}$. Then $\rho$ is also a non-normalized state with $\ker \rho = V$. Thus the second assertion (a) is proved.
with $a_1, a_4, x > 0$. Assume that $\sigma := \rho^T \geq 0$. Since $|00\rangle \in \ker \rho$, the first diagonal entry of the matrix $\sigma$ is 0. Consequently, its first row must vanish. Hence we obtain that
\begin{align}
\alpha^2 + (x - a_7)(x + a_7) &= 0, \\
a_2 a_4 + (b x + a_5)(x + a_7) &= 0, \\
a_2^2 a_4 + (x - a_7)(b x - a_5) &= 0, \\
1 - |a_0|^2 - |a_2|^2 &= 0.
\end{align}
From Eq. (24) we deduce that $a_7$ is real and $x^2 = a_7^2 + a_7^2$. From the next two we deduce that $a_5 = -ba_7$ and $a_2 = b(a_7^2 - x^2)/a_4$, and then Eq. (27) gives the contradiction $1 - |a_0|^2 = 0$.

Hence our assumption that $\sigma \geq 0$ must be false, i.e., $\rho$ must be NPT. Thus all three assertions of (a) are proved.

Next we consider the case (b). Assume that one of the Eqs. (5) holds. Say, $J_3^A = J_3^B$, i.e., $b_1 y_2 - b_2 y_1 = 0$. Then we can also assume that $b_1 = y_1 = 1$, and so $b_2 = y_2$. Hence $V$ consists of all matrices
\begin{align}
X = \begin{bmatrix}
  u & \alpha + \beta b_2 & \alpha + \beta y_3 \\
  \alpha + \beta b_3 & v & \alpha + \beta b_2 y_3 \\
  \alpha + \beta b_3 & \alpha + \beta b_2 b_3 & w
\end{bmatrix}, \quad u, v, w, \alpha, \beta \in \mathbb{C}.
\end{align}
Assume that such a matrix $X$ has rank 1. Let us also assume that $\alpha \beta \neq 0$. Then we can assume that $\beta = 1$. The following equations must hold
\begin{align}
u v &= (\alpha + b_2)^2, \\
u (\alpha + b_2 b_3) &= (\alpha + b_2)(\alpha + b_3), \\
u (\alpha + b_2 y_3) &= (\alpha + b_2)(\alpha + y_3).
\end{align}
From the last two equations we obtain that $u(\alpha + b_2 b_3)/(\alpha + y_3) = u(\alpha + b_2 y_3)/(\alpha + b_3)$, i.e., $u(\alpha - 1) = (\alpha - y_3)u = 0$. As we deal with case (b) and we assumed that $J_3^A = J_3^B$ and $b_1 = y_1 = 1$, we must have $J_3^A \neq J_2^B$, i.e., $b_3 \neq y_3$. Hence, we deduce that $u = 0$, and so $\alpha = -b_2$. Since $X$ has rank 1 and $b_2 \neq b_3$, we deduce that the $(2, 3)$ entry of $X$ must vanish. This gives the contradiction $b_2(y_3 - 1) = 0$. Consequently, we must have $\alpha \beta = 0$. Then Lemma 6 implies that $X \propto |\psi_k\rangle$ for some $k = 0, \ldots, 4$.

The case when Eq. (6) holds can be reduced to the above case by switching the states $|\psi_2\rangle$ and $|\psi_3\rangle$. After this transposition, the new values of the invariants $J_i^A$ are given by the formulæ:
\begin{align}
J_1^A &= 1 - J_1^A, \\
J_2^A &= \frac{J_2^A}{J_4^A - 1}, \\
J_3^A &= \frac{J_3^A - 1}{J_4^A (1 - J_4^A)}.
\end{align}
and the same formulæ are valid for $J_i^B$. It remains to observe that the equality $J_3^A = J_3^B$ is the same as (6).

The case when Eq. (6) holds can be reduced to the previous case by switching the states $|\psi_3\rangle$ and $|\psi_4\rangle$. After this transposition, the new values of the invariants $J_i^A$ are just the reciprocals of the old invariants $J_i^A$, and similarly for $J_i^B$. Then Eq. (6) is replaced by Eq. (7). This completes the proof of (b).

It remains to prove (c). This is a generic case; the five subcases of (b) can be intuitively viewed as the limiting cases of (c) which occur when the state $|\psi\rangle$ (which we are going to construct) becomes equal to one of the given five states so that its multiplicity increases from 1 to 2.

Since $|\psi\rangle \in V$, we have
\begin{align}
|\psi\rangle = \lambda |\psi_0\rangle + \mu |\psi_1\rangle + \nu |\psi_2\rangle + \alpha |\psi_3\rangle + \beta |\psi_4\rangle.
\end{align}
Lemma 6 implies that all coefficients must be nonzero. The six off-diagonal entries of these matrices give the following system of equations
\begin{align}
c_1 z_2 &= \alpha + \beta b_1 y_2, \\
c_1 z_3 &= \alpha + \beta b_1 y_3, \\
c_2 z_3 &= \alpha + \beta b_2 y_3, \\
c_2 z_1 &= \alpha + \beta b_2 y_1, \\
c_3 z_1 &= \alpha + \beta b_3 y_1, \\
c_3 z_2 &= \alpha + \beta b_3 y_2.
\end{align}
By eliminating $c_1$ from the first two equations, and $c_2$ and $c_3$ from the last four, we obtain a system of linear equations in the unknowns $z_i$:
\begin{align}
(\alpha + \beta b_1 y_3)z_2 - (\alpha + \beta b_1 y_2)z_3 &= 0, \\
- (\alpha + \beta b_2 y_3)z_1 + (\alpha + \beta b_2 y_1)z_3 &= 0, \\
(\alpha + \beta b_3 y_2)z_1 - (\alpha + \beta b_3 y_1)z_2 &= 0.
\end{align}
Since this system has a nontrivial solution, its determinant must vanish:

\[
\begin{vmatrix}
0 & \alpha + \beta b_1 y_3 & -(\alpha + \beta b_1 y_2) \\
-(\alpha + \beta b_2 y_3) & 0 & \alpha + \beta b_2 y_1 \\
\alpha + \beta b_3 y_2 & -(\alpha + \beta b_3 y_1) & 0
\end{vmatrix} = 0.
\]

This gives the equation

\[
(\alpha + \beta b_1 y_2)(\alpha + \beta b_2 y_3)(\alpha + \beta b_3 y_1) = (\alpha + \beta b_1 y_3)(\alpha + \beta b_2 y_2)(\alpha + \beta b_3 y_2).
\]

After expanding both sides, the terms with \(\alpha^3\) and \(\beta^3\) cancel and after dividing both sides by \(\alpha\beta\), we find that

\[
\begin{bmatrix}
\alpha \\
\beta
\end{bmatrix} \propto \begin{bmatrix}
b_2 b_3 y_1 (y_3 - y_2) + b_1 b_2 y_3 (y_1 - y_3) + b_1 b_2 y_3 (y_2 - y_1) \\
b_1 (y_1 - y_2) + b_2 (y_1 - y_3) + b_3 (y_2 - y_1)
\end{bmatrix}.
\]

We can replace the proportionality sign with the equality because \(|c\rangle\) and \(|z\rangle\) are determined only up to a scalar factor.

The system of linear equations \((36)\) for the \(z_i\) has the unique solution up to a scalar factor:

\[
|z\rangle \propto \begin{bmatrix}
(\alpha + \beta b_2 y_1)(\alpha + \beta b_3 y_1) \\
(\alpha + \beta b_2 y_1)(\alpha + \beta b_3 y_2) \\
(\alpha + \beta b_2 y_3)(\alpha + \beta b_3 y_1)
\end{bmatrix},
\]

where \(\alpha\) and \(\beta\) are given by Eq. \((41)\). After substituting the expressions for \(\alpha\) and \(\beta\) and cancelling two factors, we obtain the formulae \((42)\). From \((35)\) we have

\[
|c\rangle \propto \begin{bmatrix}
z_1 z_3 (\alpha + \beta b_1 y_2) \\
z_1 z_2 (\alpha + \beta b_3 y_3) \\
z_2 z_3 (\alpha + \beta b_3 y_1)
\end{bmatrix}
\]

and, by using \((41)\), we obtain \((43)\).

Finally by using the above expressions, we can verify that the six product states \(|\psi_k\rangle, k = 0, \cdots, 4\) and \(|\psi\rangle\) are indeed in general position. This completes the proof. \(\square\)

We remark that, by Bézout Theorem, in the case (b) exactly one of the 5 intersection points of \(\mathcal{P}^4 \cap \Sigma_{2,2}\) must have multiplicity 2 and the other multiplicity 1. If \(J^A_i = J^B_i\) holds, then the point with multiplicity 2 is \(P_{i-1}\). If Eq. \((6)\) [Eq. \((7)\)] holds, then this is the point \(P_3\) [\(P_2\)].

The case (c) is of special interest and we single it out in the following definition.

**Definition 8** A quintuple of product states \(|\psi_i\rangle^4_{i=0}\) is regular if it is in general position and the 5-dimensional subspace spanned by the \(|\psi_i\rangle\) contains exactly one additional product state (up to scalar multiple).

As an immediate consequence of the above proposition, we observe that in the case (c) the map sending \((|b\rangle, |y\rangle) \rightarrow (|c\rangle, |z\rangle)\) is involutory, i.e., it also sends \((|c\rangle, |z\rangle) \rightarrow (|b\rangle, |y\rangle)\). As another consequence, we have

**Corollary 9** Let \(|\psi_i\rangle^4_{i=0}\) be a regular quintuple of product states and \(J^A_i, J^B_i\) its invariants. Denote by \(|\psi\rangle\) the unique additional product state in the subspace spanned by the \(|\psi_i\rangle\). Then the invariants \(J^A_i, J^B_i\) of the quintuple \((|\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi\rangle)\) are given by the formulae

\[
J^A_1 = \frac{(1 - J^B_2)(J^B_3 - J^A_3)}{J^A_3(1 - J^B_2)(J^B_3 - J^A_3)}, \quad J^A_2 = \frac{(1 - J^B_3)(J^B_2 - J^A_2)}{J^A_2(1 - J^B_3)(J^B_2 - J^A_2)}, \quad J^A_3 = \frac{(1 - J^B_3)(J^B_2 - J^A_2)}{J^A_3(1 - J^B_3)(J^B_2 - J^A_2)}.
\]

\[
J^B_1 = \frac{J^A_3(1 - J^B_3)}{J^B_3(1 - J^A_3)(J^B_2 - J^A_2)}, \quad J^B_2 = \frac{(1 - J^A_3)(J^A_2 - J^B_2)}{J^B_2(1 - J^A_3)(J^A_2 - J^B_2)}, \quad J^B_3 = \frac{(1 - J^A_3)(J^A_2 - J^B_2)}{J^B_3(1 - J^A_3)(J^A_2 - J^B_2)}.
\]

All cases (a-c) of the above proposition may occur; for (b) and (c) see the last two examples in the proof of Theorem \([10]\). In particular, the proposition shows that the number of product states in \(V\) may be infinite or only 5 even when we impose the condition that the 5 given product states are in general position. Nevertheless, we will show later that the kernel of a \(3 \times 3\) PPTES of rank 4 always contains 6 product states, and that they are in general position (see Theorem \([22]\) in Sec. \([7]\)). Hence, if the kernel of a state \(\rho\) of rank 4 is of type (a) or (b) of Proposition \([7]\) then \(\rho\) must be NPT. This may shed new light on the problem of entanglement distillation of \(3 \times 3\) NPT states of rank 4 \([7]\). We investigate further the properties of 5-dimensional subspaces in the next section.
The results proved in this section may help to solve another long-standing quantum-information problem, namely the state transformation under SLOCC \([13]\). The problem is completely solved for \(2 \times M \times N\) pure states \([11, 12]\); however it becomes exceedingly difficult when all three dimensions are bigger than two, e.g., deciding the SLOCC-equivalence of two \(3 \times 3 \times 3\) states. Here we consider the transformation between two \(3 \times 3 \times 5\) states \(|\psi\rangle, |\varphi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C\) and assume that there are 5 product states \(|\mu_i, b_i\rangle \in \text{Tr}_C |\psi\rangle |\varphi\rangle\) in general position. According to the range criterion \([11\], \(\mathcal{R}(\varphi_{AB})\), we can decide the SLOCC-equivalence of \(|\psi\rangle, |\varphi\rangle\) via Proposition \(25\) and \(14\). Hence, the SLOCC-equivalence of two \(3 \times 3 \times 5\) states can be operationally decided provided that 5 product states in their range of bipartite reduced states are available. Furthermore we can expand subspaces, such as the \(3 \times 3 \times 3\) and \(3 \times 3 \times 4\) subspaces by respectively adding 2 or 1 linearly independent (product) states, to span the whole \(3 \times 3 \times 5\) space. Thus we may treat the SLOCC-equivalence of tripartite states of the former subspaces similar to the latter, when we can build 5 product states in the range of corresponding reduced states.

### III. PRODUCT STATES IN 5-DIMENSIONAL SUBSPACES

As in the previous section, let us consider the intersection \(\mathcal{P}^4 \cap \Sigma_{2,2}\) and assume that it is proper. Our main objective here is to investigate various possibilities for this intersection and provide concrete examples for each case.

#### A. Intersection patterns

Recall that because \(\mathcal{P}^4 \cap \Sigma_{2,2}\) is a finite set, consisting say of \(k\) points, we know that necessarily \(k \leq 6\). Denote by \(\mu_i\) the intersection multiplicity of the point \(P_i\). When arranged in decreasing order \(\mu_1 \geq \mu_2 \geq \cdots \geq \mu_k\), they form a partition \((\mu_1, \ldots, \mu_k)\) of the integer 6. We shall refer to this partition as the intersection pattern (see \([14\], p. 182\)). Altogether there are 11 such partitions and we shall first prove that all of them occur as intersection patterns.

**Theorem 10** All 11 partitions of 6 occur as intersection patterns of \(\mathcal{P}^4 \cap \Sigma_{2,2}\), where \(\mathcal{P}^4\) is a complex 4-dimensional projective space and \(\Sigma_{2,2}\) the Segre variety.

**Proof.** We just have to provide examples of two qutrit states \(\rho\) of rank 4 whose kernel, viewed as a complex projective 4-dimensional subspace, has the specified partition of 6 as its intersection pattern with \(\Sigma_{2,2}\). We shall subdivide the list into 6 parts corresponding to the number, say \(k\), of product states contained in \(\text{ker} \rho\). The corresponding partitions of 6 are those having exactly \(k\) parts. For \(k = 6\) the examples will be provided by the normalized projectors associated with the UPB (see Theorem \(25\)) and also by generic separable states of rank 4 (see Lemma \(21\)). However we shall include a concrete example with \(k = 6\) in our list.

In each case we assume that \(\rho = \sum_{i=0}^3 |\psi_i\rangle \langle \psi_i|\) and give the formulae for the pure states \(|\psi_i\rangle\). We also list the \(k\) product states in the \(\text{ker} \rho\) as well as their intersection multiplicities \(\mu_i\). These multiplicities were computed by means of the free software package *Singular* \([13]\) for symbolic computation in Commutative Algebra.

For \(k = 1\) we set
\[
|\psi_0\rangle = |12\rangle, \quad |\psi_1\rangle = |21\rangle, \quad |\psi_2\rangle = |01\rangle - |10\rangle - |22\rangle, \quad |\psi_3\rangle = |02\rangle + |11\rangle - |20\rangle.
\]
(46)

The kernel is spanned by the states \(|00\rangle, |01\rangle + |10\rangle, |01\rangle + |22\rangle, |02\rangle + |20\rangle\) and \(|11\rangle + |20\rangle\). The first one is the only product state in the kernel. Its multiplicity must be 6.

For \(k = 2\) we give an example for each of the patterns \((5, 1), (4, 2)\) and \((3, 3)\). For the first example we set
\[
|\psi_0\rangle = |12\rangle, \quad |\psi_1\rangle = |01\rangle - |20\rangle, \quad |\psi_2\rangle = |02\rangle - |21\rangle, \quad |\psi_3\rangle = |10\rangle - |22\rangle.
\]
(47)

The kernel is spanned by \(|00\rangle, |11\rangle, |01\rangle + |20\rangle, |02\rangle + |21\rangle\) and \(|10\rangle + |22\rangle\). The first two of them are the only product states in the kernel. Their respective multiplicities are 5 and 1.

For the second example we set
\[
|\psi_0\rangle = |01\rangle - |12\rangle, \quad |\psi_1\rangle = |10\rangle - |21\rangle, \quad |\psi_2\rangle = |02\rangle - |20\rangle, \quad |\psi_3\rangle = |22\rangle.
\]
(48)

One can readily verify that \(\text{ker} \rho\) is spanned by \(|00\rangle, |11\rangle, |01\rangle + |12\rangle, |10\rangle + |21\rangle\) and \(|02\rangle + |20\rangle\), and that \(|00\rangle\) and \(|11\rangle\) are the only product states in the kernel. Their multiplicities are 2 and 4, respectively.

For the third example we set
\[
|\psi_0\rangle = |02\rangle, \quad |\psi_1\rangle = |01\rangle - |10\rangle, \quad |\psi_2\rangle = |11\rangle - |20\rangle, \quad |\psi_3\rangle = |12\rangle - |21\rangle.
\]
(49)
The kernel is spanned by $|00\rangle$, $|22\rangle$, $|01\rangle + |10\rangle$, $|11\rangle + |20\rangle$ and $|12\rangle + |21\rangle$. The first two of them are the only product states in the kernel. Each of the two multiplicities is 3.

For $k = 3$ we give examples for each of the patterns $(4,1,1)$, $(3,2,1)$ and $(2,2,2)$. For the first example we set

$$|\psi_0\rangle = |02\rangle, \quad |\psi_1\rangle = |20\rangle, \quad |\psi_2\rangle = |01\rangle - |12\rangle, \quad |\psi_3\rangle = |10\rangle - |21\rangle.$$  \hspace{1cm} (50)

The kernel is spanned by $|00\rangle$, $|11\rangle$, $|22\rangle$, $|01\rangle + |12\rangle$ and $|10\rangle + |21\rangle$. The first three of these pure states are the only product states in the kernel. Their respective multiplicities are 1,4,1.

For the second example we set

$$|\psi_0\rangle = |20\rangle, \quad |\psi_1\rangle = |01\rangle - |22\rangle, \quad |\psi_2\rangle = |02\rangle - |12\rangle, \quad |\psi_3\rangle = |10\rangle - |21\rangle.$$  \hspace{1cm} (51)

The kernel is spanned by $|00\rangle$, $|11\rangle$, $|02\rangle + |12\rangle$, $|01\rangle + |22\rangle$ and $|10\rangle + |22\rangle$. The first three of these pure states are the only product states in the kernel. For each of them the intersection multiplicity is 2.

For the third example we set

$$|\psi_0\rangle = |11\rangle, \quad |\psi_1\rangle = |02\rangle - |12\rangle, \quad |\psi_2\rangle = |20\rangle - |21\rangle, \quad |\psi_3\rangle = |01\rangle + |10\rangle + |22\rangle.$$  \hspace{1cm} (52)

The kernel is spanned by $|00\rangle$, $|02\rangle + |11\rangle$, $|11\rangle + |20\rangle$, $|10\rangle + |22\rangle$ and $|12\rangle + |21\rangle$. The first product state in the kernel is $|00\rangle$ and the other three are given by rank one matrices:

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & \zeta & \zeta^2 & 1 \end{bmatrix}, \quad \zeta^3 = 1.$$  \hspace{1cm} (54)

For $|00\rangle$ the intersection multiplicity is 3, and for the other three points it is 1.

For the second example we set

$$|\psi_0\rangle = |10\rangle, \quad |\psi_1\rangle = |01\rangle - |22\rangle, \quad |\psi_2\rangle = |02\rangle - |12\rangle, \quad |\psi_3\rangle = |20\rangle - |21\rangle.$$  \hspace{1cm} (55)

The kernel is spanned by $|00\rangle$, $|11\rangle$, $|02\rangle + |12\rangle$, $|20\rangle + |21\rangle$ and $|01\rangle + |22\rangle$. The first four of these pure states are the only product states in the kernel. Their intersection multiplicities are 1,1,2 and 2, respectively.

For $k = 4$ we give examples with intersection patterns $(3,1,1,1)$ and $(2,2,1,1)$. For the first example we set

$$|\psi_0\rangle = |01\rangle, \quad |\psi_1\rangle = |02\rangle - |11\rangle + |20\rangle, \quad |\psi_2\rangle = |10\rangle - |22\rangle, \quad |\psi_3\rangle = |12\rangle - |21\rangle.$$  \hspace{1cm} (53)

The kernel is spanned by $|00\rangle$, $|02\rangle + |11\rangle$, $|11\rangle + |20\rangle$, $|10\rangle + |22\rangle$ and $|12\rangle + |21\rangle$. The first product state in the kernel is $|00\rangle$ and the other three are given by rank one matrices:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 1 & -i \\ -1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix}, \quad \begin{bmatrix} i & i & 1 \\ -1 & 1 & i \\ -i & i & -1 \end{bmatrix}, \quad \begin{bmatrix} -i & i & 1 \\ -1 & 1 & -i \\ i & -i & -1 \end{bmatrix}.$$  \hspace{1cm} (57)

where $i$ is the imaginary unit. For $|00\rangle$ the intersection multiplicity is 2, and for the remaining four product states each multiplicity is 1.

For $k = 5$ there is only one possible intersection pattern, namely $(2,1,1,1,1)$. We set

$$|\psi_0\rangle = |01\rangle - |20\rangle, \quad |\psi_1\rangle = |02\rangle - |11\rangle, \quad |\psi_2\rangle = |10\rangle - |22\rangle, \quad |\psi_3\rangle = |12\rangle - |21\rangle.$$  \hspace{1cm} (56)

The kernel is spanned by the states $|00\rangle$, $|01\rangle + |20\rangle$, $|02\rangle + |11\rangle$, $|10\rangle + |22\rangle$ and $|12\rangle + |21\rangle$. The first product state in the kernel is $|00\rangle$ and the other four are given by rank one matrices:

$$\begin{bmatrix} 1 & \xi & \xi^4 & \xi \\ \xi^3 & \xi^2 & \xi^4 & \xi \end{bmatrix}, \quad \xi^5 = 1.$$  \hspace{1cm} (59)

The kernel is spanned by $|00\rangle$, $|01\rangle + |20\rangle$, $|02\rangle + |11\rangle$, $|10\rangle + |22\rangle$ and $|12\rangle + |21\rangle$. The first product state in the kernel is $|00\rangle$ and the other five are given by rank one matrices:
Clearly, in this case each multiplicity must be 1.

The above example for \( k = 5 \) shows that a state of rank 4 whose range contains no product state may fail to be a PPTES. Indeed, the kernel of a PPTES of rank 4 contains exactly 6 product states (see Theorem 12 below).

On the other hand the example that we chose for \( k = 6 \) is SLOCC-equivalent to the Pyramid UPB in [11]. One way to see this is simply to verify that the quintuple of product states given by the above matrices for \( \xi = \exp(2\pi ik/5) \), \( k = 0, \ldots, 4 \) and the UPB quintuple for the Pyramid (see Eq. 11 below) have the same invariants. If we exchange the parties A, B and transform the product states in the kernel by the local operator \( S \otimes S, S = \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \oplus [\sqrt{1 + \sqrt{5}}] \), we again obtain the Pyramid.

Of course, the intersection of \( P^4 \) and \( \Sigma_{2,2} \) does not have to be proper, i.e., it may have positive dimension. For the comparison with Theorem 10 we provide a scenario where there are infinitely many product states in the kernel.

**Lemma 11** Let \( \rho \) be a \( 3 \times 3 \) state of rank 4 such that, \( \text{rank}(\langle x | \rho | x \rangle) = 1 \) for some \( |x \rangle \in \mathcal{H}_A \). Then ker \( \rho \) contains infinitely many product states.

**Proof.** Since the operator \( \sigma = \langle x | \rho | x \rangle \) has rank one, it suffices to observe that the 2-dimensional subspace \( |x \rangle \otimes \text{ker}(\sigma) \) is contained in the kernel of \( \rho \). \( \Box \)

**B. Rank-4 PPTES with no product state in the range**

In this subsection we consider a related problem of describing the product states in the kernel of states of rank 4 having no product state in the range. The set of such states properly contains all \( 3 \times 3 \) PPTES of rank 4, as one will see later in Theorem 23. It is thus important to have a general understanding of this set.

**Lemma 12** Let \( \rho \) be a \( 3 \times 3 \) state of rank 4. Then \( \mathcal{R}(\rho) \) contains at least one product state when its kernel contains either

(a) two linearly independent product states \( |a, b \rangle \) and \( |c, d \rangle \) with \( |a \rangle = |c \rangle \) or \( |b \rangle = |d \rangle \), or

(b) three linearly independent product states \( |u_i, v_i \rangle, i = 1, 2, 3 \) such that the \( |u_i \rangle \) or the \( |v_i \rangle \) are linearly dependent.

**Proof.** If (a) holds, say \( |a \rangle = |c \rangle \), then the 7-dimensional space \( \text{span}\{|a, b \rangle, |a, d \rangle\} \) contains \( \mathcal{R}(\rho) \) and the 6-dimensional subspace \( V = |a \rangle \otimes \mathcal{H}_B \). Since \( V \cap \mathcal{R}(\rho) \) has dimension \( \geq 3 \), it must contain a product state.

If (b) holds, say the \( |u_i \rangle \) are linearly dependent, then the 6-dimensional space \( \{u_i, v_i : i = 1, 2, 3\} \) contains \( \mathcal{R}(\rho) \) and the 3-dimensional subspace \( V = \{u_i, i = 1, 2, 3\} \otimes \mathcal{H}_B \). Hence, the subspace \( V \cap \mathcal{R}(\rho) \) has dimension \( \geq 1 \). Since each nonzero vector in \( V \) is a product state the assertion follows. This completes the proof. \( \Box \)

Note that the converse does not hold; i.e., both (a) and (b) may fail even though \( \mathcal{R}(\rho) \) contains a product state (see the first example for \( k = 3 \)). Nevertheless, this result will be strengthened in the case of PPTES in Sec. V.

On the other hand there may exist only 3 product states in general position in a 5-dimensional kernel, when there is no product state in the range of \( \rho \). We consider 5 states in ker \( \rho \) represented by the matrices \( C_i, i = 0, 1, 2, 3, 4 \)

\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0 \\
\end{bmatrix} \text{ or } \begin{bmatrix}
0 & a & b \\
0 & a & -1 + b \\
0 & a & -1 + b \\
0 & a & -1 + b \\
0 & a & -1 + b \\
0 & a & -1 + b \\
0 & a & -1 + b \\
0 & a & -1 + b \\
\end{bmatrix}, \quad (60)
\]

respectively, where \( a \neq 0, b \neq 1 \). Up to ILOs, this is also the generic expressions of basis in a 5-dimensional kernel where there are only 3 product states in general position and there are no product states in the range of \( \rho \).

**Lemma 13** For any \( 3 \times 3 \) state \( \rho \) of rank 4, whose kernel is spanned by the pure states above, \( \mathcal{R}(\rho) \) contains no product state while ker \( \rho \) contains only 3 product states and they are in general position.

**Proof.** First we show that there is no product state \( |a, b \rangle \in \mathcal{R}(\rho) \). Because the first three product states in the kernel are \( |00 \rangle, |11 \rangle, |22 \rangle \), we have that \( |a, b \rangle = |i\rangle(x_i(i+1) \mod 3) + y_i(i+2) \mod 3) \) or \( (x_i(i+1) \mod 3) + y_i(i+2) \mod 3) |i\rangle \), \( i = 0, 1, 2 \). Since one of them is orthogonal to the latter two states \( C_3, C_4 \) in Eq. 60, there are two parallel rows or columns in the same position of \( C_3, C_4 \). This is evidently impossible, so there is no product state in \( \mathcal{R}(\rho) \).

Second we show that \( |00 \rangle, |11 \rangle, |22 \rangle \) are the only three product states in the kernel. It is easy to see that we must use \( C_4 \). We compute the linear combination of \( C_i, i = 0, 1, 2, 3, 4 \) such that

\[
C := uC_0 + vC_1 + wC_2 + xC_3 + 4 = \begin{bmatrix}
u & a & b + x \\
a & v & -1 + b + x \\
1 + x & x & w \\
\end{bmatrix}, \quad (61)
\]
which has rank 1 when it is a product state. Evidently \( x \neq -1, 0 \). Then we can deduce that \( v = \frac{x}{1 + x} \), which leads to
\[
\det \begin{bmatrix}
a & b + x \\
v & -1 + b + x
\end{bmatrix} \neq 0.
\]
Hence \( C \) cannot be a product state \( \forall u, v, w, x \). This completes the proof. \( \square \)

Furthermore we consider 5 states in \( \ker \rho \) represented by the matrices \( C_i, i = 0, 1, 2, 3, 4 \)
\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix},
\begin{bmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{bmatrix},
\begin{bmatrix}
0 & 1 & 1 \\
0 & 0 & 0 \\
1 & -2 - c & -1 - c
\end{bmatrix},
\begin{bmatrix}
0 & c - \frac{8}{2 + c} & c \\
1 & 0 & 0 \\
0 & \frac{4c}{2 + c} & c
\end{bmatrix},
\]
(62)
respectively, where the real \( c \neq -2, 0 \). Then we have

**Lemma 14** For any \( 3 \times 3 \) state \( \rho \) of rank 4, whose kernel is spanned by the pure states \( \{ \rho \} \), \( R(\rho) \) contains no product states while \( \ker \rho \) contains only 2 product states (up to scalar multiple) and these two states are in general position.

**Proof.** The proof is similar to that for Lemma 13. First we show that there is no product state \( \{ a, b \} \in R(\rho) \). Because the first two product states in the kernel are \( |00\rangle, |11\rangle \) we have that \( \{ a, b \} = (x_0|0\rangle + x_2|2\rangle)(y_1|1\rangle + y_2|2\rangle) \), or \( (x_1|1\rangle + x_2|2\rangle)(y_0|0\rangle + y_2|2\rangle) \), or \( |2, 0 \rangle \) or \( |0, 2 \rangle \). One can check that none of them exists, so there is no product state in \( R(\rho) \). Second we show that \( |00\rangle, |11\rangle \) are the only 2 product states in the kernel. To simplify the proof, we notice that the first 4 blocks cannot generate new product states. So we must need \( C_4 \). Further we consider three cases for the linear combination \( C := uC_0 + vC_1 + wC_2 + xC_3 + C_4 \), namely \( g = 4c/(2 + c)^2 \), \( g = 1 \) and the rest. In each of these cases, one can easily show that \( C \) cannot be a product state. This completes the proof. \( \square \)

We lack examples of states whose range contains no product state, and whose kernel contains only 1 product state. This problem, as well as Lemmas 13 and 14, is more relevant for the characterization of NPT states, which is an essentially useful quantum-information resource (for a recent paper see [7]). From the next section we will focus on the main topic of this paper, namely the description of the \( 3 \times 3 \) PPTES of rank 4 via the UPB construction [3].

**IV. CHARACTERIZATION OF EQUIVALENT \( 3 \times 3 \) UPB**

Let us denote by \( \mathcal{E}_4 \) the set of all PPTES of rank 4 in a \( 3 \otimes 3 \) system. Our main objective is to prove a conjecture which was raised in [31] and gives a full description of the set \( \mathcal{E}_4 \). This has close connection with the family of PPTES constructed in [10] via UPBs.

**A. PPTES of rank 4 and UPB**

Let \( \mathcal{U} \) denote the set of all UPBs in \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). We denote by \( \mathcal{U}^\circ \) the set of all quintuples \( \{ \psi \} := (|\psi_k\rangle = |\phi_k\rangle \otimes |\chi_k\rangle)_{k=0}^4 \) of (normalized) product states such that the set \( \{ |\psi_k\rangle : 0 \leq k \leq 4 \} \) is a UPB and the following orthogonality relations hold:
\[
\langle \phi_i | \phi_{i+1} \rangle = \langle \chi_i | \chi_{i+2} \rangle = 0,
\]
(63)
where the indexes are taken modulo 5. We have a natural projection map \( \mathcal{U}^\circ \to \mathcal{U} \) which associates to a quintuple \( \{ \psi \} = (|\psi_k\rangle)_{k=0}^4 \in \mathcal{U}^\circ \) the UPB \( \{ \psi \} := \{ |\psi_k\rangle : 0 \leq k \leq 4 \} \in \mathcal{U} \). It was shown in [10] that this map is onto. It is clearly 10-to-1 map because the cyclic permutation of the \( |\psi_i\rangle \) and also the reflection which interchanges the indexes via the permutation \( (0)(14)(23) \) has no effect on the set \( \{ \psi \} \), and leaves \( \mathcal{U}^\circ \) globally invariant.

There is a natural map \( \Pi : \mathcal{U} \to \mathcal{E}_4 \) which associates to \( \{ \psi \} \in \mathcal{U} \) the state \( \Pi \{ \psi \} := (1/4)P \), where \( P \) is the orthogonal projector of rank 4 with \( \ker P = \text{span} \{ \psi \} \). The following conjecture, which gives explicit description of \( \mathcal{E}_4 \) was raised recently in [31] and supported by vast numerical evidence.

**Conjecture 15** Every state \( \rho \in \mathcal{E}_4 \) is the normalization of \( A \otimes B \Pi \{ \psi \} A^\dagger \otimes B^\dagger \) for some \( (A, B) \in \text{GL} \) and \( \{ \psi \} \in \mathcal{U} \).

The proof of this conjecture will be given in Theorem 25 of Section V.
Lemma 17

We fix orthonormal bases \( \{ |0\rangle_A, |1\rangle_A, |2\rangle_A \} \) and \( \{ |0\rangle_B, |1\rangle_B, |2\rangle_B \} \) of \( \mathcal{H}_A \) and \( \mathcal{H}_B \), respectively. It was shown in [10] that every quintuple \( |\psi_k\rangle = |\alpha_k\rangle \otimes |\beta_k\rangle \), \( k = 0, \ldots, 4 \), in \( \mathcal{U}^4 \) is LU-equivalent to one in the following 6-parameter family:

\[
\begin{align*}
|\alpha_0\rangle &= |0\rangle_A, \\
|\alpha_1\rangle &= |1\rangle_A, \\
|\alpha_2\rangle &= \cos \theta_A |0\rangle_A + \sin \theta_A |2\rangle_A, \\
|\alpha_3\rangle &= \sin \gamma_A \cos \theta_A |0\rangle_A - \sin \gamma_A \cos \theta_A |2\rangle_A + \cos \gamma_A e^{i\phi_A} |1\rangle_A, \\
|\alpha_4\rangle &= \frac{1}{N_A} \left( \sin \gamma_A \cos \theta_A e^{i\phi_A} |1\rangle_A + \cos \gamma_A |2\rangle_A \right), \\
|\beta_0\rangle &= |1\rangle_B, \\
|\beta_1\rangle &= \sin \gamma_B \sin \theta_B |0\rangle_B - \sin \gamma_B \cos \theta_B |2\rangle_B + \cos \gamma_B e^{i\phi_B} |1\rangle_B, \\
|\beta_2\rangle &= |0\rangle_B, \\
|\beta_3\rangle &= \cos \theta_B |0\rangle_B + \sin \theta_B |2\rangle_B, \\
|\beta_4\rangle &= \frac{1}{N_B} \left( \sin \gamma_B \cos \theta_B e^{i\phi_B} |1\rangle_B + \cos \gamma_B |2\rangle_B \right).
\end{align*}
\]

The 6 real parameters are the angles: \( \gamma_{A,B}, \theta_{A,B} \) and \( \phi_{A,B} \), and the normalization constants \( N_{A,B} \) are given by the formulae

\[
N_{A,B} = \sqrt{\cos^2 \gamma_{A,B} + \sin^2 \gamma_{A,B} \cos^2 \theta_{A,B}}.
\]

The first four angles are required to have nonzero sine and cosine, while the angles \( \phi_{A,B} \) may be arbitrary. It is not hard to show that the parameter domain can be further restricted as in the following lemma.

Lemma 16 Every quintuple \( |\psi\rangle = (|\psi_k\rangle)_{k=0}^4 \in \mathcal{U}^4 \) with \( |\psi\rangle = |\alpha_k\rangle \otimes |\beta_k\rangle \) is LU-equivalent to one belonging to the family \( \{64\} \) such that the four angles \( \gamma_{A,B}, \theta_{A,B} \) belong to the interval \( (0, \pi/2) \).

Proof. We may assume that \( |\alpha_0\rangle = |0\rangle_A, |\alpha_1\rangle = |1\rangle_A, |\beta_0\rangle = |1\rangle_B \) and \( |\beta_2\rangle = |0\rangle_B \). As \( |\alpha_2\rangle \) is a linear combination of \( |0\rangle_A \) and \( |2\rangle_A \), we can choose the overall phase of \( |\alpha_2\rangle \) so that the coefficient of \( |0\rangle_A \) is positive. By applying a diagonal unitary matrix \( U_A = \text{diag}(1,1,\xi) \), we can also assume that the coefficient of \( |2\rangle_A \) is positive. Thus \( |\alpha_2\rangle = \cos \theta_A |0\rangle_A + \sin \theta_A |2\rangle_A \) for some \( \theta_A \in (0, \pi/2) \).

Next, \( |\alpha_3\rangle \) is a linear combination of \( |1\rangle_A \) and \( |\alpha_0\rangle |0\rangle_A - \cos \theta_A |2\rangle_A \). We can choose the overall phase of \( |\alpha_3\rangle \) so that the coefficient of \( |0\rangle_A - \cos \theta_A |2\rangle_A \) is positive. Thus

\[
|\alpha_3\rangle = \sin \gamma_A \sin \theta_A |0\rangle_A - \sin \gamma_A \cos \theta_A |2\rangle_A + \cos \gamma_A e^{i\phi_A} |1\rangle_A
\]

for some \( \gamma_A \in (0, \pi/2) \) and some angle \( \phi_A \).

Finally, \( |\alpha_4\rangle \) is a linear combination of \( |1\rangle_A \) and \( |2\rangle_A \). We can choose the overall phase of \( |\alpha_2\rangle \) so that the coefficient of \( |2\rangle_A \) is positive. Since \( |\alpha_4\rangle \) is orthogonal to \( |\alpha_3\rangle \), we have

\[
|\alpha_4\rangle = \frac{1}{N_A} \left( \sin \gamma_A \cos \theta_A e^{i\phi_A} |1\rangle_A + \cos \gamma_A |2\rangle_A \right)
\]

with \( \gamma_A \in (0, \pi/2) \) and the positive normalization constant \( N_A \).

The same arguments can be used on Bob’s side. \( \square \)

We shall give just one example, namely the UPB quintuple known as Tiles. Its parameters, as given in [10, p. 394], are \( \phi_{A,B} = 0, \theta_{A,B} = \gamma_{A,B} = 3\pi/4 \). This quintuple is LU-equivalent to the one given by parameters \( \phi_{A,B} = \pi, \theta_{A,B} = \gamma_{A,B} = \pi/4 \). The local unitary transformation that we can use in this case fixes the vectors \( |0\rangle_A, |1\rangle_A \) and \( |0\rangle_B, |1\rangle_B \), and sends \( |2\rangle_A \) and \( |2\rangle_B \) to their negatives.

Let \( \mathcal{F} \) be the subfamily of the family \( \{64\} \) obtained by restricting the domain of parameters so that the four angles \( \gamma_{A,B}, \theta_{A,B} \) belong to the interval \( (0, \pi/2) \) while the angles \( \phi_{A,B} \) belong to \( (-\pi, \pi) \). Since the domain of parameters is connected, the family \( \mathcal{F} \) is also connected. By Lemma 16 we have \( \mathcal{U}^0 = U(3) \times U(3) \cdot \mathcal{F} \), and so the set \( \mathcal{U}^0 \) is connected too.

Lemma 17 Assume that \( A \otimes B(|\psi\rangle) = (|\psi\rangle) \) where \( (A, B) \in \text{GL} \) and the quintuples \( (|\psi\rangle) \) and \( (|\psi\rangle) \) belong to \( \mathcal{U}^0 \). Then there is a positive constant \( c \) such that \( cA \) and \( c^{-1}B \) are unitary. In particular, if \( (|\psi\rangle) \) and \( (|\psi\rangle) \) are SLOCC-equivalent then they are LU-equivalent.
Thus we may assume that since all these angles belong to $(0, 1)$, we deduce that $\langle \phi_k | \phi_{k+1} \rangle = 0$. Consequently, $A^1A$ must map the plane spanned by $|\phi_{k+1}\rangle$ and $|\phi_{k-1}\rangle$ onto itself. This clearly implies that $A^1A$ is a scalar matrix, i.e., there is a scalar $c > 0$ such that $cA$ is a unitary matrix. A similar argument shows that $c^{-1}B$ is also unitary.

Note that SLOCC-equivalence is different from the BP-equivalence which does not require the identical global scalar for simultaneous transformations $A \otimes B |\psi\rangle = |\psi'\rangle$, $k = 0, \ldots, 4$. By Lemma 17 two SLOCC-equivalent quintuples $(\psi)$ and $(\psi')$ in $\mathcal{F}$ must be connected by local unitary operators $U_A \otimes U_B$.

**Proposition 18** If two quintuples $(|\psi_k\rangle)$, $(|\psi'_k\rangle) \in \mathcal{F}$ are SLOCC-equivalent, then $|\psi_k\rangle = |\psi'_k\rangle$ for $k = 0, \ldots, 4$.

**Proof.** As in Eqs. (64) we write $|\psi_k\rangle = |\alpha_k\rangle \otimes |\beta_k\rangle$ and similarly let $|\psi'_k\rangle = |\alpha'_k\rangle \otimes |\beta'_k\rangle$. Let $(\gamma_{A,B}, \theta_{A,B})$ and $(\gamma'_{A,B}, \theta'_{A,B})$ be the parameters of the two quintuples, respectively.

The SLOCC-equivalence implies that the quintuples $(|\alpha_k\rangle)_{k=0}^4$ and $(|\alpha'_k\rangle)_{k=0}^4$ are projectively equivalent. We point out that these quintuples are in general position and so, by Proposition 14, we may assume that $J_i^A$. By using the expressions in Eq. (64) and the formulae Eq. (2), we find that these invariants $(|\psi_k\rangle)$ are given by

$$
\begin{align*}
J_1^A &= -\frac{1}{\sin^2 \theta_B}, \quad J_2^A = \frac{1}{\cos \theta_A \sin^2 \theta_B}, \quad J_3^A = -\frac{1}{\cos \theta_A \sin^2 \theta_B}, \quad J_4^A = 1 + \cos^2 \theta_B \tan^2 \gamma_B.
\end{align*}
$$

Similar formulae are valid for the quintuple $(|\psi'_k\rangle)$. The equalities $J_i^A = J_i^A'$ and $J_i^B = J_i^B'$ imply that

$$
\cos^2 \xi_X = \cos^2 \xi_X', \quad \xi = \gamma, \theta; \quad X = A, B.
$$

(80)

Since all these angles belong to $(0, \pi/2)$, we conclude that $\gamma^A_B = \gamma_{A,B}$ and $\theta^A_B = \theta_{A,B}$. It remains to prove that also $\phi^A_{A,B} = \phi_{A,B}$.

By Lemma 17 there exist unitary matrices $A = [a_{ij}]$ and $B = [b_{ij}]$ such that

$$
A |\alpha_k\rangle \otimes B |\beta_k\rangle - |\alpha'_k\rangle \otimes |\beta'_k\rangle = 0, \quad k = 0, \ldots, 4.
$$

(81)

We view each of these equations as a matrix equation. For $k = 0$ it gives $a_{11}b_{22} = 1$ and $a_{21} = a_{31} = b_{12} = b_{32} = 0$. Thus we may assume that $a_{11} = b_{22} = 1$ and, since $A$ and $B$ are unitary, we must also have $a_{12} = a_{13} = b_{21} = b_{23} = 0$. For $k = 2$, the matrix equation shows that $b_{11} = 1$ and $a_{33} = 1$. We deduce that $a_{23} = b_{31} = 0$. Now, for $k = 1$ the matrix equation implies that $a_{22} = b_{33} = 1$. This means that $A = B = I_3$ and so $\phi^A_{A,B} = \phi_{A,B}$.

**B. UPB symbols**

Let us say that a 5-dimensional subspace $W \subseteq \mathcal{H}$ is of **UPB type** if it is BP-equivalent to a subspace spanned by a UPB. We can characterize the UPB-type subspaces by using invariants. For this purpose we attach a 6-letter symbol made up of letters N, P and p to each quintuple of product states in general position having all invariants real.

Let us denote the open intervals $(-\infty, 0)$, $(0, 1)$, $(1, +\infty)$ by the letters $N$, $p$, $P$, respectively. $(N$ is for “negative”, $p$ for “positive and small” and $P$ for “positive and large”.) Let $(\psi) := (|\psi_k\rangle)_{k=0}^4$ be any quintuple of product states in general position. For convenience, we shall say that $(\psi)$ is **real** if all of its invariants are real numbers. Since the invariants do not take values 0 and 1, if $(\psi)$ is real its invariants must take the values in one of the intervals $N, P, p$. For real $(\psi)$ we define its **symbol** to be the 6-letter sequence obtained by replacing each of its invariants $J_1^A, J_2^A, J_3^A, J_4^B, J_5^B, J_6^B$ by the interval to which it belongs. For instance, each quintuple $(\psi) \in \mathcal{F}$ has $NPNPpP$ as its symbol because $J_1^A < 0$, $J_2^A > 1$, $J_3^B < 0$, $J_4^B > 1$, $0 < J_5^B < 1$ and $J_6^B > 1$. Altogether there are 144 symbols that arise in this manner. Each symbol can be broken into two parts, A and B. The A B part consists of the first [last] three letters. Because of the identity $J_1J_2J_3 = 1$, there are only 12 possibilities for each of the two parts:

$$
NNP, NNP, NPN, NpN, pNN, pPP, pPp, ppP, PNN, PPP, PpP, Ppp.
$$

(82)

We shall refer to the 12 symbols in Table 1 as the **UPB symbols**.
Table 1: UPB symbols and associated permutations

| Symbol | Associated Permutation |
|--------|------------------------|
| NNPpPp (12)(34) | id |
| PNNpPP (01)(34) | PpPpN (23) |
| pNNpPP (01) | pPPpN (03)(24) |

We can now prove the main result of this section.

**Theorem 19** Let \( W \subseteq H \) be a 5-dimensional subspace containing exactly 6 product states (up to scalar factors) and assume that these states are in general position. Denote by \( \Psi \) the collection of the 720 quintuples \( (\psi) := (|\psi_k\rangle)^I_{k=0} \), selected from these 6 product states.

(a) Assume \( (\psi) \in \Psi \) is real and its symbol is UPB. If \( \sigma \) is the permutation from Table 1 associated to this symbol, then \( (|\psi_{\sigma k}\rangle)^I_{k=0} \) has symbol \( NPNpPp \).

(b) If some \( (\psi) \in \Psi \) is real and its symbol is UPB, then \( W \) has UPB type.

(c) Conversely, if \( W \) has UPB type, then all \( (\psi) \in \Psi \) are real and their symbols are UPB.

**Proof.** The assertion (a) can be proved by straightforward verification. We shall give details for one case which we shall need later. Assume that \( (\psi) \) has symbol \( pNNpPPp \). Since we work with non-normalized states, without any loss of generality we may assume that \( (\psi) \) is given by the pair of matrices

\[
A = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & -a \\ 0 & 0 & 1 & 1 & -b \\ \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 & 0 & 1 & c \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1/d \\ \end{bmatrix}.
\]

By computing the invariants of \( (\psi) \) we obtain that

\[
J_1^A = a/b, \quad J_2^A = -b, \quad J_3^A = -1/a, \quad J_1^B = cd, \quad J_2^B = 1/d, \quad J_3^B = 1/c,
\]

and so we must have \( b > a > 0 \) and \( c, d > 1 \). From Table 1 we find that \( \sigma = (01) \) in this case. Hence, the quintuple \( (\psi') := (|\psi_{\sigma k}\rangle)^I_{k=0} \) is given by the matrices \( A' \) and \( B' \) which are obtained from \( A \) and \( B \), respectively, by switching the first two columns. For the invariants of \( (\psi') \) we obtain the formulae

\[
J_1^{A'} = -1/b, \quad J_2^{A'} = b/a, \quad J_3^{A'} = -a, \quad J_1^{B'} = d, \quad J_2^{B'} = 1/cd, \quad J_3^{B'} = c.
\]

Thus, the symbol of \( (\psi') \) is indeed \( NPNpPp \).

Next we prove (b). By using (a) we may assume that \( (\psi) \) has symbol \( NPNpPp \). Since \( J_1^A J_2^A J_3^A = 1 \) and \( J_1^B J_2^B J_3^B = 1 \), the equations (79) can be solved for the four angles \( \gamma_A, \theta_A, \gamma_B, \theta_B \). Now the assertion follows from Propositions 3 and 5.

To prove (c) we observe that any pair of real matrices

\[
U = \begin{bmatrix} 1 & 0 & \alpha & \beta & 0 \\ 0 & 1 & 0 & 1 & \alpha \\ 0 & 0 & \beta & -\alpha & 1 \\ \end{bmatrix}, \quad V = \begin{bmatrix} 1 & \delta & 0 & 0 & \gamma \\ 0 & 1 & 1 & \gamma & 0 \\ 0 & -\gamma & 0 & 1 & \delta \\ \end{bmatrix}
\]

with nonzero parameters \( \alpha, \beta, \gamma, \delta \) defines a non-normalized UPB given by the tensor products of the corresponding columns of \( U \) and \( V \). Moreover, any UPB is BP-equivalent to one of this form. The invariants of the above UPB are

\[
\left[ -\alpha^2, \alpha^2 + \beta^2, \frac{1}{\alpha^2 + \beta^2}, 1 + \gamma^2, \frac{\delta^2}{1 + (\gamma^2 + \delta^2)}, \frac{\gamma^2 + \delta^2}{\delta^2} \right].
\]

Evidently, this quintuple has the symbol \( NPNpPp \). By using these invariants and the formulae Eqs. (8) and (9) from Proposition 7 we find the sixth product state in \( W \) and extend the matrices \( U \) and \( V \) to \( 3 \times 6 \) matrices

\[
\tilde{U} = \begin{bmatrix} 1 & 0 & \alpha & \beta & 0 & \alpha[(1 + \alpha^2)(1 + \gamma^2 + \delta^2) + \beta^2(\gamma^2 + \delta^2)]/[\beta(1 + \alpha^2 + \gamma^2)] \\ 0 & 1 & 0 & 1 & \alpha & \alpha(1 + \gamma^2 + \delta^2)[\delta^2 + (\alpha^2 + \beta^2)(\gamma^2 + \delta^2)]/[\alpha^2 \gamma^2 + (\gamma^2 + \delta^2)(\beta^2 + \gamma^2(\alpha^2 + \beta^2))] \\ 0 & 0 & \beta & -\alpha & 1 & 1 \\ \end{bmatrix}, \quad (88)
\]

\[
\tilde{V} = \begin{bmatrix} 1 & \delta & 0 & 0 & \gamma & \gamma[\alpha^2(1 + \alpha^2 + \beta^2)(1 + \gamma^2 + \delta^2) + \beta^2(1 + \gamma^2 + \delta^2)]/[\beta^2 \delta(1 + \alpha^2 + \gamma^2)] \\ 0 & 1 & 1 & \gamma & 0 & \gamma(\alpha^2 + \beta^2)(1 + \alpha^2)(1 + \gamma^2 + \delta^2) + \beta^2(\gamma^2 + \delta^2)]/[\beta^2(\delta^2 + (\alpha^2 + \beta^2)(\gamma^2 + \delta^2))] \\ 0 & -\gamma & 0 & 1 & \delta & 1 \\ \end{bmatrix}, \quad (89)
\]
by appending this new product state.

The symmetric group \( S_6 \) permutes the 6 product states and induces a permutation representation on the 720 quintuples made up from these 6 product states. For instance, if we choose the quintuple corresponding to column numbers 3, 6, 2, 1, 5 (in that order) then the invariants are

\[
J^A_1 = \frac{(1 + \alpha^2 + \gamma^2)(1 + \gamma^2 + \delta^2)}{(1 + \gamma^2)(1 + \alpha^2 + \delta^2) + \beta^2(\gamma^2 + \delta^2)},
\]

\[
J^A_2 = \frac{1 + \gamma^2}{1 + \gamma^2 + \delta^2},
\]

\[
J^A_3 = \frac{(1 + \alpha^2 + \gamma^2 + \delta^2)}{1 + \alpha^2 + \gamma^2},
\]

\[
J^B_1 = -\frac{\beta^2(\gamma^2 + \delta^2)(1 + \alpha^2 + \gamma^2)}{\alpha^2\gamma^2[(1 + \alpha^2)(1 + \gamma^2 + \delta^2) + \beta^2(\gamma^2 + \delta^2)]},
\]

\[
J^B_2 = -\frac{\beta^2}{\gamma^2(\gamma^2 + \delta^2)(1 + \alpha^2 + \beta^2)},
\]

\[
J^B_3 = \frac{\gamma^2[(1 + \alpha^2)(1 + \gamma^2 + \delta^2) + \beta^2(\gamma^2 + \delta^2)]}{(\gamma^2 + \delta^2)(1 + \alpha^2 + \beta^2)(1 + \alpha^2 + \gamma^2)}
\]

and the associated symbol is \( ppPNP \).

A brute force computation shows that there are only 12 different symbols that belong to these 720 quintuples, namely the UPB symbols listed in Table 1. This completes the proof.

It is easy to see that all 144 symbols arise from some real quintuples of product states. Hence, apart from PPTES, the NPT states may also have 5 dimensional kernels with exactly 6 product states in general position.

By means of Theorem 19 we can operationally decide the UPB-type of 5-dimensional subspaces. This is the key tool in our proof of Conjecture 15 in the next section.

V. DESCRIPTION OF 3 \times 3 PPT STATES OF RANK 4

We shall first analyze the 5-dimensional subspaces which arise as kernels of 3 \times 3 PPT states of rank 4. This will help us to resolve a conjecture proposed in [31].

A. Product states in the kernel of 3 \times 3 PPT states of rank 4

We need the following lemma which we proved recently in [1, Lemma 20].

**Lemma 20** Let \( \rho \) be a 3 \times N state such that for some \( |a\rangle \in \mathcal{H}_A \), rank\( \langle a|\rho|a\rangle = 1 \). If \( \rho \) is NPT then it is distillable. If \( \rho \) is PPT and \( N = 3 \), then \( \rho \) is separable.

Let us first handle the separable states of rank 4.

**Lemma 21** Let \( \rho = \sum_{i=0}^{3} |a_i, b_i\rangle\langle a_i, b_i| \) be a separable 3 \times 3 state of rank 4. If the four product states \( |a_i, b_i\rangle \) are not in general position, then \( \ker \rho \) contains a 2-dimensional subspace \( V \otimes W \) with \( V \subseteq \mathcal{H}_A \) and \( W \subseteq \mathcal{H}_B \) (which consists of product states). Otherwise (a) \( \ker \rho \) contains exactly 6 product states, and (b) these 6 product states are not in general position.

**Proof.** Assume that the \( |a_i, b_i\rangle \) are not in general position. We consider first the case where two of the \( |a_i\rangle \) or two of the \( |b_i\rangle \) are parallel, say \( |a_0\rangle \propto |a_1\rangle \). If \( |y\rangle \in \mathcal{H}_B \) is orthogonal to \( |b_2\rangle \) and \( |b_3\rangle \), then \( |a_0\rangle \otimes |y\rangle \subseteq \ker \rho \). In the remaining case we may assume that, say \( |a_0\rangle, |a_1\rangle \) and \( |a_2\rangle \) are linearly independent while \( |b_2\rangle \) belongs to the span of \( |b_0\rangle \) and \( |b_1\rangle \). If the state \( |y\rangle \in \mathcal{H}_B \) is orthogonal to \( |b_0\rangle \) and \( |b_1\rangle \), then \( |a_3\rangle \otimes |y\rangle \subseteq \ker \rho \) and so the first assertion is proved.

Next assume that the \( |a_i, b_i\rangle \) are in general position. By the Four Point Lemma, we may assume that these product states are in the canonical form, i.e., \( |a_i, b_i\rangle \propto |ii\rangle \), for \( i = 0, 1, 2 \) and \( |a_4, b_4\rangle = \sum_{i,j=0}^{2} |ij\rangle \). The six product states \( |i\rangle \otimes (|j\rangle - |k\rangle) \) and \( (|j\rangle - |k\rangle) \otimes |i\rangle \), with \( i, j, k \) a cyclic permutation of \( (0, 1, 2) \), belong to \( \ker \rho \). To prove (a) one just needs to verify that there are no additional product states in \( \ker \rho \). We omit the details of this verification. For (b), it suffices to observe that the sum of \( |0\rangle - |1\rangle, |1\rangle - |2\rangle \) and \( |2\rangle - |0\rangle \) is 0. This completes the proof. \( \square \)
From now on we focus on the PPTES of rank 4. We recall from [7] that any state $\rho$ of rank 4 acting on a $3 \otimes 3$ system can be written as

$$\rho = \sum_{i,j=0}^{2} |i\rangle \langle j| \otimes C_i^j,$$

where the blocks $C_i$ are $4 \times 3$ matrices.

**Theorem 22** The kernel of any $3 \times 3$ PPTES of rank 4 contains exactly six product states. Moreover, these six states are in general position.

**Proof.** Let $\rho$ be a PPTES of rank 4. Assume that $\ker \rho$ contains infinitely many product states. By Lemma [14], they are all in general position. Hence we can apply Proposition [7] to any quintuple of product states in $\ker \rho$. As $\ker \rho$ contains infinitely many product states, only the case (a) of that proposition applies. The third assertion of that case contradicts our hypothesis that $\rho$ is PPT. This contradiction shows that $\ker \rho$ contains only finitely many product states.

We may assume that $\rho$ is written as in Eq. (96). We have $\rho = C^iC$, where $C = [C_0 \ C_1 \ C_2]$. We shall simplify this expression by using the techniques similar to those in [7]. We can replace $C$ with $UC$ where $U$ is a unitary matrix, without changing $\rho$. The effect of a local transformation $\rho \rightarrow (I \otimes B)^T \rho (I \otimes B)$ is to replace each $C_i$ by $C_iB$. Similarly, a local transformation $\rho \rightarrow (A \otimes I)^T \rho (A \otimes I)$ acts on $\rho$ via block-wise linear operations, such as adding a linear combination of $C_0$ and $C_1$ to $C_2$, etc. We can apply these kind of transformations repeatedly as many times as needed. Note also that if the $j$th column of $C_i$ is 0 then $|ij\rangle \in \ker \rho$. By Lemma [20], each block $C_i$ has rank at least 2.

Since $\ker \rho$ has dimension 5, it must contain a product state. We choose an arbitrary product state in $\ker \rho$. By changing the o.n. bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, we may assume that the chosen product state in $\ker \rho$ is $|00\rangle$. Since $0 = \rho|00\rangle = \sum_i |i\rangle \otimes C_i^j|C_0|0\rangle$, we must have $C_i^j|C_0|0\rangle = 0$ for each $i$. In particular, $C_i^j|C_0|0\rangle = 0$ which implies that $C_0|0\rangle = 0$, i.e., the first column of $C_0$ must be 0. Hence, the block $C_0$ must have rank 2, and we may assume that

$$C_0 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad C_1 = [b_{ij}], \quad C_2 = [c_{ij}].$$

(97)

Let $\sigma = \rho^T$ and observe that its first entry is 0. Since $\sigma \geq 0$, the first row of $\sigma$ must be 0. We deduce that $b_{11} = b_{21} = c_{11} = c_{21} = 0$. Since $\ker \rho$ contains only finitely many product states, the first columns of $C_1$ and $C_2$ must be linearly independent. By using an ILO on system $A$, we may assume that $b_{31} = c_{41} = 1$ and $b_{41} = c_{31} = 0$. Thus we have

$$C_1 = \begin{bmatrix} 0 & b_{12} & b_{13} \\ 0 & b_{22} & b_{23} \\ 1 & b_{32} & b_{33} \\ 0 & b_{41} & b_{43} \end{bmatrix}, \quad C_2 = \begin{bmatrix} 0 & c_{12} & c_{13} \\ 0 & c_{22} & c_{23} \\ 0 & c_{32} & c_{33} \\ 1 & c_{42} & c_{43} \end{bmatrix},$$

(98)

while $C_0$ did not change.

Let $\mathcal{P}^4$ be the 4-dimensional complex projective space associated to $\ker \rho$. The Segre variety $\Sigma_{2,2}$ and this $\mathcal{P}^4$ intersect properly and we claim that the intersection multiplicity at the point $P = |00\rangle$ is 1. To prove this claim, we introduce the homogeneous coordinates $\xi_{ij}$ for the projective space $\mathcal{P}^8$ associated to $\mathcal{H}$: If $|\psi\rangle = \sum_{i,j=0}^{8} \alpha_{ij}|ij\rangle$ then the homogeneous coordinates of the corresponding point $|\psi\rangle \in \mathcal{P}^8$ are $\xi_{ij} = \alpha_{ij}$. The computation will be carried out in the affine chart defined by $\xi_{00} \neq 0$ which contains the point $P = |00\rangle$. We introduce the affine coordinates $x_{ij}$, $(i,j) \neq (0,0)$, in this affine chart by setting $x_{ij} = \xi_{ij}/\xi_{00}$. Thus $P$ is the origin, i.e., all of its affine coordinates $x_{ij} = 0$.

The computation of the intersection multiplicity is carried out in the local ring, say $R$, at the point $P$. This local ring consists of all rational functions $f/g$ such that $g$ does not vanish at the origin, i.e., $f$ and $g$ are polynomials (with complex coefficients) in the 8 affine coordinates $x_{ij}$ and $g$ has nonzero constant term. By expanding these rational functions in the Taylor series at the origin, one can view $R$ as a subring of the power series ring $\mathbb{C}[\{x_{ij}\}]$ in the 8 affine coordinates $x_{ij}$. We denote by $\mathfrak{m}$ the maximal ideal of $R$ generated by all $x_{ij}$.

The range of $\rho$ is the 4-dimensional subspace spanned by the pure states $|\psi_i\rangle$, $i = 1, \ldots, 4$, given by the four columns of $C^j$ (see the proof of Proposition 6 in [7]). In the matrix notation, these pure states are represented by the following
matrices
\[
\begin{bmatrix}
0 & 1 & 0 \\
0 & b_{12} & b_{13} \\
0 & c_{12} & c_{13}
\end{bmatrix},
\begin{bmatrix}
0 & 0 & 1 \\
0 & b_{22} & b_{23} \\
0 & c_{22} & c_{23}
\end{bmatrix},
\begin{bmatrix}
0 & 0 & 0 \\
1 & b_{12}^* & c_{13} \\
0 & c_{32} & c_{33}
\end{bmatrix},
\begin{bmatrix}
0 & 0 & 0 \\
1 & b_{12} & b_{13}^* \\
0 & c_{42} & c_{43}
\end{bmatrix}.
\]

(99)

Since \( \ker \rho = R(\rho)^\perp \), the subspace \( \mathcal{P}^4 \) is the zero set of the ideal \( I_1 \) generated by the four linear polynomials:
\[
x_{01} + b_{12}x_{11} + b_{13}x_{12} + c_{12}x_{21} + c_{13}x_{22},
\]
\[
x_{02} + b_{22}x_{11} + b_{23}x_{12} + c_{22}x_{21} + c_{23}x_{22},
\]
\[
x_{10} + b_{12}x_{11} + b_{13}x_{12} + c_{32}x_{21} + c_{33}x_{22},
\]
\[
x_{20} + b_{42}x_{11} + b_{43}x_{12} + c_{42}x_{21} + c_{43}x_{22}.
\]

(100)

(101)

(102)

(103)

The piece of the Segre variety contained in our affine chart consists of all matrices
\[
\begin{bmatrix}
1 & x_{01} & x_{02} \\
x_{10} & x_{11} & x_{12} \\
x_{20} & x_{21} & x_{22}
\end{bmatrix},
\]

(104)

of rank 1. It is the zero set of the ideal \( I_2 \) generated by the four polynomials:
\[
x_{11} - x_{01}x_{10},
x_{12} - x_{02}x_{10},
x_{21} - x_{01}x_{20},
x_{22} - x_{02}x_{20}.
\]

(105)

The quotient space \( m/m^2 \) is an 8-dimensional vector space with the images of the \( x_{ij} \) as its basis. It is now easy to see that the images of the generators of \( I_1 \) and \( I_2 \) also span the space \( m/m^2 \). Hence, by Nakayama’s Lemma (see [9, p. 225]) we have \( I_1 + I_2 = m \). Consequently, \( R/(I_1 + I_2) \cong \mathbb{C} \) and so our claim is proved.

Recall that we chose in the beginning an arbitrary product state in \( \ker \rho \) and by changing the coordinates we were able to assume that this product state is \( |00 \rangle \). Since the intersection multiplicity is invariant under these coordinate changes, this means that we have shown that the intersection multiplicity is 1 at each intersection point of \( \mathcal{P}^4 \) and \( \Sigma_{2,2} \). By Bezout Theorem the sum of the multiplicities at all intersection points is 6, and since all of the multiplicities are equal to 1 we conclude that the intersection consists of exactly 6 points.

By Lemma 12 these six product states are in general position. This concludes the proof.

\[ \square \]

**B. \( \Gamma \)-invariant PPTES of rank 4**

We shall prove that every SLOCC-equivalence class in \( \mathcal{E}_4 \) contains a state which is \( \Gamma \)-invariant.

**Theorem 23** Any \( 3 \times 3 \) PPTES \( \rho \) of rank 4 is SLOCC-equivalent to one which is invariant under partial transpose, i.e., for some \( (A,B) \in \text{GL} \) and \( \sigma = A \otimes B \rho A^\dagger \otimes B^\dagger \) we have \( A^\dagger = \sigma \).

**Proof.** By Theorem 22 we may assume that \( |ii \rangle \in \ker \rho \) for \( i = 0, 1, 2 \). Hence we may assume that, in the formula (100) for \( \rho \), the column \( i + 1 \) of the block \( C_i \) vanishes for \( i = 0, 1, 2 \). By multiplying \( C = \{ C_0 \ C_1 \ C_2 \} \) by a unitary matrix on the left hand side and by performing an ILO with diagonal matrices we may assume that
\[
C_0 = \begin{bmatrix}
0 & 1 & b \\
0 & 0 & 1 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}, \quad C_1 = \begin{bmatrix}
b_{11} & 0 & b_{13} \\
b_{21} & 0 & b_{23} \\
b_{31} & 0 & b_{33} \\
b_{41} & 0 & b_{43}
\end{bmatrix}, \quad C_2 = \begin{bmatrix}
c_{11} & c_{12} & 0 \\
0 & c_{22} & 0 \\
c_{31} & c_{32} & 0 \\
c_{41} & c_{42} & 0
\end{bmatrix}.
\]

(106)

Let \( \sigma = \rho^\Gamma \) and observe that its first, fifth and ninth diagonal entries are 0. Since \( \sigma \geq 0 \), the rows of \( \sigma \) containing these entries must be 0. We deduce that \( b_{11}, b_{21}, c_{11}, c_{21}, b_{13} \) are 0 and that the second column of \( C_2 \) is orthogonal to the first and third columns of \( C_1 \). Since \( \ker \rho \) contains only finitely many product states (up to scalar multiple), the first columns of \( C_1 \) and \( C_2 \) must be linearly independent. Hence, by applying a unitary transformation to the last two rows of the \( C_1 \) and rescaling \( C_1 \) and \( C_2 \), we may assume that \( b_{31} = 0, b_{41} = 1 \) and \( c_{31} = 1 \). By the orthogonality property mentioned above, we conclude that \( c_{42} = 0 \). Thus we have
\[
C_0 = \begin{bmatrix}
0 & 1 & b \\
0 & 0 & 1 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}, \quad C_1 = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & b_{33} \\
1 & 0 & b_{43}
\end{bmatrix}, \quad C_2 = \begin{bmatrix}
0 & c_{12} & 0 \\
0 & c_{22} & 0 \\
1 & c_{32} & 0 \\
c_{41} & 0 & 0
\end{bmatrix}.
\]

(107)
Since $\rho$ is entangled and PPT, its range contains no product states. Consequently, the entries $c_{12}, c_{22}, b_{33}, b_{43}$ and $b$ must be nonzero. We choose a phase factor $z_1$ such that $c_{41}z_1 > 0$. By multiplying the first columns of all $C_i$ by $z_1$ and multiplying $C_1$ by $z_1^*$, we may assume that $d := c_{41} > 0$. By multiplying the last two columns of all $C_i$ with $1/b_{33}$ and multiplying $C_0$ by $b_{33}$, we may assume that $b_{33} = 1$. We choose the phase factor $z_2$ such that $b_{22} > 0$. By multiplying the second columns of all $C_i$ by $z_2^*$ and multiplying $C_0$ by $b_2$, we may assume that $b > 0$. Since the last row of $\sigma$ must vanish, we obtain that $b_{43} = -1/d$, $c_{12} = -c_{22}/b$ and $c_{32} = -b_{23}c_{22}$. If $b_{23} = 0$ then also $c_{32} = 0$ and $|\psi_4⟩ - d|ψ_3⟩$ is a product state (see Eq. (104)). Hence, $c := b_{23} \neq 0$. Next choose a phase factor $z_2$ such that $c_{22} > 0$. By multiplying the last two columns of all $C_i$ by $z_2$ and multiplying $C_1$ by $z_2^*$, we may assume that $c > 0$. Finally, by multiplying the second columns of all $C_i$ by $a := 1/c_{22}$ we have

$$C_0 = \begin{bmatrix} 0 & a & b \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad C_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & c \\ 0 & 0 & 1 \\ 1 & 0 & -1/d \end{bmatrix}, \quad C_2 = \begin{bmatrix} 0 & -1/b & 0 \\ 0 & 1 & 0 \\ 1 & -c & 0 \\ d & 0 & 0 \end{bmatrix}. \tag{108}$$

We claim that $a$ has to be real. For that purpose we compute the principal minor of $\sigma$ obtained by deleting the first, fifth and ninth rows and columns. We obtain the expression $c^2(a - a^*)^2$. Since this minor must be nonnegative, our claim is proved.

It is now easy to verify that $\rho' = \rho$, which completes the proof. \qed

Theorem 24 If $\rho, \rho' \in \mathcal{E}_4$ have the same range, then $\rho = \rho'$.

Proof. Clearly, in order to prove the theorem we can simultaneously transform $\rho$ and $\rho'$ by the same ILO. Thus we can assume that $\rho$ is given by Eq. (96) and that the blocks $C_i$ are as in Eq. (108). For convenience, we shall not normalize neither $\rho$ nor $\rho'$, and so we have to prove that $\rho'$ is a scalar multiple of $\rho$. The range of $\rho$ is spanned by the four pure states $|ψ_i⟩$ represented by the four matrices

$$\begin{bmatrix} 0 & a & b \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & -1/b & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1/d \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ d & 0 & 0 \end{bmatrix}. \tag{109}$$

respectively. The first of these matrices is made up in the obvious manner from the first rows of the blocks $C_i$, and the other three matrices are constructed similarly. All this information is encapsulated in the matrix $C = [C_0 \ C_1 \ C_2]$.

We also have $\rho' = \sum_{i=0}^3 |ψ'_i⟩⟨ψ_i'|$ where $|ψ'_i⟩$ are four linearly independent linear combinations of the pure states $|ψ_i⟩$. Hence, the matrix $C'$ corresponding to $\rho'$ is given by $C' = SC$, where $S$ is an invertible matrix of order 4. Thus we have $\rho' = C'^tH C'$ where $H = S^t S$ is a positive definite matrix of order 4. If $α' = (\rho')^t$, an easy computation shows that the first, fifth and ninth diagonal entries of $α'$ are 0. Consequently all entries of $α'$ in the first and fifth row must be equal to 0. These equations give immediately that $H$ is a scalar matrix, which completes the proof. \qed

C. Main result

We can now prove our main result, i.e. Conjecture 15.

Theorem 25 Up to normalization, any state $\rho \in \mathcal{E}_4$ has the form $A \otimes B \Pi\{ψ\} A^t \otimes B^t$ for some $(A, B) \in \text{GL}$ and some $\{ψ\} \in \mathcal{U}$.

Proof. The proof is based on Theorem 19. The first step is to construct the 6 product states in $\ker ρ$. Like in Theorem 23 we assume that $\rho$ is given by Eq. (96) and that the blocks $C_i$ are as in Eq. (108). A direct computation shows that the 5-dimensional space $\ker ρ$ is spanned by $|00⟩, |11⟩, |22⟩$, and any two of the pure product states

$$|ψ_i⟩ = \begin{bmatrix} (1 + b^2 + b^2 c^2) z_i - b^2 c \langle ab z_i \rangle \\ (c z_i - 1 - d^2) / d \\ z_i (c z_i - 1 - d^2) / d \\ z_i \end{bmatrix}, \tag{110}$$

for $i = 1, 2, 3, 4$. The second step is to construct the remaining product states. We know from the previous theorem that the 6 product states $|ψ_i⟩$ are not linearly independent. We can therefore find a linear relation between these states, and in particular it follows that

$$|ψ_{i+1}⟩ = |ψ_i⟩ + b|ψ_{i+1}⟩ + c|ψ_{i+2}⟩,$$
The l.h.s. is a cubic polynomial, say $f_0$. We also have

$$z_i (i = 1, 2, 3),$$

where $i = (1, 2, 3)$, are the three roots of

$$abz(cz - 1 - d^2)(c - (1 + c^2)z) + d(cz - 1)(b^2c - (1 + b^2 + b^2c^2)z) = 0. \tag{111}$$

The l.h.s. is a cubic polynomial, say $f(z)$, in the unknown $z$. We have

$$f(0) = -b^2cd < 0, \tag{112}$$
$$f\left(\frac{c}{1 + c^2}\right) = \frac{cd}{(1 + c^2)^2} > 0, \tag{113}$$
$$f\left(\frac{1 + d^2}{c}\right) = \frac{d^3}{c}(b^2c^2 - (1 + b^2 + b^2c^2)(1 + d^2)) < 0. \tag{114}$$

Since $0 < c/(1 + c^2) < (1 + d^2)/c$, we deduce that Eq. $\tag{111}$ has three distinct nonzero real roots. One of them is $z_1 \in (0, c/(1 + c^2)$), the second $z_2 \in (c/(1 + c^2), (1 + d^2)/c)$, and the third is $z_3 < 0$ if $a > 0$ and $z_3 > (1 + d^2)/c$ if $a < 0$. We also have

$$f(1/c) = abd^2/c^3 \neq 0, \tag{115}$$
$$f(\lambda) = -ab^3c^2 \cdot \frac{(1 + b^2)(1 + d^2) + b^2c^2d^2}{(1 + b^2 + b^2c^2)^3} \neq 0, \tag{116}$$

where $\lambda = b^2c/(1 + b^2 + b^2c^2)$. Hence, for $a > 0$ we have

$$z_3 < 0, \quad \lambda < z_1 < c/(1 + c^2), \quad 1/c < z_2 < (1 + d^2)/c, \tag{117}$$

and for $a < 0$

$$0 < z_1 < \lambda, \quad c/(1 + c^2) < z_2 < 1/c < (1 + d^2)/c < z_3. \tag{118}$$

The second step is to compute the invariants for one of the quintuples selected from the above 6 product states. For that purpose we shall use the quintuple $(100, |11>, |22>, |\psi_1>, |\psi_2>)$. A computation gives the formulae:

$$J_1^A = \frac{1 + d^2 - cz_2}{1 + d^2 - cz_1}, \quad J_2^A = \frac{z_2(z_1 - \lambda)}{z_1(z_2 - \lambda)}, \quad J_3^A = \frac{z_1(1 + d^2 - cz_1)(z_2 - \lambda)}{z_2(1 + d^2 - cz_2)(z_1 - \lambda)}, \tag{119}$$

$$J_1^B = \frac{z_2(1 + d^2 - cz_2)(z_2 - 1)}{z_1(1 + d^2 - cz_1)(z_2 - 1)}, \quad J_2^B = \frac{(1 + d^2 - cz_1)(z_2 - 1)}{(1 + d^2 - cz_2)(z_1 - 1)}, \quad J_3^B = \frac{z_1}{z_2}. \tag{120}$$

As the third step, we have to compute the symbol associated to this quintuple. There are two cases to consider according to whether $a > 0$ or $a < 0$. We claim that the symbol is $ppPNp$ in the former case and $pNNPp$ in the latter case. This verification is of routine nature and Figure 1 may be useful for that purpose. We shall just verify the claim in the case $a > 0$. In that case, it is obvious that $0 < J_1^A < 1$, $J_1^B < 0$, $J_2^B < 0$, and $0 < J_2^B < 1$. Since $\lambda < z_1 < z_2$ and the function $t/(t - \lambda)$ is decreasing for $t > \lambda$, we indeed have $0 < J_2^A < 1$. Since $J_1^A J_2^A J_3^A = 1$, we deduce that $J_3^A > 1$. Thus we have shown that the symbol is $ppPNp$ if $a > 0$. 

![FIG. 1: A generic picture for the function $f(z)$ for positive and negative $a$, common $b, c, d > 0$ and $\lambda = b^2c/(1 + b^2 + b^2c^2)$. The left curve represents $f(z)$ for $a > 0$ and the right curve for $a < 0$. The two curves meet at three points with abscissae $z = 0, c/(1 + c^2), (1 + d^2)/c$. The three roots of $f(z)$ are $z_1^-, z_2^-, z_3^-$ for $a < 0$, and $z_1^+, z_2^+, z_3^+$ for $a > 0$.](image)
Finally, since \( pPNNp \) and \( pNNPpp \) are UPB symbols, we conclude that \( \ker \rho \) is a 5-dimensional subspace of UPB type. Hence, we can now apply Theorem 22 to complete the proof.

It follows from the above proof that every \( 3 \times 3 \) PPTES of rank 4 is SLOCC-equivalent to one given by Eqs. (18) and (19) with positive \( a, b, c, d \).

The next corollary shows that there is no way to single out one of the six product states in the kernel of a PPTES of rank 4 in the sense that any quintuple of these states is BP-equivalent to a quintuple formed from the five states of a UPB.

**Corollary 26** Let \( \rho \in \mathcal{E}_4 \) and let \(|\psi_k\rangle, k = 0, \ldots, 4\), be any five of the six product states in \( \ker \rho \). Then there exists \((A, B) \in \text{GL}\) such that the product states \( A \otimes B |\psi_k\rangle, k = 0, \ldots, 4\), form a non-normalized UPB.

**Proof.** By Theorem 25, \( \ker \rho \) is a 5-dimensional subspace of UPB type. By Theorem 19, the symbol of the quintuple \(|\psi\rangle = (|\psi_k\rangle)_{k=0}^4\) is a UPB symbol and there exists a permutation \((k_0, \ldots, k_4)\) of the indexes \((0, \ldots, 4)\) such that the symbol of the quintuple \(|\psi'\rangle := (|\psi_{k_i}\rangle)_{i=0}^4\) is \( NPNPpP \). We can now conclude the proof by using the argument from the last paragraph of the proof of Theorem 19.

We now analyze the stabilizer of \( \rho \in \mathcal{E}_4 \) in the product \( \text{PGL} = \text{PGL}_3 \times \text{PGL}_3 \) of two projective general linear groups. Thus we have to consider \((A, B) \in \text{GL}\) such that \( A \otimes B \rho A^\dagger \otimes B^\dagger = cp \) for some scalar \( c > 0 \).

**Proposition 27** The stabilizer \( G_\rho \) of any \( \rho \in \mathcal{E}_4 \) in \( \text{PGL} \) is a finite group isomorphic to a subgroup of the symmetric group \( S_6 \). In the generic case the stabilizer is trivial.

**Proof.** Let us denote by \( P_i, i = 1, \ldots, 6 \), the six points in the projective space \( \mathbb{P}^4 \) associated with \( \ker \rho \). Assume that \((A, B) \in \text{GL}\) maps \( \rho \) to \( cp \) for some \( c > 0 \). Then \( A \otimes B \) must leave invariant \( \mathcal{R}(\rho) \) and \((A^{-1} \otimes B^{-1})^6 \) must leave invariant \( \ker \rho \) and permut the 6 product states, i.e., the points \( P_i \). The map which assigns to \((A, B)\) this permutation, say \( \pi_{A,B} \in S_6 \), is a group homomorphism. If \( \pi_{A,B} \) is the identity permutation, then the Four Point Lemma implies that \((A^{-1} \otimes B^{-1})^6 \) is a scalar operator. We conclude that the mapping sending \((A, B) \in \Gamma_\rho\) to the permutation \( \pi_{A,B} \in S_6 \) is one-to-one. This proves the first assertion.

The proof of the second assertion is based on matrices \( U \) and \( V \) from the proof of Theorem 19 and the invariants \((J_i^A, J_i^B), i = 1, 2, 3\), defined in Section 11. Let us write the product states \(|\psi_i\rangle \in \ker \rho, (i = 1, \ldots, 6)\) as \(|\psi_i\rangle = |\phi_i\rangle \otimes |\chi_i\rangle \). The first five \(|\phi_i\rangle \) and \(|\chi_i\rangle \) are determined directly by \( U \) and \( V \), respectively. One has to compute the sixth product state in \( \ker \rho \). We have done this in the proof of the theorem mentioned above. Finally, we have verified that the 720 (ordered) quintuples that one can construct from the 6 points \( P_i \) have generically different values for the invariants \((J_i^A, J_i^B)\). This completes the proof.

For special states \( \rho \in \mathcal{E}_4 \), the stabilizer may be nontrivial. For instance, the stabilizer for the **Pyramid** example is the alternating group \( A_5 \) of order 60 which permutes transitively the six product states in the kernel. The original definition of this example \( \| \) exhibits only the dihedral group of order 10 as symmetries of a regular pentagonal pyramid. A more symmetric realization is given in the recent paper \( \| \) where the full group of symmetries, \( A_5 \), can be realized by local unitary operations.

For the **Tiles** example the stabilizer is a group of order 12 isomorphic to the alternating group \( A_4 \). It also permutes transitively all six product states in the kernel of \( \rho \). Since this stabilizer is finite, it may be conjugated into the maximal compact subgroup of \( \text{PGL} \) which is just the image of the local unitary group. In this way we can obtain a more symmetric realization of **Tiles**. To be concrete, let us consider the following two \( 3 \times 6 \) matrices

\[
\dot{U} = \begin{bmatrix}
a & 0 & 1 & a & 0 & -1 \\
1 & a & 0 & -1 & a & 0 \\
0 & 1 & a & 0 & -1 & a \\
\end{bmatrix}, \quad \dot{V} = \begin{bmatrix}
-1 & 0 & a & 1 & 0 & a \\
0 & a & -1 & 0 & a & 1 \\
a & -1 & 0 & a & 1 & 0 \\
\end{bmatrix},
\]

where \( a = \sqrt[3]{3} \). Define the pure product state \(|\psi'_k,\chi\rangle, (k = 1, \ldots, 6)\), as the tensor product of the \( k \)th columns of \( \dot{U} \) and \( \dot{V} \). These states are linearly dependent since the first three and the last three have the same sum. A computation shows that the **Tiles** quintuple \(|\psi_k\rangle, k = 0, \ldots, 4\), and the quintuple \(|\psi'_0,\psi'_1,\psi'_2,\psi'_3,\psi'_4\rangle \) have the same invariants. Hence, they are BP-equivalent. The advantage of this new realization of **Tiles** is that its symmetry group (i.e., the stabilizer) is now evident. The symmetry operations are given by local unitary operations. For instance, the multiplication of \( \dot{U} \) and \( \dot{V} \) by \( \text{diag}(-1, 1, 1) \) acts on the 6 product states as the permutation \((03)(25)\). The multiplication of \( \dot{U} \) by the cyclic matrix \( Z \) with first row \([0 \ 0 \ 1]\) and the simultaneous multiplication of \( \dot{V} \) by \( Z^T \) act as the permutation \((012)(345)\). One can easily construct the unique PPTES \( \rho \) of rank 4 whose kernel is the
subspace spanned by the $|\psi_p^i\rangle$. Up to normalization, $\rho$ is given by Eq. (20) with

$$C_0 = \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad C_1 = \begin{bmatrix} 0 & 0 & a \\ a^2 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad C_2 = \begin{bmatrix} 0 & a & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a^2 \end{bmatrix}.$$  \hspace{1cm} (122)

It is now easy to verify that the above two local unitary transformations commute with $\rho$.

VI. PHYSICAL APPLICATIONS

In this section we demonstrate a few applications of our results in previous sections.

First, apart from existing numerical tests such as the semidefinite programming [11], Theorem 25 analytically provides the first bipartite system with specified dimensions and rank, in which all PPTES $\rho$ can be systematically built and characterized. The procedure is as follows. Given a 4-dimensional subspace, one can readily obtain its 5-dimensional orthogonal complement. Numerically it is possible to find the product states of this subspace. By Theorems 19 and 25, it suffices to consider the case in which this subspace contains exactly 6 product states $|\phi_i, \chi_j\rangle$, which are required to be in general position. Next by using Eq. (2) and condition (b) of Theorem 19 we can compute the invariants $(J_1^A, J_2^A, J_3^A, J_1^B, J_2^B, J_3^B)$ for any quintuple selected from these 6 product states. It is necessary that all these invariants be real and that their symbols be of UPB type. Then we compare them with Eq. (79) and derive the parameters $\gamma_{A,B}, \theta_{A,B} \in (0, \pi/2)$ of a UPB quintuple $|a_i, b_i\rangle$, see Lemma 16. Next, we find the ILOs $A, B$ such that $A \otimes B |a_i, b_i\rangle \propto |\phi_i, \chi_j\rangle$. Finally, we build the PPTES $A \otimes B (I - \sum_{i=1}^4 |a_i, b_i \rangle \langle a_i, b_i|) A^\dagger \otimes B^\dagger$, which is unique by Theorem 24. This is also succinctly stated in Theorem 25.

On the other hand it is known that the PPT condition is necessary and sufficient for detecting any $2 \times 2$ and $2 \times 3$ separable states. Likewise, Theorems 19 and 25 essentially outperform all existing criteria, such as the range criterion [27] and the covariance matrix criterion [17], which can only detect some special $3 \times 3$ PPTES of rank 4. It also follows easily from Theorem 24 that

**Corollary 28** In a two-qutrit system, the partial transpose of a PPTES of rank 4 has also rank 4.

Second, we claim that in a two-qutrit system all PPTES of rank 4 are extreme points of the set $S_{\text{PPT}}$ of PPT states. (Here our states are assumed to be normalized.) According to the definition in Sec. I, a PPTES $\rho$ is not extreme if and only if it is the midpoint of the segment joining two different PPT states. Let us prove our claim. Suppose that $2\rho = \rho_1 + \rho_2$ where $\rho_1$ and $\rho_2$ are two distinct PPT states. Since there is no product state in the range of $\rho$, the same is true for $\rho_1$ and $\rho_2$. Thus they are PPTES, and rank $\rho_1 = \rho_2 = 4$ since there is no PPTES of rank 2 or 3 [24]. Hence, these three states must have the same range, and so $\rho_1 = \rho_2 = \rho$ by Theorem 24. Thus we have a contradiction. Hence $\rho$ is always both extreme and edge PPTES [19]. The latter statement readily follows from the definition of the edge PPTES $\rho$, which contains no product state $|a, b\rangle \in R(\rho)$ such that $|a^*, b\rangle \in R(\rho^\dagger)$ [32].

Third, we can systematically build more PPTES and detect them in experiment. By following the technique in [16, 32], the entanglement witness of the PPTES $\sigma$ of rank 4 has the form

$$W_\sigma = P - cI,$$

$$\epsilon = \inf_{\langle e, f \rangle} \langle e, f | P | e, f \rangle,$$  \hspace{1cm} (123)

where $P$ is the projector onto the kernel of $\sigma$. The numerical estimation of some states $\sigma$ is also available, as well as their experimental realization in [16]. In this sense, we can detect any two-qutrit PPTES of rank 4 effectively.

On the other hand it has been proved that any PPTES has the form $\rho = p\rho_x + (1-p)\sigma$ where $\rho_x$ is a separable state and $\sigma$ is an edge PPTES [32]. In the second item, we have shown that any PPTES of rank 4 is an extreme and edge PPTES [19]. So the PPTES $\rho$ can be characterized when $\sigma$ has rank 4 and the perturbation $p$ is small, by using the entanglement witness $W_\sigma$ in Eq. (123). Building the entanglement witness for arbitrary $\rho$ requires the characterization of separable $\rho_x$, which is still an open problem. Nevertheless, if a PPTES is the convex sum of a few PPT states of rank at most 4, it is possibly characterized through the results in this paper.

Fourth, we claim that no PPTES $\rho \in E_4^4$ is symmetric, that is, $R(\rho)$ is not contained in the space spanned by the $|ii\rangle$ and the $|ij\rangle + |ji\rangle$ with $i > j$. To prove this, we use the expression in Eq. (108). Assume there is an ILO $B = [b_{ij}]$ such that $I \otimes B \rho I \otimes B^\dagger$ is symmetric. One can readily show that $b_{11} = b_{21} = b_{20} = b_{22} = 0$, which contradicts the assumption $\det B \neq 0$. Hence the simplest symmetric PPTES must have rank at least 5. Such states indeed exist, e.g., the state $\rho_{BE4}$ in [38].
Finally, up to ILO, the range of any $3 \times 3$ PPTES of rank 4 is orthogonal to a 5-dimensional subspace spanned by a UPB. Hence the product vectors of a UPB cannot be distinguished by LOCC [2]. In other words, the LOCC-indistinguishable nonlocality of the complementary subspace is a deterministic feature of any PPTES of rank 4.

VII. CONCLUSIONS

In this paper we have shown that any two-qutrit PPT entangled state of rank 4 is the normalization of

$$(A \otimes B)(I - \sum_{i=0}^{4} |a_i, b_i\rangle \langle a_i, b_i|)(A \otimes B)^\dagger, \tag{124}$$

where $A, B$ are invertible operators and the five product states $\{|a_i, b_i\rangle\}$ form an (orthogonal) UPB. Moreover, this is the only PPT entangled state among the states having the same range. The 5-dimensional subspace spanned by a UPB contains exactly 6 product states (up to scalar multiple). We have shown that any 5 of them can be converted to a UPB quintuple by a biprojective transformation. The result has been demonstrated on two well-known examples of UPB, the Pyramid and Tiles UPB [3]. Therefore we have systematically characterized all PPTES in this system.

Furthermore we have characterized the separable two-qutrit states of rank 4 whose kernel contains either infinitely many product states or exactly 6 product states but not in general position. The next goal in the future is to extend our results to higher dimensional PPT states, entangled or separable.

On the other hand, we have proposed a method of determining the BP-equivalence between two quintuples of product states of two qutrits in general position. Apart from the derivation of the main result, the method has also been applied to classify the 5-dimensional subspaces via their intersection with the set of product states. In particular all 11 partitions of the integer 6 occur as the intersection patterns of $P^4 \cap \Sigma_{2,2}$. These results are useful to characterize the distillability of NPT states of rank 4, which is another interesting open problem proposed in [7].

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