Equivalence classes and canonical forms for two-qutrit entangled states of rank four having positive partial transpose

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Let $\mathcal{E}'$ denote the set of non-normalized two-qutrit entangled states of rank four having positive partial transpose (PPT). We show that the set of SLOCC classes of states in $\mathcal{E}'$, equipped with the quotient topology, is homeomorphic to the quotient $R/A_5$ of the open rectangular box $R \subset \mathbb{R}^4$ by an action of the alternating group $A_5$. We construct an explicit map $\omega: \Omega \to \mathcal{E}'$, where $\Omega$ is the open positive orthant in $\mathbb{R}^4$, whose image $\omega(\Omega)$ meets every SLOCC equivalence class $E \subseteq \mathcal{E}'$. Although the intersection $\omega(\Omega) \cap E$ is not necessarily a singleton set, it is always a finite set of cardinality at most 60. By abuse of language, we say that any state in $\omega(\Omega) \cap E$ is a canonical form of any $\rho \in E$. In particular, we show that all checkerboard PPT entangled states can be parametrized up to SLOCC equivalence by only two real parameters. We also summarize the known results on two-qutrit extreme PPT states and edge states, and examine which other interesting properties they may have. Thus we find the first examples of SLOCC PPT states whose rank is different from the rank of its partial transpose.

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I. INTRODUCTION

Entanglement plays the essential role in quantum information processing, such as quantum teleportation \cite{1}, computing \cite{32} and cryptography \cite{17}. Entanglement also reveals a fundamental difference between the quantum and classical world which may be detected by Bell inequality and other means \cite{18}. In spite of these striking facts, it is a hard problem to decide whether a given quantum state is entangled \cite{18}.

A non-entangled state, also known as a separable state, is by definition a convex sum of product states \cite{37}. For a bipartite 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 $\rho^T = \sum_{ij} |a_j\rangle \langle a_i| \otimes \langle a_i|\rho|a_j\rangle$. The dimensions of $\mathcal{H}_A$ and $\mathcal{H}_B$ are denoted by $M$ and $N$, respectively. (We assume that $M, N \geq 2$.) We say that $\rho$ is a $k \times l$ state if its local ranks are $k$ and $l$, i.e., rank $\rho_A = k$ and rank $\rho_B = l$. We say that $\rho$ is a PPT [NPT] state if $\rho^T \geq 0$ [$\rho^T$ has at least one negative eigenvalue]. Evidently, a separable state must be PPT. The converse is true only if $MN \leq 6$ \cite{24, 33}. The first examples of two-qutrit PPT entangled states (PPTES) were constructed (in purely mathematical context) by Choi and Størmer in the 1980s \cite{12, 36}. They were introduced in 1997 \cite{25} into quantum information theory. The Choi’s example has been generalized in \cite{14}. The PPTES can be used for many tasks, e.g. the extraction of distillable key \cite{23}.

A systematic method of constructing two-qutrit PPTES $\rho$ of rank four was proposed in 1999 \cite{3} by using the unextendible product bases (UPB). This construction is indeed universal: it was proved in 2011 \cite{4, 35} that any such $\rho$ can be constructed by using a UPB. Any such $\rho$ can be converted by stochastic local operations and classical communications (SLOCC) into a canonical form depending on for positive parameters, see Eq. \cite{7} and the subsequent paragraph. This canonical form is a minor modification of the one constructed in \cite{3, Eq. (108)]. We demonstrate our result by using the well-known Pyramid and Tiles UPB \cite{14}. The set of SLOCC equivalence classes of two-qutrit PPTES carries the natural quotient topology. We show that this topological space is homeomorphic to the quotient of the open rectangular box $R \subset \mathbb{R}^4$ by an action of the alternating group $A_5$. The checkerboard family of PPTES is an early well-known example of an infinite family of two-qutrit PPTES of rank four \cite{6}. We show that, under SLOCC, the checkerboard PPTES can be parametrized by only two real parameters. These results clarify the structure of $3 \times 3$ PPTES of rank four.

We say that a PPT state $\rho$ is extreme if it is an extreme point of the compact convex set of all normalized PPT states. Every PPT state is a convex linear combination of extreme states. For convenience we say that a non-normalized state is extreme if its normalization is extreme.

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We say that a PPT state $\rho$ is an edge state if there is no product vector $|a, b\rangle \in \mathcal{R}(\rho)$ such that $|a^\dagger, b\rangle \in \mathcal{R}(\rho^T)$. Thus an edge state must be a PPTES. It is easy to see that any entangled extreme state is an edge state, but the converse is false. It has been proved that any $3 \times 3$ PPTES of rank four is an extreme state \cite{9}. They are PPTES of lowest rank. Both extreme and edge states in higher dimensions have been extensively studied in recent years \cite{8,11,33,35}. Among them, $3 \times 3$ extreme and edge states have the simplest structure. We will give a summary of these extreme cases, and point out some unknown cases. We explicitly construct states for these cases, and summarize the recent progress on $3 \times 3$ PPTES of rank four, which is invariant under the natural action of the group $G$ of local invertible transformations. In Theorem 7 we prove that any $\rho \in \mathcal{E}'$ can be converted under SLOCC into the canonical form. We also prove, see Theorem 9, that the quotient spaces $\mathcal{E}'/G$ and $R/A\mathbf{5}$ mentioned in the abstract are homeomorphic. In Sec. IV we construct a family of checkerboard PPTES depending on two positive parameters $u$ and $v$, see Proposition 14. We show that any checkerboard PPTES is SLOCC equivalent to a member of this family. By using invariants, we find a simple characterization of checkerboard PPTES (see Proposition 15). In Sec. V we summarize the recent progress on $3 \times 3$ extreme and edge states. We examine some of the known states of this type to find out what other properties they may have. E.g. we observe that there exist extreme states of birank $(r, s)$ with $r \neq s$. Apparently, this observation is new. The results are presented in Table I at the end of this section. We also propose several open problems.

II. PRELIMINARIES

We shall write $I_k$ for the identity $k \times k$ matrix. We denote by $\mathcal{R}(\rho)$ and $\ker \rho$ the range and kernel of a linear map $\rho$, respectively. From now on, unless stated otherwise, the states will not be normalized. We shall denote by $\{|i\rangle_A : i = 0, \ldots, M - 1\}$ and $\{|j\rangle_B : j = 0, \ldots, N - 1\}$ o.n. bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. The subscripts A and B will be often omitted. Any state $\rho$ of rank $r$ can be represented as

$$\rho = \sum_{i,j=0}^{M-1} |i\rangle_j \langle j| C_i^\dagger C_j,$$

where the $C_i$ are $R \times N$ matrices and $R$ is an arbitrary integer $\geq r$. In particular, one can take $R = r$. We shall often consider $\rho$ as a block matrix $\rho = C^\dagger C = [C_i^\dagger C_j]$, where $C = [C_0 \ C_1 \ \cdots \ C_{M-1}]$ is an $R \times MN$ matrix. Thus $C_i^\dagger C_j$ is the matrix of the linear operator $\langle i|_A \rho |j\rangle_A$ acting on $\mathcal{H}_B$.

In physics, the density matrix $\rho$ describes the systems $AB$. In many cases we only need to describe one system by the reduced density matrices $\rho_A = \text{Tr}_B \rho$ and $\rho_B = \text{Tr}_A \rho$. For these matrices, using Eq. (1) we have the formulae

$$\rho_B = \sum_{i=0}^{M-1} C_i^\dagger C_i; \quad \rho_A = [\text{Tr} C_i^\dagger C_j], \quad i, j = 0, \ldots, M - 1.$$

It is easy to verify that the range of $\rho$ is the column space of the matrix $C^\dagger$ and that

$$\ker \rho = \left\{ \sum_{i=0}^{M-1} |i\rangle \otimes |y_i\rangle : \sum_{i=0}^{M-1} C_i |y_i\rangle = 0 \right\}.$$  

(3)

In particular, if $C_i |j\rangle = 0$ for some $i$ and $j$ then $|i, j\rangle \in \ker \rho$.

For any bipartite state $\rho$ we have

$$\rho^\Gamma_B = \text{Tr}_A (\rho^T) = \text{Tr}_A \rho = \rho_B;$$

$$\rho^\Gamma_A = \text{Tr}_B (\rho^\Gamma) = (\text{Tr}_B \rho)^T = (\rho_A)^T.$$

(4)

(5)

(The exponent T denotes transposition.) Consequently,

$$\text{rank} (\rho^\Gamma)_{A,B} = \text{rank} \rho_{A,B}.$$  

(6)

If $\rho$ is an $M \times N$ PPT state, then $\rho^\Gamma$ is too. If $\rho$ is a PPTES so is $\rho^\Gamma$, but they may have different ranks.

Let us now recall some basic results from quantum information regarding the separability and PPT properties of bipartite states. Let us start with the basic definition.

\[\rho = \sum_{i,j} c_{ij} |i\rangle \langle j|\]

where $c_{ij} \geq 0$ and $\sum_{i,j} c_{ij} = 1$. A density matrix is PPT if it can be written in the form above with non-negative coefficients $c_{ij}$. A state $\rho$ is separable if it can be written as $\rho = \sum_{i,j} c_{ij} |i\rangle \langle j| \otimes |i\rangle \langle j|$. A state $\rho$ is entangled if it is not separable. A state $\rho$ is PPTES if it is not separable and is a pure state for any bipartition. A pure state $\rho = |\psi\rangle \langle \psi|$ is entangled if its reduced density matrix $\rho_A = \text{Tr}_B (|\psi\rangle \langle \psi|)$ is not separable.
Definition 1 We say that two bipartite states $\rho$ and $\sigma$ are equivalent under stochastic local operations and classical communications (SLOCC-equivalent, or just equivalent) if there exists an invertible local operator (ILO) $V = V_A \otimes V_B$ such that $V \rho V^\dagger = \sigma$.

This is the physical realization of ILO. Thus the equivalence classes of states are just the orbits under the action of the group $G := \text{GL}_3(\mathbb{C}) \times \text{GL}_3(\mathbb{C})$. It is easy to see that any ILO transforms PPT, entangled, or separable state into the same kind of state. We shall often use ILOs to simplify the density matrices of states.

Let us recall from [8, Theorem 22] and [9, Theorems 17,22] the main facts about the $3 \times 3$ PPTES states of rank four. Let $M = N = 3$ and let $\mathcal{U}$ denote the set of unextendible product bases in $\mathcal{H}$. For $\{\psi\} \in \mathcal{U}$ we denote by $\Pi\{\psi\}$ the normalized state $(1/4) P$, where $P$ is the orthogonal projector onto $\{\psi\}^\perp$. We say that a subspace of $\mathcal{H}$ is completely entangled (CES) if it contains no product vectors. (We require product vectors to be nonzero.) For counting purposes we do not distinguish product vectors which are scalar multiples of each other.

We give a formal definition of the term “general position” [11, Definition 7].

Definition 2 We say that a family of product vectors $\{|\psi_i\rangle = |\phi_i\rangle \otimes |\chi_i\rangle : i \in I\}$ is in general position (in $\mathcal{H}$) if for any $J \subseteq I$ with $|J| \leq M$ the vectors $|\phi_j\rangle$, $j \in J$, are linearly independent and for any $K \subseteq I$ with $|K| \leq N$ the vectors $|\chi_k\rangle$, $k \in K$, are linearly independent.

Theorem 3 ($M = N = 3$) For a $3 \times 3$ PPT state $\rho$ of rank four, the following assertions hold.

(i) $\rho$ is entangled if and only if $R(\rho)$ is a CES.

(ii) If $\rho$ is separable, then it is either the sum of four pure product states or the sum of a pure product state and a $2 \times 2$ separable state of rank three.

(iii) If $\rho$ is entangled, then

(a) $\rho$ is extreme;

(b) $\text{rank} \rho^\dagger = 4$;

(c) $\rho = V \Pi\{\psi\} V^\dagger$ for some $V \in G$ and some $\{\psi\} \in \mathcal{U}$;

(d) $\ker \rho$ contains exactly 6 product vectors, and these vectors are in general position.

The first assertion of the following proposition is [8, Theorem 23].

Proposition 4 ($M = N = 3$) Any $\rho \in \mathcal{E}'$ is SLOCC equivalent to one which is invariant under partial transpose, i.e., there exist $A,B \in \text{GL}_3(\mathbb{C})$ such that $\sigma := A \otimes B \rho A^\dagger \otimes B^\dagger$ satisfies the equality $\sigma^\dagger = \sigma$. Moreover, we may assume that $\sigma = C^\dagger C$ where $C = [C_0 \ C_1 \ C_2]$ and

$$C_0 = \begin{bmatrix} 0 & a & b \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad C_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & c \\ 1 & 0 & -1/d \end{bmatrix}, \quad C_2 = \begin{bmatrix} 0 & -1/b & 0 \\ 0 & 1 & 0 \\ 1 & -c & 0 \end{bmatrix}; \quad a,b,c,d > 0. \quad (7)$$

The weaker form of the second assertion, with $a$ being just real and nonzero, follows from the proof of [8, Theorem 23] and [10]. The stronger claim that (like $b,c,d$) $a$ can also be chosen to be positive will be proved in Theorem 7.

As an application, let us recall the following result [8, Theorem 24].

Proposition 5 ($M = N = 3$) If the normalized states $\rho$ and $\rho'$ are $3 \times 3$ PPTES of rank four with the same range, then $\rho = \rho'$.

### III. EQUIVALENCE CLASSES OF $3 \times 3$ PPTES OF RANK FOUR

The main objective of this section is to show that the set of equivalence classes of $3 \times 3$ PPTES of rank four, equipped with the quotient topology, is homeomorphic to the quotient $R/A_5$ where $R \subset \mathbb{R}^4$ is a product of four open intervals and $A_5$ is the alternating group of order 60 acting on $R$ by rational transformations. We also formulate a test for checking the equivalence of two $3 \times 3$ PPTES of rank four.

Recall that $\mathcal{E}'$ is the set of $3 \times 3$ PPTES of rank four, and that $\mathcal{E}'$ is $G$-invariant. The quotient space $\mathcal{E}'/G$ parametrizes the set of equivalence classes of $3 \times 3$ PPTES of rank four. We equip $\mathcal{E}'/G$ with the quotient topology and let $\pi : \mathcal{E}' \rightarrow \mathcal{E}'/G$ be the projection map.
Let $\Omega = \{(a, b, c, d): a, b, c, d > 0\}$ be the positive orthant of $\mathbb{R}^4$. Define the map $\omega: \Omega \to \mathcal{E}'$ by the formula $\omega(a, b, c, d) = C^tC$, where $C = [C_0 \ C_1 \ C_2]$ and the blocks $C_i$ are $4 \times 3$ matrices given by Eq. (7). Our first objective is to prove that the map $p\omega: \Omega \to \mathcal{E}'/G$ is onto. This was proved in our previous paper [3] apart from the fact that the sign of the parameter $a$ was left ambiguous. The proof uses the $G$-invariants of quintuples of product vectors which we now briefly recall.

Let $(|\alpha_i\rangle)_{i=0}^4$ be an (ordered) quintuple of vectors in $\mathcal{H}_A$ such that any three of them are linearly independent. To any such quintuple we assign three invariants $(J^A_1, J^A_2, J^A_3)$. These are certain complex numbers, different from 0 and 1, subject to the relation $J^A_1J^A_2J^A_3 = 1$. They are defined by the formulae

$$
J^A_1 = \frac{\Delta_{0,1,3}}{\Delta_{0,3,1}}, \quad J^A_2 = \frac{\Delta_{0,1,4}}{\Delta_{0,3,1}^2}, \quad J^A_3 = \frac{\Delta_{1,2,3}}{\Delta_{0,3,1}^2}.
$$

where $\Delta_{i,j,k} = \det[|\alpha_i\rangle \ |\alpha_j\rangle \ |\alpha_k\rangle]$. If two quintuples, say $(|\alpha_i\rangle)$ and $(|\alpha'_i\rangle)$, have the same invariants then there exists an invertible linear operator $V_A$ on $\mathcal{H}_A$ such that $V_A|\alpha_i\rangle \propto |\psi_i\rangle$ for each index $i$. (The proportionality constants may depend on the index.) The converse is also valid.

To any quintuple of product vectors $(|\phi_i\rangle = |\alpha_i\rangle |\beta_i\rangle)_{i=0}^4$ in $\mathcal{H}$, which are in general position, we assign six invariants $(J^A_1, J^A_2, J^A_3, J^B_1, J^B_2, J^B_3)$, where the $(J^A_1, J^A_2, J^A_3)$ are the invariants of the quintuple $(|\alpha_i\rangle)$ and $(J^B_1, J^B_2, J^B_3)$ are those of the quintuple $(|\beta_i\rangle)$. If two quintuples of product vectors, say $(|\phi_i\rangle)$ and $(|\psi_i\rangle)$, have the same invariants then there exists an ILO, say $V$, such that $V|\phi_i\rangle \propto |\psi_i\rangle$ for each index $i$, and the converse holds.

For $\rho \in \mathcal{E}'$, ker $\rho$ contains exactly six product vectors, say $|\phi_i\rangle$, $i = 0, \ldots, 5$. Moreover, these six product vectors are in general position, see [3, Theorem 22]. There are in total 720 different sextuples $(|\phi_i\rangle)$, where $\pi \in S_6$ is a permutation of the set $\{0, 1, \ldots, 5\}$. We define the six invariants of such sextuple to be the invariants of the quintuple which is obtained from the sextuple by truncation, i.e., by omitting the last product vector $|\phi_5\rangle$. It follows from [3, Theorem 25] that, for all sextuples $(|\phi_i\rangle)$, all six invariants are real. Hence, each of the invariants belongs to one of the open intervals $p = (0, 1)$, $P = (1, +\infty)$ and $N = (-\infty, 0)$. To each of the sextuples we associate a six letter symbol, with letters chosen from the set $\{p, P, N\}$. The symbol is constructed from the sequence of invariants $(J^A_1, J^A_2, J^A_3, J^B_1, J^B_2, J^B_3)$ by replacing each number by the letter designating the open interval $p$, $P$, $N$ containing it. In the generic case, the 720 sextuples of product vectors will have pairwise different sextuples of invariants. However, only 12 different symbols arise. We refer to these particular symbols as the UPB symbols (see [3, Table I]). Each of the 12 UPB symbols arises exactly 60 times. For convenience we single out one of the 12 UPB symbols, namely the symbol ppPPNp.

We assume (as we may) that the chosen sextuple $(|\phi_i\rangle)$ is of type ppPPNp. The set of all permutations $\pi \in S_6$ for which $(|\phi_i\rangle)$ is of type ppPPNp is a subgroup of $S_6$ isomorphic to the alternating group $A_5$ of order 60. We shall refer to this subgroup as the stabilizer of the symbol ppPPNp. One defines similarly the stabilizers for other UPB symbols. All these stabilizers are isomorphic to $A_5$ and are pairwise distinct. For the symbol ppPPNp, the stabilizer is generated by the 5-cycle $\alpha = (0, 1, 2, 3, 5)$ and the involution $\beta = (1, 2)(4, 5)$. Note that it permutes transitively the six product vectors $|\phi_i\rangle$. From now on we set $A_5 = (\alpha, \beta)$.

Since $J^A_1J^A_3J^A_3 = 1$ and $J^B_1J^B_2J^B_3 = 1$, it suffices to work with the following four invariants $J^A_1, J^A_2, J^B_1, J^B_2$. For each $\pi \in A_5$, the sextuple $(|\phi_\pi\rangle)$ has symbol ppPPNp and so the quadruple of its invariants $(J^A_1, J^A_2, J^B_1, J^B_2)$ belongs to the open infinite rectangular box $R = p \times p \times N \times p$ (a product of four open intervals in the Euclidean space $\mathbb{R}^4$). We shall see that $R$ parametrizes the set of equivalence classes of $3 \times 3$ PPTES $\rho$ of rank four. However, this parametrization is not one-to-one; generically it is sixty-to-one. The action of $A_5$ on sextuples of product vectors in ker $\rho$ induces an action of $A_5$ on $R$, and the equivalence classes are represented by the orbits of $A_5$ in $R$. Let us describe explicitly the action of $\alpha$ and $\beta$ on the quadruple of invariants $(a, b, c, d):=(J^A_1, J^A_2, J^B_1, J^B_2)$:

$$
\alpha: (a, b, c, d) \rightarrow \left( \frac{1 - d}{1 - c}, \frac{b}{1 - ab}(1 - acd), \frac{1}{d} \frac{1 - b}{1 - a}, \frac{1 - a}{1 - ab}(1 - acd) \right);
$$

$$
\beta: (a, b, c, d) \rightarrow \left( \frac{c}{1 - cd}, \frac{(1 - ab) - ce}{1 - c}, \frac{b}{(1 - b)(1 - ab)}, \frac{1 - a}{(1 - ab)(1 - acd)} \right),
$$

where $e = (1 - a) + ad(1 - b)$. The meaning of, say, the first formula is that its right hand member is the quadruple of invariants of the sextuple $(|\phi_\pi\rangle) = (|\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle, |\phi_5\rangle)$.

From the preceding discussion we obtain the following test for equivalence.

**Theorem 6** Let $\rho, \rho' \in \mathcal{E}'$ and let $(|\phi_i\rangle)$ and $(|\phi'_i\rangle)$ be sextuples of product vectors in ker $\rho$ and ker $\rho'$, respectively. Then $\rho$ and $\rho'$ are SLOCC equivalent if and only if there exists a permutation $\pi \in S_6$ such that the sextuples $(|\phi_\pi\rangle)$ and $(|\phi'_\pi\rangle)$ have the same invariants.
**Proof.** *Necessity.* Let \( \rho' = V \rho V^\dagger \), where \( V \) is an ILO. Since \( \rho(\phi_i) = 0 \) and \( \ker \rho = V^\dagger \ker \rho' \), we have \( V^\dagger \phi_i = c_i \pi_\pi \) for some permutation \( \pi \) and some nonzero scalars \( c_i \). It follows that the sextuples \((|\phi_{i\pi}|)\) and \((|\phi_i'|)\) have the same invariants.

*Sufficiency.* Since \((|\phi_{i\pi}|)\) and \((|\phi_i'|)\) have the same invariants, there exists an ILO, say \( V \), such that \( V^\dagger \phi_i = c_i \pi_\pi \) for some permutation \( \pi \) and some nonzero scalars \( c_i \). Since the \( |\phi_i'| \) span \( \ker \rho' \) and the \( |\phi_i| \) span \( \ker \rho \), we have \( V^\dagger \ker \rho' = \ker \rho = V^\dagger \ker(V \rho V^\dagger) \). It follows that the states \( \rho \) and \( V \rho V^\dagger \) have the same kernel and range. By Proposition 3 these two states are equivalent, and so are \( \rho \) and \( \rho' \). \( \square \)

We shall now prove that each point of \( R \) is the quadruple of invariants of some \( \rho \in \mathcal{E}' \) and that we can indeed require in Proposition 4 that \( a > 0 \). In view of Theorem 4 this implies that the map \( \pi: \Omega \rightarrow \mathcal{E}'/G \) is onto.

**Theorem 7** Every \( \sigma \in \mathcal{E}' \) is SLOCC equivalent to a state \( \rho = \omega(a,b,c,d) \) (where all \( a, b, c, d > 0 \)). For each point \( (x, y, z, w) \in R \) there exists a state \( \rho \in \mathcal{E}' \) such that \( (x, y, z, w) = (J_1^A, J_2^A, J_2^B, J_3^B) \) for some sextuple of product vectors in \( \ker \rho \).

**Proof.** To prove the first assertion we choose a sextuple of product vectors \((|\phi_i|)_{i=0}^5 \in \ker \sigma \) with invariants of type \( ppPNp \). Thus we have \((J_1^A, J_2^A, J_2^B, J_3^B) \in R \). Let us define the positive numbers \( b, c, d \) by

\[
\begin{align*}
b^2 &= \frac{J_2^B}{J_2^A} \cdot \frac{(1 - J_2^A)(1 - J_1^A J_2^A)}{(1 - J_2^B J_3^B)(1 - J_1^A J_2^B J_3^B)}, \\
c^2 &= \frac{1}{J_2^B} \cdot \frac{(1 - J_1^A J_2^B)(J_1^A - J_2^B J_3^B)}{(1 - J_3^B)(1 - J_1^A J_2^B)}, \\
d^2 &= \frac{J_1^A}{(1 - J_1^A)(1 - J_1^A J_2^B J_3^B)}. 
\end{align*}
\]

(11) (12) (13)

(It is easy to see that the right hand sides are positive.)

We can now define \( a > 0 \) by the formula

\[
a = \frac{bcd}{J_3^B} \cdot \frac{(1 - J_1^A)(1 - J_1^A J_2^B J_3^B)(J_1^A - J_2^B J_3^B)}{(1 - J_2^B)^2}. 
\]

(14)

We claim that \( \rho := \omega(a,b,c,d) \) and \( \sigma \) are equivalent. It suffices to show that we can choose a sextuple of product vectors in \( \ker \rho \) having the same invariants as the sextuple \((|\phi_i|)\). We observe that \( \ker \rho \) contains the product vectors \(|\tilde{u}\rangle\) for \( i = 0, 1, 2 \). We have to find the remaining three product vectors in this kernel. We proceed as in the proof of 2. Theorem 25. We introduce the cubic polynomial

\[
f(z) = abz(cz - 1 - d^2)(c - (1 + c^2)z) + d(cz - 1)(b^2c - (1 + b^2 + b^2c^2)z).
\]

(15)

It has three real roots \( z_1, z_2, z_3 \) such that

\[
\begin{align*}
z_3 < 0, & \quad \lambda < z_1 < c/(1 + c^2), & \quad \frac{1}{c} < z_2 < (1 + d^2)/c, 
\end{align*}
\]

(16)

where \( \lambda = b^2c/(1 + b^2 + b^2c^2) \). Explicitly, they are given by the formulae

\[
\begin{align*}
z_1 &= \frac{J_3^B}{c} \cdot \frac{1 - J_1^A J_2^B}{(1 - J_1^A J_2^B J_3^B)}, \\
z_2 &= \frac{1}{c} \cdot \frac{1 - J_1^A J_2^B}{(1 - J_1^A J_2^B J_3^B)}, \\
z_3 &= \frac{1}{c} \cdot \frac{(1 - J_2^B)(1 - J_1^A J_2^B)}{(1 - J_1^A J_2^B J_3^B)}. 
\end{align*}
\]

(17) (18) (19)

[The verification that these are indeed the roots of \( f(z) \) is a very tedious job if done by hand, but it is trivial for a package for symbolic algebraic computations such as Maple.]

The three additional product vectors in the kernel of \( \rho \) are \(|\psi_i\rangle\) \((i = 1, 2, 3)\) defined by 3, Eq. (110). By using the above expressions for \( a, b, c, d \) and \( z_1, z_2, z_3 \) and the formulae 3 Eqs. (119-120)], we can compute the invariants of the sextuple \((|00\rangle, |11\rangle, |22\rangle, |\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle)\). We obtain that they are the same as the invariants of the sextuple \((|\phi_i\rangle)\). This proves our claim and completes the proof of the first assertion.

To prove the second assertion, let us define a smooth map \( \Phi : R \rightarrow \Omega \). We set \( \Phi(x, y, z, w) = (a, b, c, d) \), where \( a, b, c, d \) are defined by the formulae 11-14 in which we replace \( J_1^A, J_2^A, J_2^B, J_3^B \) with \( x, y, z, w \), respectively. The proof
of the first assertion shows that the quadruple of invariants of the state \( \rho \), constructed above, is exactly \((x, y, z, w)\). Hence, the second assertion is proved.

It is not hard to show that the above map \( \Phi \) is a local diffeomorphism. We believe that it is a (global) diffeomorphism, but this question is beyond the scope of this paper. However, let us observe that if \((x, y, z, w) \in \Phi^{-1}(a, b, c, d)\), then \((x, y, z, w)\) is a quadruple of invariants of some ordered sextuple of the six product vectors in the kernel of \(\omega(a, b, c, d)\). Moreover, the type of this sextuple is ppPNNp. Consequently, the fibre \(\Phi^{-1}(a, b, c, d)\) is finite of cardinality at most 60.

**Corollary 8** The set, \( \mathcal{E} \), of all normalized \(3 \times 3\) PPTES of rank four on \( \mathcal{H} \) has dimension 36.

**Proof.** This set is a real semifinite set and so it has a well defined dimension, see e.g. [5]. For convenience we shall work with non-normalized states, and so the dimension will increase by one. More precisely, we have \(\mathcal{E}' = \{\lambda \rho : \lambda > 0, \rho \in \mathcal{E}\} \). Denote by \(X\) the image of \(\omega\), \(X = \{\omega(a, b, c, d) : (a, b, c, d) \in \Omega\} \subseteq \mathcal{E}'\). Each equivalence class \(E \subseteq \mathcal{E}'\) is an orbit of \(G\). It follows from [5, Proposition 27] that the identity component of the stabilizer of \(\rho \in X\) is the 3-dimensional subgroup \(\{(z_1I_3, z_2I_3) : |z_1z_2|=1\}\) of \(G\). Hence, \(\dim X = \dim G -3 = 33\). Each equivalence class \(E\) intersects \(X\) in at least one and at most 60 points. Consequently, \(\dim \mathcal{E}' = \dim X + \dim E = 37\). The normalization decreases the dimension by 1, thus \(\dim \mathcal{E} = 36\). \(\Box\)

We point out that this agrees with the computation performed in [22].

Let \(p : R \to R/A_5\) be the canonical projection map onto the quotient of \(R\) by the action of \(A_5\). As usual, the quotient space \(R/A_5\) is equipped with the quotient topology. We cannot define a map \(\mathcal{E}' \to R\) because there is no natural choice of ordering the six product vectors in the kernel of a state \(\rho \in \mathcal{E}'\). However, this ambiguity disappears when we replace \(R\) by \(R/A_5\) and specify that the sextuple of product vectors in \(\ker \rho\) is chosen to be of type ppPNNp. Thus we obtain a continuous map \(q : \mathcal{E}' \to R/A_5\). We now use the universal property of the quotient maps \(\pi : \mathcal{E}' \to \mathcal{E}'/G\) and \(p : R \to R/A_5\) to prove the following.

**Theorem 9** The quotient spaces \(\mathcal{E}'/G\) and \(R/A_5\) are homeomorphic.

**Proof.** Since the map \(q : \mathcal{E}' \to R/A_5\) is continuous and is constant on the fibers of the map \(\pi : \mathcal{E}' \to \mathcal{E}'/G\), there exists a unique continuous map \(f : \mathcal{E}'/G \to R/A_5\) such that \(q = f \pi\). At the end of the proof of the previous theorem, we have introduced the smooth map \(\Phi : R \to \Omega\). Since the map \(\pi \omega \Phi : R \to \mathcal{E}'/G\) is continuous and constant on the fibers of the map \(p : R \to R/A_5\), there exists a unique continuous map \(g : R/A_5 \to \mathcal{E}'/G\) such that \(\pi \omega \Phi = gp\). The universal property also implies that \(fg\) and \(gf\) are the identity maps. Hence, \(f\) is a homeomorphism. \(\Box\)

We shall now examine the two classical examples of UPB, namely **Pyramid** and **Tiles**.

**Example 10** The quadruple of invariants for the **Pyramid** UPB is \((- (\sqrt{5} -1)/2, (3+\sqrt{5})/2, (3-\sqrt{5})/2, (\sqrt{5}+1)/2)\) with symbol ppPNNp. If we rearrange the five vectors of this UPB in order \([2, 1, 4, 3, 5]\), the quadruple of invariants becomes \((- (\sqrt{5} -1)/2, (\sqrt{5} -1)/2, -(\sqrt{5}+1)/2, (3-\sqrt{5})/2)\). So it has the desired symbol ppPNNp and the point with these coordinates is in the region \(R\).

We claim that this point is the unique fixed point of the transformation \(\alpha\) as given by Eq. (9). Indeed, by equating the two members of Eq. (9), we obtain a system of four equations. The first two equations can be solved easily and give

\[
c = \frac{1 - b - ab + a^2b^2}{(1-a)(1-a-b)}, \quad d = \frac{a + b - 1}{1-b(1-ab)}.
\]

Then the remaining two equations factorize, and after dropping the factors that cannot vanish when \(a, b \in (0, 1)\), we obtain the system of two equations:

\[
a^2b^3 - ab^2 + ab - a - b + 1 = 0, \tag{21}
a^2b^3 - a^2b^2 - a^2b - 2ab^2 + 3ab + b - 1 = 0. \tag{22}
\]

The resultant of these two polynomials with respect to the variable \(a\) is \(b(1+b^2)(1-b)^3(1-b-b^2)\). It has a unique root in the interval \((0, 1)\) namely \(b = (\sqrt{5} -1)/2\). The proof of our claim can now be completed easily.

Moreover, one can verify that the transformation \(\beta\) fixes the unique fixed point of \(\alpha\). Hence, this point is fixed by all elements of \(A_5\). Note that this observation agrees with the fact mentioned in [4] that the stabilizer of **Pyramid** PPTES in the group \(\text{PGL}_3 \times \text{PGL}_3\) is the alternating group \(A_5\). \(\Box\)

**Example 11** Let us now consider the **Tiles** UPB. The quadruple of its invariants is \((-1/2, 2, 1/3, 3/2)\) again with symbol NPNPpP. By rearranging the five vectors in order \([2, 1, 4, 3, 5]\), we obtain the quadruple of invariants

\[
(1, 4, 3, 5, 2), \quad (1, 5, 4, 3, 2), \quad (1, 5, 3, 4, 2).
\]
(1/2, 2/3, −1, 1/2) having the desired symbol ppPNNp. The orbit of $A_5$ containing the point $(1/2, 2/3, −1, 1/2) \in R$ has size five. The other four points of this orbit are $(1/2, 1/2, −2, 1/4), (2/3, 1/2, −2, 1/2), (2/3, 3/4, −3, 1/3)$ and $(3/4, 2/3, −1, 1/3). Each of these five points $(x, y, z, w)$ gives the parameters $(a, b, c, d) = \Phi(x, y, z, w) \in \Omega$ such that the state $\omega(a, b, c, d) \in \mathcal{E}'$ is equivalent to the PPTES obtained from Tiles. For instance, by substituting the coordinates of the first point for the invariants $J_1^A, J_2^A, J_2^B, J_3^B$ in Eqs. (11)-(14), we obtain that $a = 7\sqrt{21}/27, b = 2/3\sqrt{5}$, $c = \sqrt{21}/2$ and $d = 2\sqrt{5}$.

At the referee’s suggestion, we shall also consider the one-parameter generalization of Choi’s PPTES.

Example 12 This one-parameter family $\rho_\lambda$ of $3 \times 3$ PPTES of rank four is given in [19, p. 169] by its density matrix

\[
A = \begin{bmatrix}
1 & \lambda^2 & 1 \\
\lambda^{-2} & 1 & \lambda^{-2} \\
1 & \lambda^2 & 1 \\
\end{bmatrix}
\]

(23)

(The blank entries are zeros.) The parameter $\lambda$ is assumed to be positive and different from 1. For simplicity, we shall assume that $0 < \lambda < 1$. The six product vectors in $\ker \rho_\lambda$ are the tensor products of the corresponding columns in the following two $3 \times 6$ matrices

\[
\begin{bmatrix}
1 & 0 & \lambda & 1 & 0 & -\lambda \\
\lambda & 1 & 0 & -\lambda & 1 & 0 \\
0 & \lambda & 1 & 0 & -\lambda & 1 \\
\end{bmatrix}, \begin{bmatrix}
-\lambda & 0 & 1 & \lambda & 0 & 1 \\
1 & -\lambda & 0 & 1 & \lambda & 0 \\
0 & 1 & -\lambda & 0 & 1 & \lambda \\
\end{bmatrix}.
\]

(24)

This sextuple of product vectors has symbol pNNPpp. After interchanging the third and fourth columns of both matrices, the symbol becomes ppPNNp and a computation shows that the quadruple of invariants of the reordered sextuple is given by

\[
J_1^A = \frac{1 + \lambda^3}{2}, \quad J_2^A = \frac{1 - \lambda^3}{1 + \lambda^3}, \quad J_2^B = \frac{1 + \lambda^3}{1 - \lambda^3}, \quad J_3^B = \frac{2\lambda^3}{1 + \lambda^3}.
\]

(25)

By applying the formulae (11)-(14), we conclude that $\rho_\lambda$ is equivalent to the state $\sigma$ defined in Proposition 4 with $a, b, c, d > 0$ given by

\[
b^2 = \frac{2\lambda^6}{1 + \lambda^6}, \quad c^2 = \frac{(3 + \lambda^6)(1 + 3\lambda^6)}{(1 - \lambda^6)^2}, \quad d^2 = \frac{2}{1 + \lambda^6}, \quad a = \frac{bcd}{2\lambda^6} \cdot \frac{(1 - \lambda^{12})(1 + 3\lambda^6)}{(3 + \lambda^6)^2}.
\]

(26)

Finally we show a simple result on PPTES.

Lemma 13 Given $\rho \in \mathcal{E}'$, there is no $3 \times 3$ extreme state $\sigma$ of rank five, such that $\mathcal{R}(\sigma) = \ker \rho$.

Proof. Suppose such $\sigma$ exists. We may assume that $\rho = \omega(a, b, c, d)$ for some $a, b, c, d > 0$. Using Eq. (7), the product vector $|00\rangle$ belongs to $\mathcal{R}(\sigma)$ and $\mathcal{R}(\sigma^\dagger)$. So $\sigma$ is not an edge state, and we have reached a contradiction. □

IV. CHECKERBOARD STATES

One of the early examples of PPTES was the multi-parameter family of checkerboard states constructed in [8], see also [12]. We will show that, up to equivalence, all checkerboard PPTES can be parametrized by just two real parameters. By using invariants, we have devised a test for checking whether an arbitrary $3 \times 3$ PPTES of rank four is equivalent to a checkerboard state.
We define the checkerboard states (see \[8\] section 7) to be the states $\rho$ which can be written as $\rho = C^\dagger C$, where $C = [C_1 C_2 C_3]$ and the $C_i$ are complex matrices having the following form:

$$C_1 = \begin{pmatrix} a & 0 & d \\ 0 & g & 0 \\ j & 0 & m \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & c & 0 \\ f & 0 & i \\ 0 & l & 0 \end{pmatrix}, \quad C_3 = \begin{pmatrix} b & 0 & e \\ 0 & h & 0 \\ k & 0 & n \end{pmatrix}.$$  

(27)

**Proposition 14** Every checkerboard PPTES is equivalent to one with

$$C_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & u & 0 \\ 1 & 0 & 0 \\ 0 & l & 0 \end{pmatrix}, \quad C_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & v & 0 \\ v & 0 & 1 \end{pmatrix}, \quad u, v > 0.$$  

(28)

Consequently, there exist $3 \times 3$ PPTES of rank four not equivalent to any checkerboard state.

**Proof.** Let $\rho = C^\dagger C$ be a $3 \times 3$ PPTES of rank four, where $C = [C_1 C_2 C_3]$ with the $C_i$ given by (27). Then any linear combination of the $C_i$ must have rank at least two. By replacing $C_1$ with a suitable linear combination of $C_1$ and $C_3$, we can assume that $ami = dj$. By applying an ILO and premultiplying $C$ by a unitary matrix, we may assume that

$$C_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & c & 0 \\ f & 0 & i \\ 0 & l & 0 \end{pmatrix}, \quad C_3 = \begin{pmatrix} b & 0 & e \\ 0 & h & 0 \\ k & 0 & n \end{pmatrix}.$$  

(29)

Since $\rho^F \geq 0$, we must have $e = i = 0$. By using another ILO, we can further simplify these matrices to obtain

$$C_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & c & 0 \\ 1 & 0 & 0 \\ 0 & l & 0 \end{pmatrix}, \quad C_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & h & 0 \\ k & 0 & 1 \end{pmatrix}.$$  

(30)

As $\rho$ is entangled, $\mathcal{R}(\rho)$ must be a CES and so $chl r = 0$. By using an argument from the proof of \[8\] Theorem 28], we obtain that $h = rk^*, |c| = 1$ and $l = cr^* k/k^*$. Thus

$$C_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & c & 0 \\ 1 & 0 & 0 \\ 0 & l & 0 \end{pmatrix}, \quad C_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & rk^* & 0 \\ k & 0 & 1 \end{pmatrix}.$$  

(31)

Let us choose $u_2$ such that $u_2^2 = c$ and premultiply $C$ with the unitary matrix diag(1, $u_2$, $u_3$, $u_4$), where $u_3 = |r| k^*/r^* k$ and $u_4 = u_2 |k|/k$. Next we postmultiply each $C_i$ with diag($1$, $u_2^2/|r|$, $|k|/k^*$), and multiply $C_2$ and $C_3$ with $u_2^2$ and $|rk|/rk^*$, respectively. (Note that these transformations form an ILO.) Now we have

$$C_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/|r| & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & 1/|r| & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad C_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & |k| & 0 \\ |k| & 0 & 1 \end{pmatrix}.$$  

(32)

Thus the first assertion is proved, and the second follows from the first because the matrices (28) depend only on two positive parameters.

We can now characterize the checkerboard PPTES up to equivalence.

**Proposition 15** A $3 \times 3$ PPTES of rank four is equivalent to a checkerboard state if and only if, for some ordering of the product vectors in its kernel, its invariants are of type PNNpPP and satisfy the equations $J_2^A = J_3^A$ and $J_2^B = J_3^B$.

**Proof.** *Necessity.* Let $\rho$ be a $3 \times 3$ checkerboard PPTES of rank four and $(J_1^A, J_2^A, J_3^A, J_1^B, J_2^B, J_3^B)$ its invariants with symbol PNNpPP. By Proposition 14 we have $\rho = C^\dagger C$ where $C = [C_1 C_2 C_3]$ and the $C_i$ are given by (28). We
have to find the six product vectors in ker $\rho$. First observe that the product vectors $|\phi_0\rangle = |02\rangle$ and $|\phi_3\rangle = |20\rangle - v|22\rangle$ belong to ker $\rho$. Let us exhibit the remaining four.

Let $\pm x_1, \pm x_2$ be the roots of the biquadratic polynomial $f(x) = u^2(1 + v^2)x^4 - (u^2v^2 + 2u^2 + v^2)x^2 + u^2$. Since $f(1) = -v^2 < 0$, we may assume that $0 < x_1 < 1 < x_2$. For any real $t$ let $|\phi(t)\rangle = |\alpha(t)\rangle \otimes |\beta(t)\rangle$, where $|\alpha(t)\rangle = v|0\rangle + tv|1\rangle + u(t^2 - 1)|2\rangle$ and $|\beta(t)\rangle = uv^2|0\rangle - tv(1) + (t^2 - 1)|2\rangle$. One can easily verify that the product vectors $|\phi_1\rangle = |\phi(x_1)\rangle$, $|\phi_2\rangle = |\phi(-x_1)\rangle$, $|\phi_3\rangle = |\phi(x_2)\rangle$, $|\phi_4\rangle = |\phi(-x_2)\rangle$ belong to ker $\rho$.

A computation shows that the invariants of the sextuple $|\phi_i\rangle_i$ are $(1/\mu^2, -\mu, -\mu, 1/\lambda^2, \lambda, \lambda)$, where $\lambda = (x_2 + x_1)/(x_2 - x_1) > 1$ and $\mu = (1 - x_1x_2)/(1 + x_1x_2) < \lambda$. As $x_2^2 - x_1^2 = 1/(1 + v^2) < 1$, we have $\mu > 0$. From the equality $x_1^2 = (\lambda - \mu)(\lambda - 1)/(\lambda + \mu)(\lambda + 1)$ we deduce that $\mu < 1$. Hence, the invariants indeed have the required symbol PNNpP, and the equalities $J_2^A = J_3^A$ and $J_2^B = J_3^B$ hold.

**Sufficiency.** Now assume that $\sigma$ is a 3 × 3 PPTES of rank four and that $(J_1^A, J_2^A, J_3^A, J_1^B, J_2^B, J_3^B)$ are the invariants, having the symbol PNNpP, of some sextuple of product vectors in ker $\sigma$. We also assume that $J_2^A = J_3^A$ and $J_2^B = J_3^B$, and so we can write these invariants as $(1/\mu^2, -\mu, -\mu, 1/\lambda^2, \lambda, \lambda)$, where $\lambda > 1$ and $\mu > 0$. Since the first letter of the above symbol is $P$, we have $\mu < 1$. We set

$$v = 2\sqrt{\lambda\mu}/\lambda - \mu > 0, \quad w = 2\lambda - \mu\sqrt{\lambda^2 + 1}/\lambda^2 - 1.$$  

(33)

It is not hard to verify that

$$(1 + v^2)(w - 1) - 1 = 4\lambda^2(1 - \mu^2)/(\lambda^2 - 1)(\lambda - \mu)^2 > 0,$$  

(34)

and so we can define $u > 0$ by the equation $u^2((1 + v^2)(w - 1) - 1) = v^2$.

Let $\rho = C^ TC$ be the checkerboard state where $C = [C_1 \ C_2 \ C_3]$ and the $C_i$ are given by (28) with the parameters $u$ and $v$ as defined above. The biquadratic polynomial $f(x) = u^2(1 + v^2)x^4 - (u^2v^2 + 2u^2 + v^2)x^2 + u^2$ has roots $\pm x_1, \pm x_2$, where $x_1, x_2 > 0$ are given by

$$x_1^2 = (\lambda - \mu)(\lambda - 1)/(\lambda + \mu)(\lambda + 1), \quad x_2^2 = (\lambda - \mu)(\lambda + 1)/(\lambda + \mu)(\lambda - 1).$$  

(35)

The computation performed in the first part of the proof shows that $(1/\mu^2, -\mu, -\mu, 1/\lambda^2, \lambda, \lambda)$ are also the invariants of a sextuple of product vectors in ker $\rho$. Hence, $\rho$ and $\sigma$ are equivalent.

We remark that if we use the invariants of type ppPNNp (instead of PNNpP) then the two equations in the proposition should be replaced by $J_2^A + J_3^A = 2J_2^A J_3^A$ and $J_2^B + J_3^B = 2J_2^B J_3^B$. Since in Theorems 17 we use only the invariants $J_1^A, J_2^A, J_2^B$ and $J_3^B$, we mention that the former equation can be rewritten as $J_2^A(1 - J_1^A J_2^A) = 1 - J_2^A$.

**V. EXTREME AND EDGE 3 × 3 STATES**

In recent years extreme and edge 3 × 3 states have been extensively studied. A primary reason is that PPTES do not exist in any bipartite extreme or of smaller dimension. On the other hand, many important problems are open for 3 ⊗ 3 systems. For example, a 3 × 3 PPT state of rank four is separable if and only if there is a product vector in the range of this state. But there is no analytical criterion for deciding which 3 × 3 states of rank larger than four are separable. It is also unknown whether two-qutrit entangled states of rank larger than three are distillable. Characterizing 3 × 3 extreme and edge PPTES may provide a better understanding of these problems.

We begin with extreme states. There is a simple necessary condition for extremality of states.

**Proposition 16** Let $\rho$ be an $M \times N$ PPT state of birank $(r, s)$. If $r^2 + s^2 > M^2N^2 + 1$ then $\rho$ is not extreme.

By this proposition, the birank of an extreme 3 × 3 PPTES $\rho$ must be (up to ordering) one of the following five pairs:

$$(4, 4), (5, 5), (6, 6), (5, 6), (5, 7).$$  

(36)

Examples for the first three pairs have been known for some time. First, the extreme states $\rho$ of birank $(4, 4)$ were thoroughly analyzed and characterized by UPB. Second, the edge states $\rho$ of biranks $(5, 5)$ and $(6, 6)$ have been analytically constructed. They were proved to be extreme in Ref. 20. Third, families of edge states $\rho$ for the remaining two pairs, $(5, 6)$ and $(5, 7)$, have been constructed very recently. In Table I at the end of this section, we will show that for suitable parameter values, these edge states turn out to be extreme. They are the first
examples of extreme states \( \rho \) with rank \( \rho \neq \operatorname{rank} \rho^F \). Hence, each of the pairs \( (36) \) is the birank of some \( 3 \times 3 \) extreme state.

Next we consider the \( 3 \times 3 \) edge states \( \rho \) of birank \( (r, s) \).

By \( (36) \) we have \( r = 4 \) if and only if \( s = 4 \). It is known that \( r + s \leq 14 \) \( (29, 30) \). (It has been claimed in \( (34) \) that this claim is false.) The birank \( (r, s) \) cannot be equal to \( (5, 9) \) because any 5-dimensional subspace of \( \mathcal{H} \) contains at least one product vector.

We conclude that, up to ordering, \( (r, s) \) must be one of the following eight pairs:

\[
(4, 4), \ (5, 5), \ (6, 6), \ (5, 6), \ (5, 7), \ (5, 8), \ (6, 7), \ (6, 8).
\] (37)

Recall that there exist extreme states for the first five pairs. As any extreme state of rank bigger than one is also an edge state, it remains to consider only the last three pairs in this list. Such edge states have been constructed recently in \( (30) \). Since the examples for the first five pairs in \( (37) \) are extreme states, it is an interesting question to ask whether in these five cases there exist \( 3 \times 3 \) edge states \( \rho \) which are not extreme.

We have constructed such states \( \rho \) (see Table I) for pairs \( (6, 6), (5, 6) \) and \( (5, 7) \). Since every PPTES of birank \( (4, 4) \) is extreme, only the case \( (5, 5) \) remains in doubt. We have tested a few known \( 3 \times 3 \) edge states of birank \( (5, 5) \), but all of them turned out to be extreme (see Table I). We conjecture that any \( 3 \times 3 \) edge state of birank \( (5, 5) \) is extreme. This should be compared with the known result that any \( 2 \times 4 \) PPTES of birank \( (5, 5) \) is extreme \( (1) \). The \( 3 \times 3 \) case is more challenging because there exist \( 3 \times 3 \) PPTES of birank \( (5, 5) \) which are not edge states. An example is \( \rho = \sigma + \epsilon |00\rangle \langle 00| \) where \( \sigma \) is a \( 3 \times 3 \) PPTES of birank \( (4, 4) \), and \( \epsilon > 0 \) is sufficiently small.

Another interesting problem is whether our results can be extended to higher dimensions. For instance, examples of extreme \( M \times N \) PPTES of rank \( M + N - 2 \) have been constructed recently \( (11) \). One may ask how many parameters are necessary to describe such states.

Table I of \( 3 \times 3 \) edge and extreme states \( \rho \).
(Computations performed using Maple.)

1. Birank (5, 5)

   (a) [13, Section II]
   Extreme state.
   \( \ker \rho \): 2 product vectors.
   \( \mathcal{R}(\rho) \): Infinitely many product vectors.
   \( \mathcal{R}(\rho^F) \): Infinitely many product vectors.

   (b) [21, 28] with \( s = 1 \) and \( t = 2 \).
   Extreme state.
   \( \ker \rho \): 2 product vectors.
   \( \mathcal{R}(\rho) \): Infinitely many product vectors.
   \( \mathcal{R}(\rho^F) \): Infinitely many product vectors.

   (c) [30, Sec. 4] with \( b = 2 \) and \( \theta = \pi/6 \).
   Extreme state.
   \( \ker \rho \): CES.
   \( \mathcal{R}(\rho) \): 6 product vectors.
   \( \mathcal{R}(\rho^F) \): 6 product vectors.

2. Birank (6, 5)

   (a) [21] with \( s = 2 \).
   Edge state, but not extreme.
   \( \ker \rho \): 2 product vectors.
   \( \mathcal{R}(\rho^F) \): 3 product vectors.

   (b) [30, Sec. 4] with \( b = 2, \theta = \pi/4 \) and \( r = 0 \).
   Extreme state.
   \( \ker \rho \): CES.
   \( \mathcal{R}(\rho^F) \): 6 product vectors.

3. Birank (6, 6)

   (a) [13, Section III]
   Extreme state.
   \( \ker \rho \): CES.
(b) [30, Sec. 4] with $b = 2$, $\theta = \pi/6$, $(\xi|\eta) = 0$ and $(\eta|\zeta) = (\zeta|\xi) = 1$. Edge state, but not extreme. 
$\ker \rho$: CES.

4. Birank (7, 5)

(a) [21] with $s = 2$.
Edge state, but not extreme.
$\ker \rho$: CES.
$\mathcal{R}(\rho^F)$: 6 product vectors.

(b) [30] Sec. 4] $r = 3/7$, $b = 2$ and $\theta = \arccos(9/14)$. Extreme state.
$\ker \rho$: CES.
$\mathcal{R}(\rho^F)$: 6 product vectors.

5. Birank (7, 6)

(a) [21] with $s = 2$.
Edge state, but not extreme.
$\ker \rho$: CES.

6. Birank (8, 5)

(a) [30] Sec. 4] with $b = 2$, $\theta = \pi/4$ and $r = 3/7$.
Edge state, but not extreme.
$\ker \rho$: CES.
$\mathcal{R}(\rho^F)$: 6 product vectors.

7. Birank (8, 6)

(a) [30] Sec. 3] with $b = 2$ and $\theta = \pi/4$.
Edge state, but not extreme.
$\ker \rho$: CES.

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