Nonexistence of *n*-qubit unextendible product bases of size $2^n - 5$

Lin Chen^{1,2,*} and Dragomir Ž Đoković^{3,†}

¹School of Mathematics and Systems Science, Beihang University, Beijing 100191, China ²International Research Institute for Multidisciplinary Science, Beihang University, Beijing 100191, China ³Department of Pure Mathematics and Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada (Dated: May 8, 2019)

It is known that the *n*-qubit system has no unextendible product bases (UPBs) of cardinality $2^n - 1$, $2^n - 2$ and $2^n - 3$. On the other hand the *n*-qubit UPBs of cardinality $2^n - 4$ exist for all $n \ge 3$. We prove that they do not exist for cardinality $2^n - 5$.

PACS numbers: 03.65.Ud, 03.67.Mn

I. INTRODUCTION

The notion of UPBs is fundamental in quantum information theory and has various applications. First, UPBs have been constructed to characterize the nonlocality without entanglement that appears when locally distinguishing product vectors [22]. Second, UPBs have been used to construct positive-partial-transpose (PPT) entangled states [3]. All two-qutrit UPBs have been constructed as well as all two-qutrit PPT entangled states of rank four [6]. Furthermore, the multiqubit UPBs have been used to construct Bell inequalities without quantum violation [21]. Recently, it has been shown that the structure of multiqubit UPBs is related to the socalled orthogonality complete graphs, and many multiqubit UPBs have been thus constructed [11]. However the main problem, namely to determine the cardinalities of multiqubit UPBs is still unresolved.

For convenience we denote by Θ_n the set of cardinalities of UPBs in the n-qubit systems. As we allow a UPB to span the whole Hilbert space, we have $2^n \in \Theta_n$. It is known that $2^n - 1$, $2^n - 2$ and $2^n - 3$ do not belong to Θ_n for any n, and $2^n - 4 \in \Theta_n$ for all $n \geq 3$ [12, 13]. In these references, extensive computer computations failed to find any example of n-qubit UPBs of cardinality 2^n-5 . In the cases n = 3, 4 it is known that they do not exist. Hence, the question was raised whether such UPBs exist for some $n \geq 5$. In Theorem 9 we prove that they do not exist. Our proof is based on the study of the hypothetical entangled PPT projector ρ of rank 5 which a UPB of size $2^n - 5$ would provide. As a result we constructed a couple of examples of 5-qubit bound entangled states of rank 5, which give the affirmative answer to a question raised by Johnston in [12, Sec. 6], open problem (1).

The rest of this paper is organized as follows. In Sec. II we introduce our notation and recall some known facts. Then we prove two auxilliary lemmas and our main result in Sec. III. We conclude in Sec. IV.

II. PRELIMINARIES

Let $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ be the Hilbert space of dimension D representing a quantum system A_1, \ldots, A_n consisting of n parties. We are mainly interested in the case where all parties are qubits, i.e. each Hilbert space \mathcal{H}_j has dimension two. In that case, we fix an orthonormal basis $|0\rangle_j, |1\rangle_j$ of \mathcal{H}_j . Usually, the subscript j will be suppressed.

We say that a vector $|v\rangle \in \mathcal{H}$ is a unit vector if |v| = 1. As a rule, we shall not distinguish two unit vectors which differ only in the phase. When $\operatorname{Dim} \mathcal{H}_j = 2$, by using this convention, we can say that for any unit vector $|v_j\rangle \in \mathcal{H}_j$ there exists a unique unit vector $|v_j\rangle \in \mathcal{H}_j$ perpendicular to $|v_j\rangle$.

A product vector is a nonzero vector $|x\rangle = |x_1\rangle \otimes \cdots \otimes$ $|x_n\rangle$, which will be written also as $|x\rangle = |x_1, \dots, x_n\rangle$. If ||x|| = 1 we shall assume (as we may) that each $||x_j|| = 1$. Two product vectors $|x\rangle = |x_1, \dots, x_n\rangle$ and $|y\rangle = |y_1, \dots, y_n\rangle$ are orthogonal if and only if $|x_i\rangle \perp |y_i\rangle$ for at least one index j. We use the abbreviation OPS to denote any set of pairwise orthogonal unit product vectors in \mathcal{H} . The cardinality of an OPS cannot exceed D, the dimension of \mathcal{H} . We say that an OPS is an OPB, $orthogonal \ product \ basis$, if its cardinality is D. As an example, in the n-qubit system, the 2^n product vectors $|x_s\rangle = |s_1, \ldots, s_n\rangle$, where $s := (s_1, \ldots, s_n)$ runs through all binary $\{0,1\}$ -sequences of length n, is an OPB. We refer to this OPB as the *standard OPB*. However, there are many other n-qubit OPBs and describing or classifying them for any n is a very hard problem, see [3-5, 7-11, 14]and our paper [7] for the case n = 4.

An unextendible product basis (UPB) is an OPS such that there is no product vector orthogonal to all vectors of the OPS [3, 4]. Originally it was required that UPB does not span the whole Hilbert space \mathcal{H} , but for the sake of convenience we have dropped that restriction. We say that a UPB is proper if it does not span \mathcal{H} . We record some facts from the introduction section in the following lemma.

Lemma 1 For $n \geq 3$, the two largest integers in Θ_n are 2^n and $2^n - 4$.

^{*} linchen@buaa.edu.cn (corresponding author)

[†] djokovic@uwaterloo.ca

On the other hand, the problem of finding the smallest element of Θ_n has been considered by several authors [1, 2, 5] and it was finally resolved by Johnston [11, Theorem 1]. We state his theorem as follows.

Theorem 2 (Jonhston, 2013) The smallest integer in Θ_n is:

- (i) n+1 if n is odd;
- (ii) n+2 if $n \equiv 2 \pmod{4}$;
- (iii) n + 4 if $n \equiv 0 \pmod{4}$ and n > 8;
- (iv) 6 if n = 4 and 11 if n = 8.

For small values of n, we have $\Theta_1 = \{2\}$, $\Theta_2 = \{4\}$, $\Theta_3 = \{4, 8\}$. Further, from [12, Table 3] we see that

$$\Theta_4 = \{6, 7, 8, 9, 10, 12, 16\},\tag{1}$$

$$\Theta_5 \supseteq \{6, 8, 9, 10, 12 - 26, 28, 32\},$$
 (2)

$$\Theta_6 \supseteq \{8, 9, 12, 14 - 58, 60, 64\},$$
 (3)

$$\Theta_7 \supseteq \{8, 12, 16, 17, 18, 20 - 122, 124, 128\},$$
 (4)

where i-j means that all integers k in the range $i \leq k \leq j$ are included. Johnston [12] asks whether the integers 11, 27 belong to Θ_5 ; 10, 11, 13, 59 to Θ_6 ; and 10, 11, 13, 14, 15, 19, 123 to Θ_7 .

The main result of this note, Theorem 9, asserts that $2^n - 5 \notin \Theta_n$ for any n. In particular, we obtain partial answers to the above questions, namely $27 \notin \Theta_5$, $59 \notin \Theta_6$, and $123 \notin \Theta_7$.

In what follows we recall some known results which we need for the proof of our main result. Here we allow the spaces \mathcal{H}_i to have any finite dimension ≥ 2 .

Let ρ denote an n-partite state $\rho := \rho_{12...n}$ on the space $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$. We say that ρ is a PPT state if the partial transpose of ρ with respect to any subsystem is positive semidefinite. We use the acronym PPTES to denote entangled PPT states. If ρ is a separable state, then $L(\rho)$ denotes its length. For any linear operator ρ we denote its range by $\mathcal{R}(\rho)$ and its nullspace by $\ker \rho$.

We say that a bipartite state ρ is a $k \times l$ state if its reduced states ρ_1 and ρ_2 have ranks k and l, respectively. In the bipartite case, ρ^{Γ} will denote the partial transpose of ρ with respect to the first system. We refer to the ordered pair (rank ρ , rank ρ^{Γ}) as the birank of ρ .

Lemma 3 (i) Let ρ be a $2 \times N$ PPT state and $|a,b\rangle \in \ker \rho \cap (\mathcal{R}(\rho_1) \otimes \mathcal{R}(\rho_2))$ a unit product vector. Then there exists $\lambda > 0$ such that $\sigma := \rho - \lambda |a,b\rangle \langle a,b| \geq 0$, rank $\sigma = \operatorname{rank} \rho - 1$, rank $\sigma^{\Gamma} = \operatorname{rank} \rho^{\Gamma} - 1$, rank $\sigma_2 = \operatorname{rank} \rho_2 - 1 = N - 1$, and the state σ is PPT.

(ii) If ρ is a 2×2 or 2×3 separable state of birank (r,s), then $L(\rho) = \max(r,s)$.

Proof. (i) For all assertions, except the PPT property of σ , see [15, Lemma 7] and its proof. We shall prove the PPT property. By tracing out the first party in the equation $\rho = \sigma + \lambda |a,b\rangle\langle a,b|$, we obtain that $\rho_2 = \sigma_2 + \lambda |b\rangle\langle b|$. It follows that $|b\rangle \notin \mathcal{R}(\sigma_2)$. Hence, there exists an invertible linear operator W on

 \mathcal{H}_2 which makes $P:=W\sigma_2W^\dagger$ into an orthogonal projector and such that $PW|b\rangle=0$. If $V:=W^{-1}PW$ then $(I\otimes V)\rho=(I\otimes V)\sigma$ because $PW|b\rangle=0$, and so we have $(I\otimes V)\rho(I\otimes V^\dagger)=(I\otimes V)\sigma(I\otimes V^\dagger)$. Thus to prove that σ is PPT it suffices to verify that $(I\otimes V)\sigma(I\otimes V^\dagger)=\sigma$. This can be done as follows.

Let $\sigma_2 = \sum_{i=1}^{N-1} |b_j\rangle\langle b_j|$ and $P = \sum_{i=1}^{N-1} |j\rangle\langle j|$. Since $P = W\sigma_2W^{\dagger}$ we may assume that $W|b_j\rangle = |j\rangle$. Since σ_2 is a reduced density operator of σ , we have $\sigma = \sum_i |\alpha_i\rangle\langle \alpha_i|$ where $|\alpha_i\rangle = \sum_{j=1}^r |a_{j,i},b_j\rangle$ for some vectors $|a_{j,i}\rangle$. Then one can verify that $(I \otimes V)\sigma(I \otimes V^{\dagger}) = \sigma$.

(ii) is proved in [9, Proposition 3].

In the following lemma, r_j denotes the rank of the jth reduced density operator, ρ_j , of the state ρ .

Lemma 4 (see [8]). (i) Any n-partite PPT state of rank at most three is separable.

(ii) If ρ is an n-partite PPTES of rank four then either n=2 and $r_1=r_2=3$ or n=3 and $r_1=r_2=r_3=2$.

The following lemma is a special case of Kruskal's theorem (see [19] and [20, Theorem 12.5.3.1, p. 306]).

Lemma 5 Let $|a\rangle = |a_1, a_2, a_3\rangle$, $|b\rangle = |b_1, b_2, b_3\rangle$, $|c\rangle = |c_1, c_2, c_3\rangle$ and $|d\rangle = |d_1, d_2, d_3\rangle$ be product vectors of a tripartite system and let the vectors $|a_i\rangle$ and $|b_i\rangle$ be linearly independent for i = 1, 2, 3. Then the equality $|a\rangle + |b\rangle = |c\rangle + |d\rangle$ implies that, up to phase factors, $\{|a\rangle, |b\rangle\} = \{|c\rangle, |d\rangle\}$.

For the convenience of the reader, let us state [7, Remark, p. 7] as a lemma.

Lemma 6 All OPBs of a bipartite system $\mathcal{H}_1 \otimes \mathcal{H}_2$ with $\operatorname{Dim} \mathcal{H}_1 = 2$ can be constructed by the following method. First choose an orthogonal decomposition $\mathcal{H}_2 = X_1 \oplus \cdots \oplus X_m$ with $k_j := \operatorname{Dim} X_j \geq 1$ and $\sum k_j = \operatorname{Dim} \mathcal{H}_2$. Next choose m pairwise different o.n. bases $\{|v_j\rangle, |v_j^{\perp}\rangle\}$, $j \in \{1, 2, \ldots, m\}$ of \mathcal{H}_1 . Finally, for each j, choose two arbitrary o.n. bases $\{|x_{j,1}\rangle, |x_{j,2}\rangle, \ldots, |x_{j,k_j}\rangle\}$ and $\{|y_{j,1}\rangle, |y_{j,2}\rangle, \ldots, |y_{j,k_j}\rangle\}$ of X_j . Then the product vectors

$$|v_j, x_{j,1}\rangle, \dots, |v_j, x_{j,k_j}\rangle, |v_j^{\perp}, y_{j,1}\rangle, \dots, |v_j^{\perp}, y_{j,k_j}\rangle, j = 1, \dots, m,$$

form an OPB of \mathcal{H} .

III. MAIN RESULT

In this section we present our main result on the multiqubit UPBs in Theorem 9. In addition to the known results in Sec. II we shall need two more lemmas.

Lemma 7 Suppose there is a UPB $U \subset \mathcal{H}$ of cardinality $2^n - 5$ which is orthogonal to five mutually orthogonal

states $|a\rangle \otimes |\varphi_j\rangle$, j = 1, ..., 5, with $|a\rangle \in \mathcal{H}_1$ a unit vector. Then $\mathcal{H}' := \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$ has a UPB of cardinality $2^{n-1} - 5$ which is orthogonal to the states $|\varphi_j\rangle$.

Proof. The set $\mathcal{V} := \mathcal{U} \cup \{|a\rangle \otimes |\varphi_j\rangle : j = 1, ..., 5\}$ is an OPB when we view \mathcal{H} as a bipartite system $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}'$. By Lemma 6, \mathcal{V} has the form

$$\mathcal{V} = \{ |a_i, \varphi_{ij}\rangle : i = 1, \dots, m, \ j = 1, \dots, k_i \}
\cup \{ |a_i^{\perp}, \psi_{ij}\rangle : i = 1, \dots, m, \ j = 1, \dots, k_i \},$$
(5)

where the $\{|a_i\rangle, |a_i^{\perp}\rangle\}$ are m different o.n. bases of \mathcal{H}_1 . We may assume that $|a\rangle = |a_1\rangle$ and $|\varphi_j\rangle = |\varphi_{1j}\rangle$, $j=1,\ldots,5$. As $\langle a_i|a_j\rangle \neq 0$ for $i\neq j$, the set $\mathcal{W}:=\{|\varphi_{ij}\rangle: i=1,\ldots,m,\ j=1,\ldots,k_i\}$ is an o.n. basis of \mathcal{H}' . It consists of five entangled states $|\varphi_j\rangle = |\varphi_{1j}\rangle$ and $2^{n-1}-5$ product states $|\varphi_{ij}\rangle$ for which $|a_i,\varphi_{ij}\rangle \in \mathcal{U}$. Since the subspace spanned by the former contains no product vector, the latter vectors form a UPB in \mathcal{H}' of cardinality $2^{n-1}-5$.

Lemma 8 We shall view the n-qubit Hilbert space \mathcal{H} also as a bipartite space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}'$, where $\mathcal{H}' := \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$. Let ρ be a state of rank five on \mathcal{H} which is PPTES as n-partite state and $2 \times m$ as a bipartite state. Assume further that $\ker \rho$ has an o.n. basis consisting of n-partite product vectors. Then ρ is separable as a bipartite state and has length five, say $\rho = \sum_{j=1}^5 |a_j, \psi_j \rangle \langle a_j, \psi_j|$. If ρ is a projector then the $|a_j, \psi_j \rangle$ form an o.n. basis of $\mathcal{R}(\rho)$.

Proof. Since rank $\rho = 5$ we must have $n \geq 3$. Let $\{|b_j,\phi_j\rangle: j=1,\ldots,2^n-5\}$ be the o.n. basis of $\ker \rho$ mentioned in the lemma. Since the $|b_j,\phi_j\rangle \in \ker \rho$, we have $\langle b_j,\phi_j|\rho|b_j,\phi_j\rangle = 0$ which is equivalent to $\langle b_j^*,\phi_j|\rho^{\Gamma}|b_j^*,\phi_j\rangle = 0$. As ρ is PPT, this implies that all $|b_j^*,\phi_j\rangle \in \ker \rho^{\Gamma}$. We conclude that $\operatorname{rank} \rho^{\Gamma} \leq 5$.

Let $\rho' = \operatorname{Tr}_1 \rho$, be the state obtained from ρ by tracing out the first qubit, and note that $m = \operatorname{rank} \rho'$. As $\operatorname{rank} \rho = 5$, we must have $3 \le m \le 5$. If m = 5 then all assertions follow easily from [15, Corollary 3(a)]. Thus we may assume that m is 3 or 4.

Since rank $\rho = 5$, the vectors $|\phi_j\rangle$ span a subspace of dimension at least $2^{n-1} - 2$. As $m \geq 3$, for some k we have $|\phi_k\rangle \notin \ker \rho'$. Thus we have a decomposition $|\phi_k\rangle = |\alpha\rangle + |\beta\rangle$ with $|\alpha\rangle \in \mathcal{R}(\rho')$, $|\beta\rangle \in \ker \rho'$. Since $|b_k,\phi_k\rangle \in \ker \rho$ and $|b_k,\beta\rangle \in \mathcal{H}_1 \otimes \ker \rho' \subseteq \ker \rho$, we deduce that $|b_k,\alpha\rangle \in (\mathcal{H}_1 \otimes \mathcal{R}(\rho')) \cap \ker \rho$. By Lemma 3 (i) there is a $\lambda > 0$ such that $\sigma := \rho - \lambda |b_k,\alpha\rangle \langle b_k,\alpha| \geq 0$ is a PPT state of birank (4,r-1) and rank $\sigma' = m-1$, where $\sigma' = \operatorname{Tr}_1 \sigma$. As m = 3 or m = 4, by the Peres-Horodecki criterion σ is separable. Hence, ρ is separable as a bipartite state. Since $r \leq 5$, it follows from Lemma 3 (ii) that $L(\sigma) = 4$.

The last assertion follows from the fact that rank $\rho = L(\rho) = 5$.

Let us give an example of a state ρ satisfying the conditions of the above lemma. We take n=4 and

$$\rho = |0, 0, 0, 0\rangle\langle 0, 0, 0, 0| + |1\rangle\langle 1| \otimes \sigma,$$

where σ is a well-known 3-qubits PPTES of rank four constructed from the 3-qubit UPB of size 4 (see [4]).

On the other hand there exist multiqubit PPTES of rank five not of this type. An example is the extremal four-qubit symmetric PPTES with three-rank (5,7,8) constructed in [16] at the end of Sec. III.

Each of the above two PPTESs answers affirmatively a question raised in [12, Sec. 6], open problem (1). The range of the first PPTES contains the product state $|0,0,0,0\rangle$. The range of the second PPTES is the 5-qubit symmetric subspace spanned by symmetric product states. So, the kernel of neither of these two PPTESs is spanned by a multiqubit UPB.

Another interesting example is the so-called X-type multiqubit PPT state of rank five [17, 18], which may be yet another example of a multiqubit PPTES of rank five, but so far we have no proof that this is the case.

Now we are in a position to prove our main result.

Theorem 9 There are no n-qubit UPBs of cardinality $2^n - 5$, i.e., $2^n - 5 \notin \Theta_n$.

Proof. Since $\Theta_3 = \{4,8\}$ and $\Theta_4 = \{6,7,8,9,10,12,16\}$, the assertion is true for n=3,4. Assume that the assertion fails for some n>4 and let n be the smallest such integer. We have to derive a contradiction.

By our assumtion, there exists a UPB $\mathcal{U} \subset \mathcal{H}$ of cardinality $2^n - 5$. We can write it as

$$\mathcal{U} = \{ |u_i, \phi_i\rangle : i = 1, 2, \dots, 2^n - 5 \},$$

where $|u_i\rangle \in \mathcal{H}_1$ are unit vectors and the $|\phi_i\rangle$ are product vectors in $\mathcal{H}' := \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$.

Denote by ρ the projector onto the 5-dimensional subspace \mathcal{U}^{\perp} . By Lemma 8 we have

$$\rho = \sum_{j=1}^{5} |a_j\rangle\langle a_j| \otimes |\psi_j\rangle\langle \psi_j|, \tag{6}$$

where the vectors $|a_j, \psi_j\rangle$ form an o.n. basis of \mathcal{U}^{\perp} and the $|a_j\rangle \in \mathcal{H}_1$ are unit vectors. If all the $|a_j\rangle$ are equal, then Lemma 7 implies that \mathcal{H}' has a UPB of cardinality $2^{n-1} - 5$. This contradicts our choice of n. We conclude that the vectors $|a_j\rangle$ span \mathcal{H}_1 . We shall now distinguish three cases.

Case 1. $\{|a_i\rangle\}$ contains two o.n. bases of \mathcal{H}_1 .

Without any loss of generality we may assume that $|a_2\rangle = |a_1^{\perp}\rangle$, $|a_4\rangle = |a_3^{\perp}\rangle$ and either $|a_5\rangle \neq |a_j\rangle$ for j < 5 or $|a_5\rangle = |a_4\rangle$. Since the $|a_j, \psi_j\rangle$ are pairwise orthogonal, we have $|\psi_3\rangle \perp |\psi_1\rangle, |\psi_2\rangle$. By using Lemma 6, one can verify that $\{|\psi_1\rangle, |\psi_3\rangle\}^{\perp}$ has an o.n. basis consisting of product vectors. Consequently, $\alpha := |\psi_1\rangle\langle\psi_1| + |\psi_3\rangle\langle\psi_3|$ is an (n-1)-partite PPT state of rank two. By [8, Lemma 11] it is separable of length two. The same is true for $\beta := |\psi_2\rangle\langle\psi_2| + |\psi_3\rangle\langle\psi_3|$, and so we have

$$\alpha = |b_2, \dots, b_n\rangle\langle b_2, \dots, b_n| + |c_2, \dots, c_n\rangle\langle c_2, \dots, c_n|,$$

$$\beta = |d_2, \dots, d_n\rangle\langle d_2, \dots, d_n| + |e_2, \dots, e_n\rangle\langle e_2, \dots, e_n|(7)$$

where $|b_2, \ldots, b_n\rangle \perp |c_2, \ldots, c_n\rangle$ and $|d_2, \ldots, d_n\rangle \perp |e_2, \ldots, e_n\rangle$ are unit vectors. Hence

$$|\psi_1\rangle, |\psi_3\rangle \in \operatorname{span}\{|b_2, \dots, b_n\rangle, |c_2, \dots, c_n\rangle\},$$

 $|\psi_2\rangle, |\psi_3\rangle \in \operatorname{span}\{|d_2, \dots, d_n\rangle, |e_2, \dots, e_n\rangle\}.$ (8)

By permuting the last n-1 qubits, we may assume that for some $m \geq 2$ we have $|b_j\rangle \neq |c_j\rangle$ for $2 \leq j \leq m$ and $|b_j\rangle = |c_j\rangle$ for j > m. As no $|\psi_j\rangle$ is a product vector, it follows from (8) that m > 2.

Suppose that m > 3. Then Lemma 5 implies that the sets $\{|b_2, \ldots, b_n\rangle, |c_2, \ldots, c_n\rangle\}$ and $\{|d_2, \ldots, d_n\rangle, |e_2, \ldots, e_n\rangle\}$ are the same (up to phase factors). It follows that the vectors $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle$ belong to the same 2-dimensional subspace, and since $|\psi_3\rangle \perp |\psi_1\rangle, |\psi_2\rangle$ we deduce that $|\psi_1\rangle = |\psi_2\rangle$. Since $|a_1, \psi_1\rangle$ and $|a_2, \psi_2\rangle = |a_1^{\perp}, \psi_1\rangle$ belong to $\mathcal{R}(\rho)$, so does $|a_3, \psi_1\rangle$. Since also $|a_3, \psi_3\rangle \in \mathcal{R}(\rho)$, we deduce that $|a_3, b_2, \ldots, b_n\rangle \in \mathcal{R}(\rho)$. This contradicts the assumption that \mathcal{U} is a UPB.

Hence, we must have m=3 and so

$$|b_4,\ldots,b_n\rangle = |c_4,\ldots,c_n\rangle = |d_4,\ldots,d_n\rangle = |e_4,\ldots,e_n\rangle.$$
(9

As mentioned earlier, we have to consider two possibilities for $|\psi_5\rangle$.

The first one is that $|a_5\rangle \neq |a_j\rangle$ for j < 5. By using Lemma 6, one can verify that the subspace $\{|\psi_1\rangle, |\psi_3\rangle, |\psi_5\rangle\}^{\perp}$ of \mathcal{H}' has an o.n. basis consisting of product vectors. As the vectors $|a_j, \psi_j\rangle$ are mutually orthogonal, we have $|\psi_5\rangle \perp |\psi_1\rangle, |\psi_3\rangle$. Hence, by adjoining the product vectors $|b_2, \ldots, b_n\rangle$ and $|c_2, \ldots, c_n\rangle$ to the above mentioned o.n. basis, we obtain an o.n. basis for the hyperplane of \mathcal{H}' orthogonal to $|\psi_5\rangle$. As $|\psi_5\rangle$ is not a product vector and \mathcal{H}' has no UPBs of cardinality $2^{n-1} - 1$, we have a contradiction.

The second possibility is that $|a_5\rangle = |a_4\rangle$. As the vectors $|a_j,\psi_j\rangle$ are mutually orthogonal, the same is true for the vectors $|\psi_1\rangle$, $|\psi_4\rangle$ and $|\psi_5\rangle$. By using Lemma 6, one can verify that the subspace $\{|\psi_1\rangle, |\psi_4\rangle, |\psi_5\rangle\}^{\perp}$ of \mathcal{H}' has an o.n. basis consisting of product vectors. Since $2^{n-1} - k \notin \Theta_{n-1}$ for $k \in \{1, 2, 3\}$, the subspace spanned by $|\psi_1\rangle$, $|\psi_4\rangle$ and $|\psi_5\rangle$ has an o.n. basis consisting of product vectors, say $|p\rangle = |p_2, \dots, p_n\rangle$, $|q\rangle = |q_2, \dots, q_n\rangle$ and $|r\rangle = |r_2, \dots, r_n\rangle$. It follows that there exists an order-3 unitary matrix $[u_{ij}]$ such that

$$|\psi_{1}\rangle = u_{11}|p\rangle + u_{12}|q\rangle + u_{13}|r\rangle,$$

$$|\psi_{4}\rangle = u_{21}|p\rangle + u_{22}|q\rangle + u_{23}|r\rangle,$$

$$|\psi_{5}\rangle = u_{31}|p\rangle + u_{32}|q\rangle + u_{33}|r\rangle.$$
 (10)

By the argument we used above to prove that the $|a_j\rangle$ are not all equal, we can show that there is no j>3 such that $|p_j\rangle=|q_j\rangle=|r_j\rangle=|b_j\rangle$.

If $u_{11} = 0$ then we have $u_{22}u_{33} - u_{23}u_{32} = 0$ and by taking a suitable linear combination of $|a_4, \psi_4\rangle$ and $|a_4, \psi_5\rangle$ we obtain that the product vector $|a_4, p\rangle \in \mathcal{R}(\rho)$, i.e. we have a contradiction. Thus $u_{11} \neq 0$, and similarly

 $u_{12} \neq 0$ and $u_{13} \neq 0$. From the equations (8) and (9) we obtain that

$$|\psi_1\rangle = (\xi|b_2, b_3\rangle + \eta|c_2, c_3\rangle) \otimes |b_4, \dots, b_n\rangle$$

= $u_{11}|p_2, \dots, p_n\rangle + u_{12}|q_2, \dots, q_n\rangle + u_{13}|r_2, \dots, r_n\rangle,$ (11)

where $\xi \eta \neq 0$ and $|b_j\rangle \neq |c_j\rangle$ for j=2,3. Since we have shown that for j>3 at least one of the three unit vectors $|p_j\rangle$, $|q_j\rangle$, $|r_j\rangle$ is not equal to $|b_j\rangle$, the equation (11) implies that at most one of the same three vectors can be equal to $|b_j\rangle$.

We claim that $|p_j\rangle \neq |b_j\rangle$ for j>3. We shall prove it by contradiction. Assume that, say, $|p_n\rangle = |b_n\rangle$. Then the equation (11) implies that $|q_2,\ldots,q_{n-1}\rangle = |r_2,\ldots,r_{n-1}\rangle$ and so

$$|\psi_1\rangle = u_{11}|p_2,\dots,p_n\rangle + |q_2,\dots,q_{n-1}\rangle \otimes (u_{12}|q_n\rangle + u_{13}|r_n\rangle).$$
(12)

From (11) we see that $\langle b_4,\ldots,b_n|\psi_1\rangle=\xi|b_2,b_3\rangle+\eta|c_2,c_3\rangle$ has Schmidt rank 2. From (12) we deduce that also $|p_2,p_3\rangle+|q_2,q_3\rangle$ has Schmidt rank 2. As $\langle b_{n-1}^{\perp}|\psi_1\rangle=0$, from the same equation we obtain that

$$u_{11}\langle b_{n-1}^{\perp}|p_{n-1}\rangle|p_{2},\dots,p_{n-2},p_{n}\rangle + \langle b_{n-1}^{\perp}|q_{n-1}\rangle|q_{2},\dots,q_{n-2}\rangle \otimes (u_{12}|q_{n}\rangle + u_{13}|r_{n}\rangle) = 0.$$

This equation implies that $\langle b_{n-1}^{\perp}|p_{n-1}\rangle = \langle b_{n-1}^{\perp}|q_{n-1}\rangle = 0$ which gives the contradiction: $|p_{n-1}\rangle = |q_{n-1}\rangle = |b_{n-1}\rangle$. Thus our claim is proved.

Let $|\theta\rangle = |\psi_1\rangle - u_{11}|p\rangle$. By switching the tensor factors \mathcal{H}_3 and \mathcal{H}_4 , $|\theta\rangle$ is mapped to

$$\xi|b_2,b_4\rangle\otimes|b_3,b_5,\ldots,b_n\rangle+\eta|c_2,b_4\rangle\otimes|c_3,b_5,\ldots,b_n\rangle$$

 $-u_{11}|p_2,p_4\rangle\otimes|p_3,p_5,\ldots,p_n\rangle.$

The three first tensor factors, namely $|b_2, b_4\rangle$, $|c_2, b_4\rangle$ and $|p_2, p_4\rangle$, are linearly independent and the same holds true for the second tensor factors. It follows that $|\theta\rangle$ considered as bipartite tensor has tensor rank 3. Now the equation (11) gives a contradiction.

Case 2. $\{|a_j\rangle\}$ contains only one o.n. basis of \mathcal{H}_1 . Say, $|a_2\rangle = |a_1^{\perp}\rangle$. We have $\rho = |a_1\rangle\langle a_1| \otimes \alpha + |a_1^{\perp}\rangle\langle a_1^{\perp}| \otimes \beta + \gamma$, where α is a sum of p terms $|\psi_i\rangle\langle\psi_i|$, β is a sum of q terms $|\psi_j\rangle\langle\psi_j|$, and γ is a sum of q terms $|a_l,\psi_l\rangle\langle a_l,\psi_l|$. We may also assume that $p\leq q$. By using Lemma 6, one can verify that the orthogonal complement in \mathcal{H}' of the set of the $|\psi_i\rangle$ which appear in α has an o.n. basis consisting of product vectors. Hence, $|\alpha\rangle$ is a PPT state of rank $p\leq 2$. By Lemma 4 α is separable. It follows that $\mathcal{R}(\rho)$ contains a product vector and we have a contradiction.

Case 3. $\{|a_i\rangle\}$ contains no o.n. basis of \mathcal{H}_1 .

We may assume that $|a_i\rangle = |a_1\rangle$ for $i \leq p$ and $|a_j\rangle \neq |a_1\rangle$ for j > p. Let $V \subseteq \mathcal{H}'$ be the subspace spanned by the $|\psi_i\rangle$ for $i \leq p$. By the same argument as in case 2, the subspace $V^{\perp} \subseteq \mathcal{H}'$ has an o.n. basis consisting of product vectors. Note that $p \notin \Theta_{n-1}$. This is clear

when p < 5 and it is true for p = 5 by our choice of n. Consequently V contains a product vector, say $|\phi\rangle$. Then $|a_1,\phi\rangle$ is a product vector in $\mathcal{R}(\rho)$ and we have a contradiction.

This completes the proof.

Let ρ be an n-qubit PPTES of rank five. Since any 3-qubit subspace of dimension five contains a product vector, we must have n>3. Theorem 9 shows that $\ker \rho$ is not spanned by a UPB. However $\mathcal{R}(\rho)$ may contain a product vector. Indeed we have shown that this is the case for the PPTESs mentioned below Lemma 8. If such ρ exists for n=4 then $\rho\otimes |a\rangle\langle a|$, with $|a\rangle$ a product vector, would be also a multiqubit PPTES of rank five whose range contains no product vectors. Intuitively we believe that

Conjecture 10 The range of any multiqubit PPTES of rank five contains a nonzero product vector.

Note that this conjecture is stronger than Theorem 9.

IV. CONCLUSIONS

The problem of constructing UPBs in multipartite quantum systems, which is more than 15 years old, is still of interest due to its role in various applications such as those mentioned in the Introduction. Some important advances in the case of multiqubit systems have been

made recently regarding the cardinalities of UPBs in such systems. For instance the minimal size of the n-qubit UPB is known for all n. Recall that Θ_n denotes the set of sizes of the UPBs of the n-qubit system. In this paper we have proved, see Theorem 9, that $2^n - 5 \notin \Theta_n$ for any n. In particular, $27 \notin \Theta_5$, $59 \notin \Theta_6$, and $123 \notin \Theta_7$. This gives a partial answer to a question raised in [12]. We propose a conjecture about multiqubit entangled PPT states of rank 5, Conjecture 10.

Let us also point out that the improper UPBs (known as OPBs) of n-qubit systems, i.e. those of cardinality 2^n , can be studied by using special combinatorial matrices of size $2^n \times n$ as in our paper [7]. With some minor modifications, the same combinatorial technique is applicable to the study of proper UPBs.

ACKNOWLEDGEMENTS

LC was supported by Beijing Natural Science Foundation (4173076), the NNSF of China (Grant No. 11501024), and the Fundamental Research Funds for the Central Universities (Grant Nos. KG12001101, ZG216S1760 and ZG226S17J6). The second author was supported in part by the National Sciences and Engineering Research Council (NSERC) of Canada Discovery Grant 5285.

- N. Alon and L. Lovsz, Unextendible product bases. J. Combinatorial Theory, Ser. A, 95:169179, 2001.
- [2] K. Feng. Unextendible product bases and 1-factorization of complete graphs. Discrete Appl. Math., 154:942949, 2006
- [3] C. H. Bennett, D. P. DiVincenzo, T. Mor, P. W. Shor, J. A. Smolin, and B. M. Terhal, Unextendible product bases and bound entanglement, Phys. Rev. Lett.82, 5385 (1999).
- [4] D. P. DiVincenzo, T. Mor, P. W. Shor, J. A. Smolin, and B. M. Terhal, Unextendible product bases, uncompletable product bases and bound entanglement, Commun. Math. Phys. 238, 379-410 (2003).
- [5] S. B. Bravyi, Unextendible Product Bases and Locally Unconvertible Bound Entangled States, Quantum Information Processing, 3, 309 (2004).
- [6] L. Chen and D. Ž. Đoković, Description of rank four entangled states of two qutrits having positive partial transpose, J. Math. Phys., 52, 122203 (2011).
- [7] L. Chen and D. Ž. Đoković, Orthogonal product bases of four qubits, quant-ph/1606.06254 (2016).
- [8] L. Chen and D. Ž. Đoković, Separability problem for multipartite states of rank at most 4, J. Phys. A. Math. Theor. 46, 275304 (2013).
- [9] L. Chen and D. Ž. Đoković, Qubit-qudit states with positive partial transpose, Phys. Rev. A 86, 062332 (2012).
- [10] Y. Feng and Y. Shi, Characterizing locally indistinguishable orthogonal product states, IEEE Trans. Inform.

- Theory 55 (2009).
- [11] N. Johnston, The minimum size of qubit unextendible product bases. In Proceedings of the 8th Conference on the Theory of Quantum Computation, Communication and Cryptography (TQC) (2013).
- [12] N. Johnston, The structure of qubit unextendible product bases, J. Phys. A. Math. Theor. 47, 424034 (2014).
- [13] N. Johnston, 2014, Complete characterization of all unextendible product bases on 4 qubits www.njohnston.ca/4qubitupbs.txt
- [14] Jianxin Chen and Nathaniel Johnston, The Minimum Size of Unextendible Product Bases in the Bipartite Case (and Some Multipartite Cases), Commun. Math. Phys. **333**, 351-365 (2015).
- [15] B. Kraus, J. İ. Cirac, S. Karnas, and M. Lewenstein, Phys. Rev. A 61, 062302 (2000).
- [16] J. Tura, R. Augusiak, P. Hyllus, M. Kus, J. Samsonowicz, M. Lewenstein, Four-qubit entangled symmetric states with positive partial transpositions, Phys. Rev. A 85, 060302 (2012).
- [17] Otfried Guhne, and Michael Seevinck, Separability criteria for genuine multiparticle entanglement, New J. Phys. 12, 053002 (2010).
- [18] Kyung Hoon Han and Seung-Hyeok Kye, Construction of multi-qubit optimal genuine entanglement witnesses, J. Phys. A 49, 175303 (2016).
- [19] Joseph B. Kruskal, Three-way arrays: rank and uniqueness of of trilinear decompositions, with application to

- arithmetic complexity and statistics, Linear Algebra and Appl. ${\bf 18}~(1977),$ no. 2, 95-138.
- [20] J.M. Landsberg, Tensors: Geometry and Applications, Amer. Math. Society, Graduate Studies in Mathematics v. 128, 2012.
- [21] R. Augusiak, T. Fritz, M. Kotowski, M. Kotowski, M. Pawlowski, M. Lewenstein, and A. Acin. Tight bell inequalities with no quantum violation from qubit unextendible product bases. Phys. Rev. A, 8, 042113 (2012).
- [22] C. H. Bennett, D. P. DiVincenzo, C. A. Fuchs, T. Mor, E. Rains, P. W. Shor, J. A. Smolin and W. K. Wootters, Quantum nonlocality without entanglement, Phys. Rev. A, 59, 1070 (1999).