# Graph-theoretic characterization of unextendible product bases

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Unextendible product bases (UPBs) play a key role in the study of quantum entanglement and nonlocality. Here we provide an equivalent characterization of UPBs in graph-theoretic terms. Different from previous graph-theoretic investigations of UPBs, which focused mostly on the orthogonality relations between different product states, our characterization includes a graph-theoretic reformulation of the unextendibility condition. Building on this characterization, we develop a constructive method for building UPBs in low dimensions and shed light on the open question of whether there exist genuinely unextendible product bases (GUPBs), that is, multipartite product bases that are unextendible with respect to every possible bipartition. We derive a lower bound on the size of any candidate GUPB, significantly improving over the state of the art. Moreover, we show that every minimal GUPB saturating our bound must be associated to regular graphs and discuss a possible path towards the construction of a minimal GUPB in a tripartite system of minimal local dimension. Finally, we apply our characterization to the problem of distinguishing UPB states under local operations and classical communication, deriving a necessary condition for reliable discrimination in the asymptotic limit.

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## I. INTRODUCTION

An important notion in the study of quantum entanglement and nonlocality is the notion of unextendible product basis (UPB) [1]. Mathematically, a UPB is a set of orthogonal product vectors whose complementary subspace contains no product vector [1]. UPBs have a number of properties that make them important in quantum information and quantum foundations. For example, the complementary subspace of a UPB is a completely entangled subspace, that is, a subspace containing only entangled states [2–4]. The normalized projector on the complementary subspace of a UPB is a bound entangled state, that is, a state from which no pure entanglement can be distilled [1,5]. UPBs also play a central role in the study of Bell inequalities with no quantum violation [6–9], where they offer insights into the foundations of quantum theory.

The construction and characterization of UPBs has attracted great attention over the past two decades [5,10–21]. A famous open question in the field is whether there exists a multipartite UPB that is a UPB with respect to every possible bipartition. Such a UPB is called a *genuinely unextendible product basis (GUPB)* [22] and its complementary subspace is a genuinely entangled subspace, that is, a subspace that contains only genuinely entangled states [2,22,23].

Sets of orthogonal product states that cannot be completed to full product bases in every bipartion were found in Ref. [24]. However, these sets do not provide examples of GUPBs, because noncompletability to a full product basis for the whole Hilbert space is a weaker property than nonextendibility to a larger set of orthogonal product states. A universal construction for genuinely entangled subspaces was given in [25]. However, determining whether the orthogonal complement of such subspaces admits a product basis and, in the affirmative case, constructing the product basis is highly nontrivial. For these reasons, the existence of GUPBs is still an open question.

Recently, Demianowicz gave a lower bound on size that GUPBs must have, if they exist [26]: for an $N$-partite GUPB in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ the number of vectors in the basis, denoted by $k$, must satisfy the bound

$$k \geqslant \frac{D}{d_{\max}} + \left\lfloor \frac{\frac{D}{d_{\max}} - 2}{N-1} \right\rfloor + 1, \tag{1}$$

where $D := d_1 d_2 \cdots d_N$ and $d_{\max} := \max\{d_1, d_2, \ldots, d_N\}$ (here and in the rest of the paper, we always assume the condition $d_m \geqslant 3$ for every $m \in \{1, \ldots, N\}$ because no bipartite

UPB—and therefore no GUPB—exists when one of the local dimensions is smaller than 3 [1,5]).

In this paper, we provide a graph-theoretic characterization of UPBs and GUPBs. Similarly to previous graph-theoretic investigations of UPBs [10–14], our characterization uses the notion of orthogonality graph [27], a central notion in classical and quantum information theory [28–36]. While the previous works mostly focused on the orthogonality relations between different basis vectors, our work also includes a graph-theoretic characterization of the unextendibility condition. This characterization translates directly into a constructive method for building UPBs, which we illustrate by building a new UPB for a two-qubits and two-qutrits quantum system. For GUPBs, the characterization implies a new lower bound, which significantly improves over the state of the art. Specifically, we show that the size of a GUPB in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ is lower bounded as

$$k \geqslant \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N - 1}. \tag{2}$$

In general, the estimate of $k$ provided by Eq. (2) is always larger than or equal to the estimate of $k$ provided by Eq. (1). The difference between the two bounds becomes visible when the component systems have different local dimensions. For example, consider a tripartite system where the component systems have local dimensions $d_1 = d_2 = 2p$ and $d_3 = 3p$ for some integer $p$. In this case, bounds (1) and (2) read $k \geqslant 6p^2$ and $k \geqslant 8p^2$, respectively, and the difference between them becomes arbitrarily large as $p$ increases.

The connection between UPBs/GUPBs and orthogonality graphs also implies other constraints on the structure of UPBs/GUPBs. In particular, we show that minimal UPBs saturating a bound by Bennett *et al.* [1] must necessarily correspond to regular graphs and we show that the same holds for minimal GUPBs saturating our bound (2). Finally, we use the regularity condition to discuss a possible path to the construction of a minimal GUPB in a tripartite quantum system of minimal local dimension.

An important property of UPBs is that they consist of product states that cannot be perfectly distinguished using local operations and classical communication (LOCC), a phenomenon that has become known as *quantum nonlocality without entanglement* [1,37] and has been recently shown to admit a device-independent certification [38]. Asymptotic LOCC is the topological closure of LOCC [39], which means that an error is allowed but must vanish in the limit of an infinite number of rounds. Using our characterization of UPBs, we provide a necessary condition for perfect discrimination of UPBs with asymptotic LOCC and show that certain UPBs cannot be perfectly discriminated even within asymptotic LOCC.

The rest of this paper is organized as follows. In Sec. II, we review the concepts of UPBs, GUPBs, and orthogonality graphs. In Sec. III, we establish a connection between UPBs and orthogonality graphs and derive upper and lower bounds on the degrees of vertices of the orthogonality graphs associated to UPBs. In Sec. IV, we derive Eq. (2) and discuss its relations with other bounds on the size of GUPBs. In Sec. V, we provide an improved bound valid for certain local dimensions. In Sec. VI, we show that minimal GUPBs saturating the bound (2) should be associated to regular graphs and we use this result to discuss a possible route to construct a minimal GUPB. In Sec. VII, we give an efficient necessary condition for perfect discrimination of UPBs within asymptotic LOCC. Finally, the conclusions are provided in Sec. VIII.

## II. PRELIMINARIES

In this section, we review a few basic facts about notation, unextendible product bases, orthogonality graphs, and orthogonal representations.

*Notation.* In this paper, the number of vectors in a UPB will always be denoted by $k$ and will be called the *size* of the UPB. The total dimension of the space $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ will always be denoted by $D := d_1 d_2 \cdots d_N$. Moreover, we will assume that the local dimensions are listed in nondecreasing order, namely $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_N$. Finally, we will often work with unnormalized product states, which simplifies some of the expressions.

*Unextendible product bases.* Let us start from the mathematical definition.

*Definition 1.* A set of orthogonal product states $\mathcal{U} = \{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}\cdots|\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^{k} \subset \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ is an unextendible product basis (UPB) if the orthogonal complement of $\mathsf{Span}\{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}\cdots|\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^{k}$ has nonzero dimension and contains no product state. A UPB is called a genuinely unextendible product basis (GUPB) if it is a UPB with respect to every possible bipartition of the tensor product $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$.

A well-known result about bipartite UPBs is that they can only exist if the local dimensions are strictly larger than 2 [1,5]: in other words, there is no UPB for bipartite systems of the form $\mathbb{C}^2 \otimes \mathbb{C}^n$ or of the form $\mathbb{C}^n \otimes \mathbb{C}^2$, for some $n \geqslant 2$.

In the multipartite case, it is important to stress that the notion of GUPB is much stronger than the notion of multipartite UPB. A multipartite UPB cannot be extended by any vector of the fully product form $|\psi_1\rangle_{A_1}|\psi_2\rangle_{A_2}\cdots|\psi_N\rangle_{A_N}$, where $|\psi_m\rangle_{A_m}$ is a state of subsystem $A_m$. In contrast, a GUPB cannot even be extended by vectors of the form $|\Psi_1\rangle_{S_1} \otimes |\Psi_2\rangle_{S_2}$, where $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are (possibly entangled) states of the quantum systems associated to a partition of the composite system $A_1 \cdots A_N$ into two disjoint parts $S_1$ and $S_2$.

The fact that no bipartite UPB can exist with local dimensions smaller than 3 implies that an $N$-partite GUPB can only exist if

$$d_m \geqslant 3, \quad \forall m \in \{1, \ldots, N\}. \tag{3}$$

Another important type of constraint on multipartite UPBs and GUPBs concerns their size. A first bound was provided by Bennett *et al.* [1], who showed that the size of a multipartite UPB is lower bounded as

$$k \geqslant \sum_{m=1}^{N} (d_m - 1) + 1. \tag{4}$$

Later, Alon and Lovász [10] showed that the above inequality holds with the ">" sign if at least one of the dimensions $(d_m)_{m=1}^{N}$ is even and the sum $\sum_{m=1}^{N}(d_m - 1) + 1$ is odd. Applying the above bounds to the bipartition $(A_1|A_2 \cdots A_N)$

yields the following bounds on the size of GUPBs [26]:

$$k \geqslant \begin{cases} d_1 + \frac{D}{d_1}, & \text{if } d_1 \text{ and } \frac{D}{d_1} \text{ are even,} \\ d_1 + \frac{D}{d_1} - 1, & \text{otherwise.} \end{cases} \tag{5}$$

In the rest of the paper, we will call a lower bound *nontrivial* if it improves over Eq. (5) for some values of $N$ and of the local dimensions. An example of a nontrivial lower bound is Demianowicz's bound (1) in the case when $(N-1)d_N < N\, d_1$ and when certain conditions on the local dimensions are satisfied [26]. Another example of a nontrivial lower bound is our bound (2), which is nontrivial for a larger set of values of the local dimensions.

*Orthogonality graphs.* An undirected simple graph $G = (V, E)$ is an ordered pair consisting of a set $V$ of vertices and a set $E$ of edges, which is an irreflexive, symmetric relation on $V$. A vertex $u$ is a neighbor of a vertex $v$ if $u$ and $v$ are adjacent, namely $(u, v) \in E$. The neighborhood $N_G(v)$ of a vertex $v$ is the set of all neighbors of $v$. The degree $\deg_G(v)$ is the number of vertices in the neighborhood $N_G(v)$, i.e., $\deg_G(v) = |N_G(v)|$. If the degree of each vertex is $k$, the graph is called $k$-regular. A complete graph $K_n$ is an $(n-1)$-regular graph with $n$ vertices, that is, a graph in which every two different vertices are connected. For two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, the union of graphs $G_1$ and $G_2$ is the graph $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$.

The *orthogonality graph* of a set of vectors $\{|\varphi^{(1)}\rangle, \ldots, |\varphi^{(k)}\rangle\} \subset \mathbb{C}^d$ is the graph $G = (V, E)$ with vertex set $V = \{v_1, \ldots, v_k\}$ and edge set $E = \{(v_i, v_j) \mid \langle\varphi^{(i)}|\varphi^{(j)}\rangle = 0\}$.

A connection between UPBs and orthogonality graphs was made by Alon and Lovász in Ref. [10], where it was used to prove existence results about minimal UPBs satisfying Bennett *el al.'s* bound (4). We now introduce a new definition that will allow us to provide an if and only if characterization of UPBs in terms of orthogonality graphs.

*Definition 2.* Let $G = (V, E)$ be the orthogonality graph of the set $\{|\varphi^{(1)}\rangle, \ldots, |\varphi^{(k)}\rangle\} \subset \mathbb{C}^d$ and let $W \subseteq V$ be a subset of the vertices. We say that the subset $W$ is *saturated* if the corresponding vectors $\{|\varphi^{(i)}\rangle \mid v_i \in W\}$ span the whole space $\mathbb{C}^d$. Otherwise, we call the set $W$ *unsaturated.*

For a set of $N$-partite product vectors $\{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2} \cdots |\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k$ in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$, one can define $N$ orthogonality graphs.

*Definition 3.* Let $\{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2} \cdots |\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k$ in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ be a set of $N$-partite product vectors. For $m \in \{1, \ldots, N\}$, the orthogonality graph $G_m = (V, E_m)$ is the graph with vertex set $V = \{v_1, v_2, \ldots, v_k\}$ and edge set $E_m = \{(v_i, v_j) \mid \langle\varphi_m^{(i)}|\varphi_m^{(j)}\rangle_{A_m} = 0\}$.

Note that all the graphs $G_m$ have the same vertex set and (generally) different edges due to the (generally) different orthogonality relations between the vectors in different subsystems.

We now give a necessary and sufficient condition, formulated in terms of orthogonality graphs, for a set of product states to be a UPB.

*Lemma 1.* Let $\mathcal{U}$ be a set of $k$ product vectors in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ and let $(G_m)_{m=1}^N$ be the corresponding orthogonality graphs. The set $\mathcal{U}$ is a UPB if and only if the following conditions hold.

(i) $\bigcup_{m=1}^N G_m = K_k$.

(ii) $\bigcup_{m=1}^N W_m \neq V$ for every $N$-tuple $(W_1, W_2, \ldots, W_N)$ in which $W_m$ is an unsaturated set for $G_m$ for every $m \in \{1, \ldots, N\}$.

The proof of Lemma 1 is provided in Appendix A. To illustrate the lemma, we consider the following example.

*Example 1.* The following product vectors form a UPB in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^3$:

$$\begin{aligned}
|\psi_1\rangle &= |0\rangle_{A_1}|0\rangle_{A_2}|0\rangle_{A_3}|0\rangle_{A_4}, \\
|\psi_2\rangle &= (|0\rangle + |1\rangle)_{A_1}(|0\rangle + |1\rangle)_{A_2}(|0\rangle + |1\rangle)_{A_3}|1\rangle_{A_4}, \\
|\psi_3\rangle &= (|0\rangle + 2|1\rangle)_{A_1}(|0\rangle + 2|1\rangle)_{A_2}(|0\rangle + 2|1\rangle)_{A_3}|2\rangle_{A_4}, \\
|\psi_4\rangle &= |1\rangle_{A_1}(2|0\rangle - |1\rangle)_{A_2}(|0\rangle - |1\rangle)_{A_3}(|0\rangle + |1\rangle + |2\rangle)_{A_4}, \\
|\psi_5\rangle &= (|0\rangle - |1\rangle)_{A_1}|1\rangle_{A_2}(2|0\rangle - |1\rangle)_{A_3}(|0\rangle + 2|1\rangle - 3|2\rangle)_{A_4}, \\
|\psi_6\rangle &= (2|0\rangle - |1\rangle)_{A_1}(|0\rangle - |1\rangle)_{A_2}|1\rangle_{A_3}(5|0\rangle - 4|1\rangle - |2\rangle)_{A_4}.
\end{aligned} \tag{6}$$

The UPB $\{|\psi_i\rangle\}_{i=1}^6$ has the minimum size compatible with Bennett *et al.*'s bound (4), which in this case reads $k \geqslant \sum_{m=1}^4 (d_m - 1) + 1 = 6$.

*Analysis of Example 1.* For the vectors in Example 1, the orthogonality graphs $(G_m)_{m=1}^4$ and their common vertex set are shown in Fig. 1. It is then easy to check that the union of the graphs $(G_m)_{m=1}^4$ is the complete graph $K_6$. Hence the first condition in Lemma 1 is satisfied. Regarding the second condition, note that every two vectors in the set $\{|0\rangle, (|0\rangle + |1\rangle), (|0\rangle + 2|1\rangle), |1\rangle, (|0\rangle - |1\rangle), (2|0\rangle - |1\rangle)\} \subset \mathbb{C}^2$ are linearly independent and therefore form a basis for $\mathbb{C}^2$. Hence the size of any unsaturated set $W_m$ in $G_m$ can be at most 1 for every $m \in [1, 3]$. Similarly, since any three vectors in the set $\{|0\rangle, |1\rangle, |2\rangle, (|0\rangle + |1\rangle + |2\rangle), (|0\rangle + 2|1\rangle - 3|2\rangle), (5|0\rangle - 4|1\rangle - |2\rangle)\} \subset \mathbb{C}^3$ are linearly independent, the size of any unsaturated set $W_4$ in $G_4$ is at most 2. Putting everything together, we obtain that the union of any four unsaturated sets $(W_m)_{m=1}^4$ cannot contain all vertices in $V$. Since both conditions in Lemma 1 are satisfied, we conclude that the vectors $\{|\psi_i\rangle\}_{i=1}^6$ form a UPB.

Lemma 1 also implies an upper bound on the number of elements in the unsaturated sets associated to a UPB.

*Lemma 2.* Let $(G_m)_{m=1}^N$ be the orthogonality graphs associated to a UPB of size $k$. Then, the size of any unsaturated set $W_m$ in $G_m$ is upper bounded as

$$|W_m| \leqslant k - 1 - \sum_{i \in \{1,\ldots,N\} \setminus \{m\}} (d_i - 1). \tag{7}$$

The proof is provided in Appendix A.

*Orthogonal representations of a graph.* An *orthogonal representation* [27] of a graph $G = (V, E)$ in dimension $d$ is a set of $k = |V|$ vectors $\{|\varphi^{(1)}\rangle, \ldots, |\varphi^{(k)}\rangle\} \subset \mathbb{C}^d$ such that $\langle\varphi^{(i)}|\varphi^{(j)}\rangle = 0$ for every pair of adjacent vertices $v_i$ and $v_j$. The representation is called *faithful* if $\langle\varphi^{(i)}|\varphi^{(j)}\rangle = 0$ only if $v_i$ and $v_j$ are adjacent.

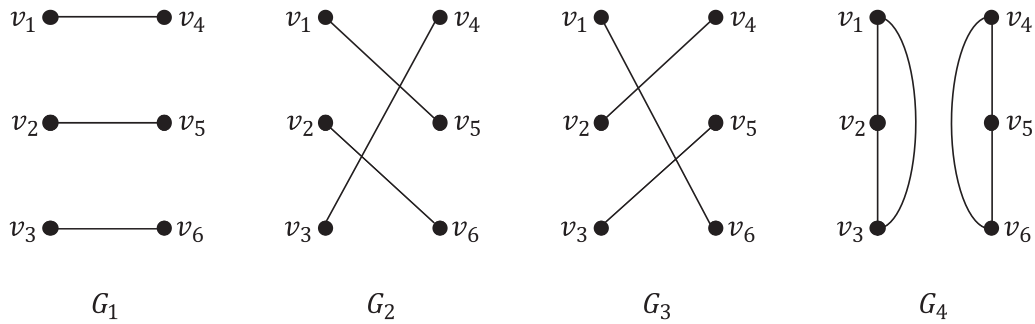


FIG. 1. Orthogonality graphs of the UPB in Example 1.

One way to search for an orthogonal representation of a given graph is to solve the following optimization problem:

$$\text{minimize} \sum_{(v_i,v_j)\in E} |\langle\varphi^{(i)}|\varphi^{(j)}\rangle|$$
$$\text{subject to } \langle\psi|\varphi^{(i)}\rangle = 1, \quad \forall i = 1,\dots,k, \tag{8}$$

where $|\varphi^{(i)}\rangle$ are variable vectors and $|\psi\rangle$ is an arbitrarily chosen nonzero constant vector. Here, the constraint (8) ensures that every $|\varphi^{(i)}\rangle$ is nonzero. This constraint does not restrict the search space of orthogonal representations since, for any given valid orthogonal representation, one can always rotate the vectors globally so that each vector has a nonzero overlap with $|\psi\rangle$ and scale each vector individually to make every overlap be one. In our realization of this algorithm, we fix the first component of each vector $|\varphi^{(i)}\rangle$ to be one, which is equivalent to setting $|\psi\rangle$ to be the unit vector along the first axis. After optimization, if the objective function reaches zero, then the vectors $\{|\varphi^{(i)}\rangle\}_{i=1}^{k}$ satisfy the desired orthogonality relations.

Equation (8) shows that the search for orthogonal representations of a graph is an optimization problem with linear constraints. Various algorithms for this task are known, such as sequential least squares programing [40,41]. Notice that the problem in Eq. (8) is not a convex optimization and therefore optimization algorithms are not guaranteed to find the global minimum. Still, when an algorithm returns the value zero, this value is automatically guaranteed to be the global minimum and the result of the optimization is an orthogonal representation of the given graph. In general, the solution may not be faithful, meaning there may exist vectors $|\varphi^{(i)}\rangle$ and $|\varphi^{(j)}\rangle$ that are orthogonal even if the corresponding vertices $v_i$ and $v_j$ are not adjacent.

Lemma 1 suggests a systematic route to construct UPBs of any desired size $k$ in $\mathbb{C}^{d_1}\otimes\mathbb{C}^{d_2}\otimes\cdots\otimes\mathbb{C}^{d_N}$ as follows.

(1) Decompose the complete graph $K_k$ into $N$ subgraphs $(G_m)_{m=1}^{N}$.

(2) For each $G_m$, find an orthogonal representation in $\mathbb{C}^{d_m}$.

(3) For each arbitrary $N$-tuple $(W_m)_{m=1}^{N}$ of unsaturated sets $W_m$ in $G_m = (V, E_m)$, check that $\bigcup_{m=1}^{N} W_m \neq V$.

The first step, namely the decomposition of the complete graph into subgraphs $(G_m)_{m=1}^{N}$ will be discussed in the next section of the paper. Once a decomposition is given, the second step can be attempted by optimization algorithms that search for an orthogonal representation of the graphs $G_m$, as discussed in the previous paragraph. Computationally, this step is the most challenging one. Finally, the third step can be achieved by brute force enumerating all the unsaturated sets of the graphs $G_m$, once the decomposition $(G_m)_{m=1}^{N}$ and an orthogonal representation of the graphs $G_m$ are known. The computational cost of this step is tolerable for instances of the problem where $N$ and $D$ are small. In general, the size of every unsaturated set in $G_m$ is upper bounded by $k-1-\sum_{i\in\{1,\dots,N\}\setminus\{m\}}(d_i-1)$ (by Lemma 2) and further inspection of the structure of the orthogonality graphs $G_m$ and their orthogonal representations can further reduce this number. Hence, as long as the number of systems $N$ and the total dimension $D$ are small, the enumeration of all $N$-tuples of unsaturated sets remains computationally feasible.

To illustrate our method, we construct here a new UPB of size 8 for a two-qubits and two-qutrits system. The basis and its orthogonality graphs are shown in Example 3 in Appendix A. This UPB has the minimum size compatible with Alon and Lovász's bound (4), which in this case reads $\sum_{m=1}^{4}(d_m-1)+1=7$ is odd and at least one of the local dimensions (2,2,3,3) is even.

Later in the paper, we will further discuss the minimal case $N=3$, with $d_1=d_2=d_3=3$. In this case, $k$ can be generally bounded as $7\leqslant k\leqslant 23$ for UPBs and $13\leqslant k\leqslant 23$ for GUPBs [the lower bounds come from Eq. (4) for UPBs and from Eqs. (1) and (2) for GUPBs, while the upper bound comes from the fact that the projector on the span of a UPB is the orthogonal complement of a bound entangled state with positive partial transpose, and no such state can have a rank smaller than 4 [42].

## III. ORTHOGONALITY GRAPHS OF UPBS

In this section, we show that the orthogonality graphs associated to UPBs must satisfy nontrivial conditions on the degree of their vertices. In particular, we show that every minimal UPB saturating Bennett *et al.*'s bound (4) must correspond to regular graphs.

*Lemma 3.* For every UPB in $\mathbb{C}^{d_1}\otimes\mathbb{C}^{d_2}\otimes\cdots\otimes\mathbb{C}^{d_N}$, the degrees of the vertices in the orthogonality graphs $(G_m)_{m=1}^{N}$ must satisfy the condition

$$d_m-1\leqslant \deg_{G_m}(v_i)\leqslant k-1-\sum_{i\in\{1,\dots,N\}\setminus\{m\}}(d_i-1),$$
$$\forall v_i\in V,\quad \forall m\in\{1,\dots,N\}. \tag{9}$$

The proof of Lemma 3 is provided in Appendix A.

Our bounds on the degrees of the vertices are satisfied with the equality sign when the UPB has the minimal size compatible with Bennett *et al.*'s bound (4) as follows.

*Proposition 1.* For a minimal UPB saturating Bennett *et al.*'s bound (4), the orthogonality graph $G_m$ is a $(d_m - 1)$-regular graph for every $m \in \{1, \ldots, N\}$.

An example of this situation is Example 1. There, $G_i$ is a 1-regular graph for $1 \leqslant i \leqslant 3$ and $G_4$ is a 2-regular graph.

Since regularity is a strong graph-theoretic property, Proposition 1 establishes strong constraint on every minimal UPB saturating Bennett *et al.*'s bound. In the next section, we build on the connection with orthogonality graphs to derive the bound (2) on the size of candidate GUPBs. Later in the paper, we will show that the bound (2) plays for GUPBs a similar role as Bennett *et al.*'s bound for UPBs: as we will show, every minimal GUPB saturating bound (2) must be associated to regular orthogonality graphs.

## IV. BOUND ON THE GUPB SIZE

In this section, we derive the bound (2) and discuss its relations with other bounds on the size of GUPBs.

*Theorem 1.* Every GUPB in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ must satisfy the bound (2) or equivalently

$$k \geqslant \left\lceil \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N-1} \right\rceil. \tag{10}$$

*Proof.* Let us assume there exists a GUPB $\mathcal{U}$ in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$. Since $\mathcal{U}$ is a UPB with respect to the bipartition $A_m \mid \{A_1 A_2 \cdots A_N\} \setminus \{A_m\}$ for $1 \leqslant m \leqslant N$, Lemma 3 implies that the degree of every vertex $v_i$ of $G_m$ satisfies the condition

$$\deg_{G_m}(v_i) \leqslant k - 1 - \left(\frac{D}{d_m} - 1\right) = k - \frac{D}{d_m}. \tag{11}$$

Now, Lemma 1 tells us that the union of the graphs $(G_m)_{m=1}^N$ is the complete graph $K_k$. Since the complete graph $K_k$ is $(k-1)$ regular, we have the bound

$$\sum_{m=1}^{N} \deg_{G_m}(v_i) \geqslant k - 1. \tag{12}$$

Combining Eqs. (11) and (12), we then obtain the relation

$$\sum_{m=1}^{N} \left(k - \frac{D}{d_m}\right) \geqslant k - 1, \tag{13}$$

which implies the desired bound

$$k \geqslant \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N-1}. \tag{14}$$

Since $k$ is (by definition) an integer, the bound also holds with the ceiling sign, as in Eq. (10). ■

Our lower bound coincides with Demianowicz's bound (1) when the local dimensions are all equal, i.e., if $d_m = d, \forall m \in \{1, \ldots, N\}$. In general, however, our bound is strictly more accurate, as shown in the following proposition.

*Proposition 2.* The right-hand side (RHS) of Eq. (10) is always larger than or equal to the RHS of Eq. (1).

TABLE I. Comparison among three lower bounds on the GUPB size for different values of the local dimensions.

| Local dimensions | Bound (1) [26] | Bound (5) [1,10,26] | Our bound (2) |
|---|---|---|---|
| (3,3,4) | 13 | 14 | 16 |
| (3,3,5) | 13 | 17 | 19 |
| (3,3,3,4) | 36 | 38 | 45 |
| (3,3,4,4) | 48 | 50 | 56 |
| (3,3,3,3,4) | 101 | 110 | 128 |
| (3,3,3,4,4) | 135 | 146 | 162 |

The proof of Proposition 2 is provided in Appendix B.

Another benefit of the new bound (2) is that it provides a nontrivial lower bound in new cases, including values of the local dimensions for which no previous bound could improve over Eq. (5). Some examples of this situation are illustrated in Table I.

In Ref. [26], Demianowicz showed that Eq. (1) is a nontrivial lower bound if and only if $(N-1)d_{\max} < N d_{\min}$, where $d_{\min} = \min\{d_1, d_2, \ldots, d_N\}$, and the local dimensions satisfy the conditions $(d_1, d_2, d_3) \neq (2p, 2p, 3p-1)$ and $(d_1, d_2, d_3) \neq (2p-1, \tilde{d}, 3p-2)$ for every integer $p \geqslant 2$ and every integer $\tilde{d}$ satisfying $2p - 1 \leqslant \tilde{d} \leqslant 3p - 2$. In contrast, we now show that our lower bound (2) remains nontrivial even when the local dimensions are of the form $(d_1, d_2, d_3) = (2p, 2p, 3p-1)$ or $(d_1, d_2, d_3) = (2p-1, \tilde{d}, 3p-2)$.

*Proposition 3.* In the tripartite case, the bound (2) is nontrivial when $(d_1, d_2, d_3) = (2p, 2p, 3p-1)$ for some integer $p \geqslant 2$ and when $(d_1, d_2, d_3) = (2p-1, \tilde{d}, 3p-2)$ for some integer $p \geqslant 2$ and some integer $\tilde{d} \in [2p-1, 3p-2]$.

The proof of Proposition 3 is provided in Appendix B.

## V. IMPROVED BOUND UNDER CONDITIONS ON THE LOCAL DIMENSIONS

We now show that our bound (2) can be slightly improved if the local dimensions satisfy certain conditions as follows.

*Proposition 4.* If at least one of the local dimensions $(d_m)_{m=1}^N$ is even and the sum $\sum_{m=1}^{N} \frac{D}{d_m} - 1$ is an odd multiple of $N-1$, then the size of any GUPB in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ is lower bounded as

$$k \geqslant \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N-1} + 1. \tag{15}$$

The proof of Proposition 4 is provided in Appendix B. For example, if $(d_1, d_2, d_3) = (3, 4, 5)$, then $k \geqslant 24$ for a GUPB of size $k$ in $\mathbb{C}^3 \otimes \mathbb{C}^4 \otimes \mathbb{C}^5$ by Proposition 4. Similarly, if $(d_1, d_2, d_3, d_4) = (4, 4, 4, 4)$, then $k \geqslant 86$. This second example can be generalized to all situations in which the number of system $N$ is even and all local dimensions are equal to $N$.

*Corollary 1.* If $N$ is even and $d_m = N$ for every $m \in \{1, \ldots, N\}$, then the minimum size of a GUPB in $(\mathbb{C}^N)^{\otimes N}$ is lower bounded as

$$k \geqslant \frac{N^N - 1}{N-1} + 1. \tag{16}$$

The bound (16) is another example of a nontrivial bound, i.e., of a bound that improves over bound (5). Here the improvement is exponential: for asymptotically large $N$, the difference between the RHS of Eq. (16) and the RHS of Eq. (5) grows as $N^{N-2}$. It is also worth noting that the bound (16) provides also a small improvement over bound (1) in a scenario where all local dimensions are equal.

## VI. ORTHOGONALITY GRAPHS FOR MINIMAL GUPBS

We now derive an analog of Proposition 1 for GUPBs, showing that a certain kind of minimal GUPBs must be associated to regular graphs.

*Proposition 5.* For a minimal GUPB saturating the bound (2), the orthogonality graph $G_m$ is a $(k-\frac{D}{d_m})$-regular graph for every $m \in \{1,\dots,N\}$.

The proof of Proposition 5 is provided in Appendix B. We now use Proposition 5 to put forward a possible approach to construct a GUPB of minimal size and local dimension. Since UPBs do not exist in $\mathbb{C}^2 \otimes \mathbb{C}^n$ [1,5], the minimal setting for a GUPB is a three-qutrits system. By bounds (1) and (2), we know that the size of a candidate GUPB must be at least 13.

Now, Proposition 5 shows that, if there exists a GUPB of size 13 in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$, then each orthogonality graph $G_m$ is a 4-regular graph. We then have the following proposition.

*Proposition 6.* A set of product states $\{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}|\varphi_3^{(i)}\rangle_{A_3}\}_{i=1}^{13}$ in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$ is a GUPB if the following three conditions hold.

(i) $\bigcup_{m=1}^{3} G_m = K_{13}$, where each orthogonality graph $G_m$ is a 4-regular graph.

(ii) The subspace spanned by any five states in $\{|\varphi_m^{(i)}\rangle_{A_m}\}_{i=1}^{13}$ has dimension 3 for any $m = 1, 2, 3$.

(iii) The subspace spanned by any nine states in $\{|\varphi_{j_1}^{(i)}\rangle_{A_{j_1}} \otimes |\varphi_{j_2}^{(i)}\rangle_{A_{j_2}}\}_{i=1}^{13}$ has dimension 9 for any $(j_1, j_2) \in \{(1,2),(1,3),(2,3)\}$.

*Proof.* Immediate from Lemma 1 and the fact that the orthogonality graphs $(G_m)_{m=1}^{3}$ are 4-regular. ■

Proposition 6 provides a possible approach to construct a tripartite GUPB of the minimum local dimension. There are three steps for constructing a GUPB of size 13 in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$:

(1) decompose the complete graph $K_{13}$ into three 4-regular graphs $(G_m)_{m=1}^{3}$;

(2) find an orthogonal representation for each $G_m$ in $\mathbb{C}^3$;

(3) check the conditions (ii) and (iii) of Proposition 6.

We now discuss the possible ways forward and the challenges arising in the above steps. Regarding step (1), there are many ways to decompose $K_{13}$ into three 4-regular graphs. In particular, one can decompose $K_{13}$ into three Cayley graphs [43]. To do this, one has to consider the group of integers modulo 13, $\mathbb{Z}_{13} = \{0, \pm1, \pm2, \pm3, \pm4, \pm5, \pm6\}$. Given a 2-element set $S = \{p, q\}$, where $1 \leqslant p \neq q \leqslant 6$, one can construct the Cayley graph $G^{(S)} = (V, E)$, where $V = \mathbb{Z}_{13}$ and $E = \{(a, b) \mid a - b \in S \cup (-S)\}$. By construction, $G^{(S)}$ is a 4-regular graph. By partitioning the set $\{1, 2, 3, 4, 5, 6\}$ into three 2-element subsets $S_1 = \{p_1, q_1\}$, $S_2 = \{p_2, q_2\}$, and $S_3 = \{p_3, q_3\}$, we then obtain the desired decomposition $K_{13} = \bigcup_{m=1}^{3} G^{(S_m)}$. Note that there are $\frac{\binom{6}{2}\times\binom{4}{2}\times\binom{2}{2}}{3\times2\times1} = 15$ distinct partitions of $\{1, 2, 3, 4, 5, 6\}$ into three 2-element subsets, where $\binom{n}{i}$ is the binomial coefficient. Hence there are 15 distinct decompositions of $K_{13}$ into three Cayley graphs. While step (1) is relatively straightforward, a bottleneck arises in step (2), where one has to find an orthogonal representation of the graphs in the decomposition of $K_{13}$. For each decomposition, our algorithm in Sec. II can find the orthogonal representations of at most two graphs, leaving the third unspecified.

The bottleneck of the orthogonal representations remains even if one replaces the decomposition into Cayley graphs with some other decomposition of $K_{13}$ in terms of regular graphs. To better understand the origin of the problem, we point out that it is not overwhelmingly difficult to find orthogonal representations for all 4-regular graphs with 13 vertices, as the total number of such graphs, up to isomorphism, is 10 880 [44]. However, our algorithm for searching orthogonal representation does not ensure the fulfillment of condition (ii) or (iii) of Proposition 6. By iterating the algorithm on the same graph, one may hope to find orthogonal representations fulfilling condition (ii) by chance. Unfortunately, we did not encounter any such solutions. One way to circumvent the problem would be to translate the condition (ii) into a constraint that has to be satisfied while searching for the orthogonal representation with our algorithm in Sec. II. The problem with this approach is that condition (ii) results in nonlinear constraints, which heavily slow down the convergence of the optimization process. We managed to run the modified algorithm twice on all 4-regular 13-vertex graphs, but did not find any orthogonal representation satisfying condition (ii). Due to these obstacles, finding an example of GUPB through the above route still requires a major investment of computational resources.

## VII. APPLICATION: LOCAL APPROXIMATION FOR PERFECT DISCRIMINATION OF UPBS

In this section, we consider local approximation for perfect discrimination of UPBs. It is known that UPBs cannot be perfectly distinguished under LOCC, which shows the phenomenon of quantum nonlocality without entanglement [5,37]. More generally, some UPBs still cannot be perfectly distinguished by using asymptotic LOCC (denoted by $\overline{\text{LOCC}}$), wherein an error is allowed but must vanish in the limit of an infinite number of rounds [45,46]. $\overline{\text{LOCC}}$ is the topological closure of LOCC and the LOCC class is a proper subset of the $\overline{\text{LOCC}}$ class [39], that is,

$$\text{LOCC} \subsetneq \overline{\text{LOCC}}. \tag{17}$$

Cohen gave a necessary condition for perfect discrimination of orthogonal product states within $\overline{\text{LOCC}}$ [46].

*Lemma 4.* (Ref. [46]). Consider a set of orthogonal product states $\mathcal{S} = \{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}\cdots|\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^{k} \subset \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$. For each party $A_s$, define the subset of all index pairs $J_{A_s} = \{(i,j) \mid \langle\varphi_s^{(i)}|\varphi_s^{(j)}\rangle_{A_s} = 0; \langle\varphi_t^{(i)}|\varphi_t^{(j)}\rangle_{A_t} \neq 0, \forall t \neq s\}$. If for each party $A_s$ the set $\{|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|\}_{(i,j)\in J_{A_s}}$ spans a space of dimension $d_s^2 - 1$, then $\mathcal{S}$ cannot be perfectly discriminated within $\overline{\text{LOCC}}$.

It is not easy to check this condition when the size of the set is large. Next, we transform this condition into another condition.

A positive operator-valued measure (POVM) on $\mathbb{C}^d$ is a set of positive semidefinite operators $\{E_m = M_m^\dagger M_m\}$, which satisfy the completeness relation $\sum_m E_m = \mathbb{I}$, and $\mathbb{I}$ is the identity operator on $\mathbb{C}^d$. Each $E_m$ is called a POVM element. A measurement is *trivial* if all the POVM elements are proportional to the identity operator. Otherwise, it is called nontrivial.

For a set of orthogonal product states $\{|\Psi_i\rangle = |\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}\cdots|\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k \subset \mathbb{C}^{d_1}\otimes\mathbb{C}^{d_2}\otimes\cdots\otimes\mathbb{C}^{d_N}$, a measurement $\{E_m = M_m^\dagger M_m\}$ on party $A_s$ is called an *orthogonality-preserving local measurement* if the postmeasurement states $\{\mathbb{I}_{A_1}\otimes\cdots\otimes\mathbb{I}_{A_{s-1}}\otimes M_m\otimes\mathbb{I}_{A_{s+1}}\otimes\cdots\otimes\mathbb{I}_{A_N}|\Psi_i\rangle\}_{i=1}^k$ keep being mutually orthogonal for each $m$.

*Lemma 5.* Consider an orthogonal set of product states $\{|\Psi_i\rangle = |\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}\cdots|\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k$. For each party $A_s$, the set $\{|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|\}_{(i,j)\in J_{A_s}}$ spans a subspace of dimension $d_s^2 - 1$ if and only if the only orthogonality-preserving local measurements on $A_s$ are trivial.

*Proof.* First, we prove the necessity. Assume an orthogonality-preserving local measurement $\{E_m\}$ is performed on $A_s$ party; then we obtain

$$\begin{aligned}&\langle\Psi_i|\mathbb{I}_{A_1}\otimes\cdots\otimes\mathbb{I}_{A_{s-1}}\otimes E_m\otimes\mathbb{I}_{A_{s+1}}\otimes\cdots\otimes\mathbb{I}_{A_N}|\Psi_j\rangle\\&\quad=\langle\varphi_s^{(i)}|E_m|\varphi_s^{(j)}\rangle_{A_s}\prod_{1\leqslant t\neq s\leqslant N}\langle\varphi_t^{(i)}|\varphi_t^{(j)}\rangle_{A_t}=0,\quad\forall i\neq j.\end{aligned}$$

If $(i, j)\in J_{A_s}$, then

$$\langle\varphi_s^{(i)}|E_m|\varphi_s^{(j)}\rangle_{A_s}=0. \tag{18}$$

We obtain

$$\mathrm{Tr}\left(E_m|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\right)=0,\quad\forall(i,j)\in J_{A_s}. \tag{19}$$

Let $\mathcal{Q}$ be the subspace spanned by the set $\{|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|\}_{(i,j)\in J_{A_s}}$ and $\mathcal{Q}^\perp$ be the orthogonal complement of $\mathcal{Q}$. By Eq. (19), $E_m\in\mathcal{Q}^\perp$. If $E_m$ is proportional to the identity operator, then it must satisfy Eq. (19). Further, since $\mathrm{Dim}(\mathcal{Q}) = d_s^2-1$, then $\mathrm{Dim}(\mathcal{Q}^\perp)=1$, and $E_m$ must be proportional to the identity operator. Thus the only orthogonality-preserving local measurements on party $A_s$ are trivial.

Now we prove the sufficiency by contradiction. Note that $\mathrm{Dim}(\mathcal{Q})\leqslant d_s^2-1$, as the identity operator belongs to $\mathcal{Q}^\perp$. Assume $\mathrm{Dim}(\mathcal{Q})\leqslant d_s^2-2$. Let $\mathcal{P}_\mathbb{C}$ be the subspace spanned by the set of Hermitian matrices $\{|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}| + |\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|, i|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}| - i|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\}_{(i,j)\in J_{A_s}}$, i.e.,

$$\begin{aligned}\mathcal{P}_\mathbb{C}=\Bigg\{&\sum_{(i,j)\in J_{A_s}}a_{i,j}\left(|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|+|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\right)\\&+b_{i,j}\left(i|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|-i|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\right)\mid a_{i,j},b_{i,j}\in\mathbb{C}\Bigg\}.\end{aligned}$$

Since any element of $\{|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|, |\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\}$ is a linear combination of the two Hermitian matrices $\{|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}| + |\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|, i|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}| - i|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\}$, and vice versa, then $\mathcal{P}_\mathbb{C}=\mathcal{Q}$. Further, we define the $R$ subspace

$$\begin{aligned}\mathcal{P}_\mathbb{R}=\Bigg\{&\sum_{(i,j)\in J_{A_s}}a_{i,j}\left(|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|+|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\right)\\&+b_{i,j}\left(i|\varphi_s^{(i)}\rangle_{A_s}\langle\varphi_s^{(j)}|-i|\varphi_s^{(j)}\rangle_{A_s}\langle\varphi_s^{(i)}|\right)\mid a_{i,j},b_{i,j}\in\mathbb{R}\Bigg\}.\end{aligned}$$

Then $\mathcal{P}_\mathbb{R}$ contains only Hermitian matrices and $\mathcal{P}_\mathbb{R}\subset\mathcal{P}_\mathbb{C}$. Assume $\{H_1, H_2, \ldots, H_n\}$ is a linearly independent set in $\mathcal{P}_\mathbb{R}$. Let

$$\sum_{k=1}^n(x_k+iy_k)H_k=0, \tag{20}$$

where $x_k+iy_k\in\mathbb{C}$, $x_k, y_k\in\mathbb{R}$. Taking the Hermitian conjugate on both sides, we have

$$\sum_{k=1}^n(x_k-iy_k)H_k=0. \tag{21}$$

Then by Eqs. (20) and (21), we have $\sum_{k=1}^n x_kH_k=0$ and $\sum_{k=1}^n y_kH_k=0$. This means that $x_k=y_k=0$ and $x_k+iy_k=0$ for any $1\leqslant k\leqslant n$. Thus any linearly independent set in $\mathcal{P}_\mathbb{R}$ is also a linearly independent set $\mathcal{P}_\mathbb{C}$. We obtain

$$\mathrm{Dim}(\mathcal{P}_\mathbb{R})\leqslant\mathrm{Dim}(\mathcal{P}_\mathbb{C})=\mathrm{Dim}(\mathcal{P}_\mathbb{Q})\leqslant d_s^2-2. \tag{22}$$

Since the dimension of subspace consisting of all Hermitian matrices on $\mathbb{C}^{d_s}$ is $d_s^2$, we have $\mathrm{Dim}(\mathcal{P}_\mathbb{R}^\perp)\geqslant 2$. There must exist $E\in\mathcal{P}_\mathbb{R}^\perp$, which is not proportional to the identity matrix. Furthermore, there must exist $c\in\mathbb{R}$ such that each eigenvalue $\lambda$ of $cE$ satisfies $|\lambda|<\frac{1}{2}$. Then $\{\frac{1}{2}\mathbb{I}+cE, \frac{1}{2}\mathbb{I}-cE\}$ is a nontrivial orthogonality-preserving local measurement on $A_s$. ■

Then by using Lemmas 4 and 5, we obtain the following.

*Proposition 7.* Consider a set of orthogonal product states $\mathcal{S}=\{|\varphi_1^{(i)}\rangle_{A_1}|\varphi_2^{(i)}\rangle_{A_2}\cdots|\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k$. For each party $A_s$, if the only orthogonality-preserving local measurements on $A_s$ are trivial, then $\mathcal{S}$ cannot be perfectly discriminated within $\overline{\text{LOCC}}$.

There are a lot of sets of orthogonal product states that cannot be perfectly discriminated within LOCC [47–63] and the main method is to show that the only orthogonality-preserving local measurements on each party are trivial. By Proposition 7, these sets of orthogonal product states cannot be perfectly discriminated within $\overline{\text{LOCC}}$ either.

Cohen showed that, when $\sum_{m=1}^N(d_m-1)+1\geqslant 2d_{\max}-1$, the UPB with the minimum size $k=\sum_{m=1}^N(d_m-1)+1$ in $\mathbb{C}^{d_1}\otimes\mathbb{C}^{d_2}\otimes\cdots\otimes\mathbb{C}^{d_N}$ cannot be perfectly discriminated within $\overline{\text{LOCC}}$ [46]. However, when $\sum_{m=1}^N(d_m-1)+1<2d_{\max}-1$, there are still some UPBs with the minimum size that cannot be perfectly discriminated within $\overline{\text{LOCC}}$.

*Example 2.* Let

$$\begin{aligned}&|\Psi_1\rangle=|0\rangle_{A_1}|0\rangle_{A_2}|0\rangle_{A_3},\\&|\Psi_2\rangle=(|0\rangle+|1\rangle)_{A_1}(|0\rangle+|1\rangle)_{A_2}|1\rangle_{A_3},\\&|\Psi_3\rangle=(|0\rangle+2|1\rangle)_{A_1}(|0\rangle+2|1\rangle)_{A_2}|2\rangle_{A_3},\\&|\Psi_4\rangle=|1\rangle_{A_1}(2|0\rangle-|1\rangle)_{A_2}(|0\rangle-|2\rangle+|3\rangle)_{A_3},\\&|\Psi_5\rangle=(|0\rangle-|1\rangle)_{A_1}|1\rangle_{A_2}(|0\rangle+|1\rangle-|3\rangle)_{A_3},\\&|\Psi_6\rangle=(2|0\rangle-|1\rangle)_{A_1}(|0\rangle-|1\rangle)_{A_2}(|1\rangle+|2\rangle+|3\rangle)_{A_3}.\end{aligned} \tag{23}$$

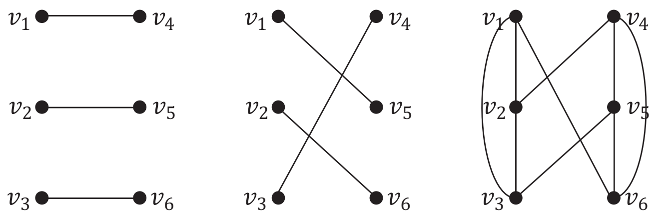


FIG. 2. Orthogonality graphs of the UPB in Example 2.

Then $\{|\Psi_i\rangle\}_{i=1}^6$ is a UPB with the minimum size 6 in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^4$ and it cannot be perfectly discriminated within $\overline{\text{LOCC}}$.

*Proof.* The orthogonality graphs $(G_m)_{m=1}^3$ of $\{|\Psi_i\rangle\}_{i=1}^6$ are shown in Fig. 2. Then it is easy to check that $\cup_{m=1}^3 G_m = K_6$. Hence the first condition in Lemma 1 is satisfied. Regarding the second condition, note that every two vectors in the set $\{|0\rangle, (|0\rangle + |1\rangle), (|0\rangle + 2|1\rangle), |1\rangle, (|0\rangle - |1\rangle), (2|0\rangle - |1\rangle)\} \subset \mathbb{C}^2$ are linearly independent; the size of any unsaturated set $W_m$ in $G_m$ can be at most 1 for every $m = 1, 2$. Similarly, since any four vectors in the set $\{|0\rangle, |1\rangle, |2\rangle, (|0\rangle - |2\rangle + |3\rangle), (|0\rangle + |1\rangle - |3\rangle), (|1\rangle + |2\rangle + |3\rangle)\} \subset \mathbb{C}^4$ are linearly independent, the size of any unsaturated set $W_4$ in $G_4$ is at most 3. Putting everything together, we obtain that the union of any three unsaturated sets $(W_m)_{m=1}^3$ cannot contain all vertices in $V$. Since both conditions in Lemma 1 are satisfied, we conclude that the vectors $\{|\Psi_i\rangle\}_{i=1}^6$ form a UPB.

Next, we show that $\{|\Psi_i\rangle\}_{i=1}^6$ cannot be perfectly discriminated within $\overline{\text{LOCC}}$.

Assume an orthogonality-preserving local measurement $\{E_m\}$ is performed on $A_1$ party, where each POVM element $E_m$ can be written as a $2 \times 2$ matrix $E_m = (a_{i,j})_{i,j \in \mathbb{Z}_2}$ under the basis $\{|i\rangle\}_{i \in \mathbb{Z}_2}$. By the orthogonality graph $G_1$, we know that $v_1$ and $v_4$ are adjacent; then we obtain $\langle 0|E_m|1\rangle_{A_1} = \langle 1|E_m|0\rangle_{A_1} = 0$, that is, $a_{0,1} = a_{1,0} = 0$. Moreover, since $v_2$ and $v_5$ are adjacent, we have $(\langle 0| + \langle 1|)E_m(|0\rangle - |1\rangle)_{A_1} = 0$ and it implies $a_{0,0} = a_{1,1}$. Thus the orthogonality-preserving local measurements $\{E_m\}$ on $A_1$ are trivial.

Since the orthogonality graph $G_2$ is similar to $G_1$, we can also show that the only orthogonality-preserving local measurements on $A_2$ are trivial in the same way.

Assume an orthogonality-preserving local measurement $\{E_m\}$ is performed on $A_3$ party, where each POVM element $E_m$ can be written as a $4 \times 4$ matrix $E_m = (a_{i,j})_{i,j \in \mathbb{Z}_4}$ under the basis $\{|i\rangle\}_{i \in \mathbb{Z}_4}$. By the orthogonality graph $G_3$, we known that $v_1$, $v_2$, and $v_3$ are two adjacent to each other; then we obtain $\langle 0|E_m|1\rangle_{A_3} = \langle 1|E_m|0\rangle_{A_3} = \langle 0|E_m|2\rangle_{A_3} = \langle 2|E_m|0\rangle_{A_3} = \langle 1|E_m|2\rangle_{A_3} = \langle 2|E_m|1\rangle_{A_3} = 0$, that is, $a_{0,1} = a_{1,0} = a_{0,2} = a_{2,0} = a_{1,2} = a_{2,1} = 0$. Since $v_1$ and $v_6$ are adjacent, we have $\langle 0|E_m(|1\rangle + |2\rangle + |3\rangle)_{A_3} = (\langle 1| + \langle 2| + \langle 3|)E_m|0\rangle_{A_3} = 0$ and it implies $a_{0,3} = a_{3,0} = 0$. By using $v_2$ and $v_4$, we have $\langle 1|E_m(|0\rangle - |2\rangle + |3\rangle)_{A_3} = (\langle 0| - \langle 2| + \langle 3|)E_m|1\rangle_{A_3} = 0$ and it implies $a_{1,3} = a_{3,1} = 0$. By using $v_3$ and $v_5$, we have $\langle 2|E_m(|0\rangle + |1\rangle - |3\rangle)_{A_3} = (\langle 0| + \langle 1| - \langle 3|)E_m|2\rangle_{A_3} = 0$ and it implies $a_{2,3} = a_{3,2} = 0$. By using $v_4$ and $v_5$, we have $(\langle 0| - \langle 2| + \langle 3|)E_m(|0\rangle + |1\rangle - |3\rangle)_{A_3} = 0$ and this implies $a_{0,0} = a_{3,3}$. By using $v_4$ and $v_6$, we have $(\langle 0| - \langle 2| + \langle 3|)E_m(|1\rangle + |2\rangle + |3\rangle)_{A_3} = 0$ and this implies $a_{2,2} = a_{3,3}$. By using $v_5$ and $v_6$, we have $(\langle 0| + \langle 1| - \langle 3|)E_m(|1\rangle + |2\rangle + |3\rangle)_{A_3} = 0$ and this implies $a_{1,1} = a_{3,3}$. Then we obtain $a_{0,0} = a_{1,1} = a_{2,2} = a_{3,3}$. This means that the only orthogonality-preserving local measurements on $A_3$ are trivial.

By Proposition 7, the UPB $\{|\Psi_i\rangle\}_{i=1}^6$ cannot be perfectly discriminated within $\overline{\text{LOCC}}$. ■

We can also use Proposition 7 to show that other UPBs are indistinguishable within $\overline{\text{LOCC}}$. This does not mean that this approach is applicable to all UPBs. For example, let $\{|\Psi_i\rangle\}_{i=1}^5$ be the UPB with the minimum size in $\mathbb{C}^3 \otimes \mathbb{C}^3$ [5]; then $\{|\Psi_i\rangle\}_{i=1}^5 \bigcup \{|0\rangle_{A_1}|3\rangle_{A_2}, |1\rangle_{A_1}|3\rangle_{A_2}, |2\rangle_{A_1}|3\rangle_{A_2}\}$ is a UPB with size 8 in $\mathbb{C}^3 \otimes \mathbb{C}^4$. However, a nontrivial orthogonality-preserving local measurement $\{|0\rangle_{A_2}\langle 0| + |1\rangle_{A_2}\langle 1| + |2\rangle_{A_2}\langle 2|, |3\rangle_{A_2}\langle 3|\}$ can be performed on party $A_2$. Moreover, all UPBs with the minimum size appear to be indistinguishable within $\overline{\text{LOCC}}$.

## VIII. CONCLUSIONS

In this paper, we established a graph-theoretic characterization of UPBs and GUPBs. Building on this characterization, we developed a constructing method for finding UPBs in low dimensional systems and we derived a new lower bound on the number of elements in any GUPB. Our bound significantly improves on the state of the art [26], thus placing stronger restrictions on potential candidates of GUPBs. Equivalently, our bound implies an upper bound on the rank of any bound entangled state built from a GUPB. Our results indicate a potential route to find a minimal tripartite GUPB consisting of 13 product vectors. While the numerical search for such GUPB is still challenging, our construction helps clarify where the problems lie and may eventually help find a suitable modification that is amenable to numerical search. Moreover, we presented an efficient necessary condition for perfect discrimination of UPBs within asymptotic LOCC, which can be used to show that some UPBs cannot be perfectly discriminated within asymptotic LOCC.

Besides addressing the open problem of the existence of GUPBs, we provided a systematic route to the construction of multipartite UPBs of any desired size between the minimum and the maximum. Equivalently, our construction can be viewed as a systematic way of constructing bound entangled states of different ranks. In addition, our results have an application to the study of nonlocality without entanglement. In Ref. [38] it was shown that quantum measurements exhibiting nonlocality without entanglement can be certified in a device-independent way. Since our results provide a systematic construction of multipartite UPBs, the corresponding scenarios of nonlocality without entanglement are likely to give rise to new self-testing procedures. Finally, another interesting direction is the study of nontrivial Bell inequalities with no quantum violation [6–8]. In this context, our work can be used to construct such inequalities in multipartite systems with larger local dimensions, going beyond the multiqubit scenario typically considered in the literature.

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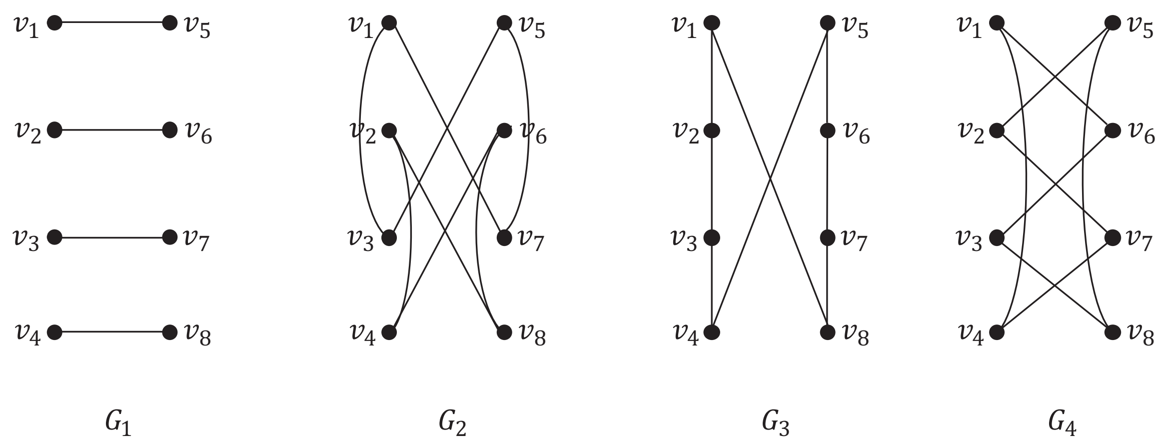


FIG. 3. Orthogonality graphs of the UPB in Example 3.

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## APPENDIX A: PROOFS OF LEMMAS 1, 2, AND 3

*Lemma 1.* Let $\mathcal{U}$ be a set of $k$ product vectors in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ and let $(G_m)_{m=1}^N$ be the corresponding orthogonality graphs. The set $\mathcal{U}$ is a UPB if and only if the following conditions hold.

(i) $\bigcup_{m=1}^N G_m = K_k$.

(ii) $\bigcup_{m=1}^N W_m \neq V$ for every $N$-tuple $(W_1, W_2, \dots, W_N)$ in which $W_m$ is an unsaturated set for $G_m$ for every $m \in \{1, \dots, N\}$.

*Proof.* The proof builds on arguments by Bennett *et al.* (cf. Lemma 1 of [1]), which are translated here into the graph theoretic framework of our paper by using the notion of saturated set. First, we observe that the product states in the set $\mathcal{U}$ are mutually orthogonal if and only if $\bigcup_{m=1}^N G_m = K_k$. Hence we only need to show that a set of orthogonal product states $\mathcal{U}$ is unextendible if and only if condition (ii) holds.

The "only if" part is proven by contrapositive: we show that if condition (ii) is violated, then the set $\mathcal{U}$ must be extendible. The proof is as follows: if there exists an unsaturated set $W_m$ of $G_m$ for every $1 \leqslant m \leqslant N$ such that $\bigcup_{m=1}^N W_m = V$, then we can find a state $|\psi\rangle_{A_m} \in \mathbb{C}^{d_m}$ that is orthogonal to any state in $\{|\varphi_m^{(i)}\rangle_{A_m} \mid v_i \in W_m\}$ for every $1 \leqslant m \leqslant N$ and $|\psi_1\rangle_{A_1}|\psi_2\rangle_{A_2} \cdots |\psi_N\rangle_{A_N}$ is orthogonal to any state in $\mathcal{U}$.

For the "if" part, we also proceed by contrapositive: we assume that $\mathcal{U}$ is extendible and show that condition (ii) must be violated. If $\mathcal{U}$ is extendible, then there exists a product state $|\psi_1\rangle_{A_1}|\psi_2\rangle_{A_2} \cdots |\psi_N\rangle_{A_N}$ that is orthogonal to any state in $\mathcal{U}$. Let $W_m = \{v_i \mid \langle\psi_m|\varphi_m^{(i)}\rangle_{A_m} = 0\}$ for every $1 \leqslant m \leqslant N$; then $W_m$ must be an unsaturated set of $G_m$ for every $1 \leqslant m \leqslant N$ and $\bigcup_{m=1}^N W_m = V$. ■

*Lemma 2.* Let $(G_m)_{m=1}^N$ be the orthogonality graphs associated to a UPB of size $k$. Then, the size of any unsaturated set $W_m$ in $G_m$ is upper bounded as

$$|W_m| \leqslant k - 1 - \sum_{i \in \{1,\dots,N\} \setminus \{m\}} (d_i - 1). \tag{A1}$$

*Proof.* The proof is by contradiction. Suppose that there existed an integer $m_0 \in \{1, \dots, N\}$ and an unsaturated set $W_{m_0}$ such that $|W_{m_0}| \geqslant k - \sum_{i \neq m_0} (d_i - 1)$. Then, the set $V \setminus W_{m_0}$ contains $l \leqslant \sum_{i \neq m_0} (d_i - 1)$ vertices. These $l$ vertices can be divided into $N - 1$ subsets, putting at most $d_m - 1$ vertices in the $m$th subset, for every $m \in \{1, \dots, N\} \setminus \{m_0\}$. The $m$th subset, denoted by $W_m$, is by construction an unsaturated set in $G_m$. Also, the above construction guarantees that $\bigcup_{m=1}^N W_m = V$. But this condition is in contradiction with the fact that the graphs $(G_m)_{m=1}^N$ are the orthogonality graphs of a UPB, because Lemma 1 showed the relation $\bigcup_{m=1}^N W_m \neq V$ for every $N$-tuple of unsaturated subsets $(W_1, \dots, W_N)$. This concludes the proof by contradiction. ■

*Lemma 3.* For every UPB in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$, the degrees of the vertices in the orthogonality graphs $(G_m)_{m=1}^N$ must satisfy the condition

$$d_m - 1 \leqslant \deg_{G_m}(v_i) \leqslant k - 1 - \sum_{i \in \{1,\dots,N\} \setminus \{m\}} (d_i - 1),$$
$$\forall v_i \in V, \quad \forall m \in \{1, \dots, N\}. \tag{A2}$$

*Proof.* The upper bound is immediate from the fact that the degree $\deg_{G_m}(v_i) = |N_{G_m}(v_i)|$, where $N_{G_m}(v_i)$ is the neighborhood of $v_i$ in $G_m$. Since the neighborhood of a vertex in an orthogonality graph is, by definition, an unsaturated set, the upper bound on its size follows from Lemma 2.

For the lower bound, we assume that there exists an orthogonality graph $G_m = (V, E_m)$ and a vertex $v_j \in V$ such that $\deg_{G_m}(v_j) \leqslant d_m - 2$. Then we can find a state $|\phi\rangle_{A_m}$ in $\mathbb{C}^{d_m}$ which is orthogonal to any state in $\{|\varphi_m^{(i)}\rangle_{A_m} \mid v_i \in \{v_j\} \cup N_{G_m}(v_j)\}$. The product state $|\varphi_1^{(j)}\rangle_{A_1} \cdots |\varphi_{m-1}^{(j)}\rangle_{A_{m-1}} |\phi\rangle_{A_m} |\varphi_{m+1}^{(j)}\rangle_{A_{m+1}} \cdots |\varphi_N^{(j)}\rangle_{A_N}$ is orthogonal to any state in $\{|\varphi_1^{(i)}\rangle_{A_1} |\varphi_2^{(i)}\rangle_{A_2} \cdots |\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k$, which contradicts that $\{|\varphi_1^{(i)}\rangle_{A_1} |\varphi_2^{(i)}\rangle_{A_2} \cdots |\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^k$ is a UPB. ■

*Example 3.* The following product vectors form a UPB of size 8 in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$:

$$\begin{aligned}
|\psi_1\rangle &= |0\rangle_{A_1}|0\rangle_{A_2}(|0\rangle + |1\rangle + |2\rangle)_{A_3}(|0\rangle + |1\rangle + |2\rangle)_{A_4},\\
|\psi_2\rangle &= (|0\rangle + |1\rangle)_{A_1}(|0\rangle + |1\rangle)_{A_2}(|0\rangle + |1\rangle - 2|2\rangle)_{A_3}(2|0\rangle - |1\rangle - 2|2\rangle)_{A_4},\\
|\psi_3\rangle &= (|0\rangle + 2|1\rangle)_{A_1}|1\rangle_{A_2}(4|0\rangle + 2|1\rangle + 3|2\rangle)_{A_3}(3|0\rangle + 6|1\rangle - 2|2\rangle)_{A_4},\\
|\psi_4\rangle &= (|0\rangle + 3|1\rangle)_{A_1}(|0\rangle - |1\rangle)_{A_2}(2|0\rangle - |1\rangle - 2|2\rangle)_{A_3}(|0\rangle + |1\rangle - 2|2\rangle)_{A_4},\\
|\psi_5\rangle &= |1\rangle_{A_1}|0\rangle_{A_2}(|0\rangle + 4|1\rangle - |2\rangle)_{A_3}(|0\rangle + 4|1\rangle - |2\rangle)_{A_4},\\
|\psi_6\rangle &= (|0\rangle - |1\rangle)_{A_1}(|0\rangle + |1\rangle)_{A_2}(2|0\rangle + |1\rangle + 6|2\rangle)_{A_3}(-8|0\rangle + 5|1\rangle + 3|2\rangle)_{A_4},\\
|\psi_7\rangle &= (2|0\rangle - |1\rangle)_{A_1}|1\rangle_{A_2}(3|0\rangle + 6|1\rangle - 2|2\rangle)_{A_3}(4|0\rangle + 2|1\rangle + 3|2\rangle)_{A_4},\\
|\psi_8\rangle &= (3|0\rangle - |1\rangle)_{A_1}(|0\rangle - |1\rangle)_{A_2}(-8|0\rangle + 5|1\rangle + 3|2\rangle)_{A_3}(2|0\rangle + |1\rangle + 6|2\rangle)_{A_4}.
\end{aligned} \tag{A3}$$

*Proof.* The orthogonality graphs $(G_m)_{m=1}^4$ of $\{|\psi_i\rangle\}_{i=1}^8$ are shown in Fig. 3. Then it is easy to check that $\cup_{m=1}^4 G_m = K_8$. Hence the first condition in Lemma 1 is satisfied. Regarding the second condition, note that every two vectors in the set $\{|0\rangle, (|0\rangle + |1\rangle), (|0\rangle + 2|1\rangle), (|0\rangle + 3|1\rangle), |1\rangle, (|0\rangle - |1\rangle), (2|0\rangle - |1\rangle), (3|0\rangle - |1\rangle)\} \subset \mathbb{C}^2$ are linearly independent. Hence the size of any unsaturated set $W_1$ in $G_1$ can be at most 1. Since every three vectors in the set $\{|0\rangle, (|0\rangle + |1\rangle), |1\rangle, (|0\rangle - |1\rangle), |0\rangle, (|0\rangle + |1\rangle), |1\rangle, (|0\rangle - |1\rangle)\} \subset \mathbb{C}^2$ are linearly independent, the size of any unsaturated set $W_2$ in $G_2$ can be at most 2. Moreover, since any three vectors in the set $\{(|0\rangle + |1\rangle + |2\rangle), (|0\rangle + |1\rangle - 2|2\rangle), (4|0\rangle + 2|1\rangle + 3|2\rangle), (2|0\rangle - |1\rangle - 2|2\rangle), (|0\rangle + 4|1\rangle - |2\rangle), (2|0\rangle + |1\rangle + 6|2\rangle), (3|0\rangle + 6|1\rangle - 2|2\rangle), (-8|0\rangle + 5|1\rangle + 3|2\rangle)\} \subset \mathbb{C}^3$ are linearly independent, the size of any unsaturated set $W_m$ in $G_m$ is at most 2 for every $3 \leqslant m \leqslant 4$. Putting everything together, we obtain that the union of any four unsaturated sets $(W_m)_{m=1}^4$ cannot contain all vertices in $V$. Since both conditions in Lemma 1 are satisfied, we conclude that the vectors $\{|\psi_i\rangle\}_{i=1}^8$ form a UPB. ■

### APPENDIX B: PROOFS OF PROPOSITIONS 2, 3, 4, AND 5

*Proposition 2.* The RHS of Eq. (10) is always larger than or equal to the RHS of Eq. (1).

*Proof.* First, we show that the RHS of Eq. (10) satisfies the equality

$$\left\lceil \frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1} \right\rceil = \left\lfloor \frac{\sum_{m=1}^N \frac{D}{d_m} - 2}{N-1} \right\rfloor + 1. \tag{B1}$$

If the number $s := \frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1}$ is an integer, then one has the relations $s = \lceil \frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1} \rceil$ and $\lfloor \frac{\sum_{m=1}^N \frac{D}{d_m} - 2}{N-1} \rfloor + 1 = \lfloor \frac{s(N-1)-1}{N-1} \rfloor + 1 = s$. If instead $\frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1}$ is not an integer, it can be written as $\frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1} = s + \frac{t}{N-1}$ for some integer $s$ and some integer $1 \leqslant t \leqslant N-2$. Then, $\lceil \frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1} \rceil = s + 1$ and $\lfloor \frac{\sum_{m=1}^N \frac{D}{d_m} - 2}{N-1} \rfloor + 1 = s + \lfloor \frac{t-1}{N-1} \rfloor + 1 = s + 1$. Thus $k \geqslant \lceil \frac{\sum_{m=1}^N \frac{D}{d_m} - 1}{N-1} \rceil = \lfloor \frac{\sum_{m=1}^N \frac{D}{d_m} - 2}{N-1} \rfloor + 1$.

To conclude, we use the bound

$$\begin{aligned}
\left\lfloor \frac{\sum_{m=1}^N \frac{D}{d_m} - 2}{N-1} \right\rfloor + 1 &\geqslant \left\lfloor \frac{N \frac{D}{d_{\max}} - 2}{N-1} \right\rfloor + 1\\
&= \frac{D}{d_{\max}} + \left\lfloor \frac{\frac{D}{d_{\max}} - 2}{N-1} \right\rfloor + 1,
\end{aligned} \tag{B2}$$

where the last term in the inequality is the RHS of Eq. (1). Combining Eqs. (B1) and (B2) we then obtain that the RHS of Eq. (10) is larger than or equal to the RHS of Eq. (1). ■

*Proposition 3.* In the tripartite case, the bound (2) is nontrivial when $(d_1, d_2, d_3) = (2p, 2p, 3p-1)$ for some integer $p \geqslant 2$, and when $(d_1, d_2, d_3) = (2p-1, \tilde{d}, 3p-2)$ for some integer $p \geqslant 2$ and some integer $\tilde{d} \in [2p-1, 3p-2]$.

*Proof.* In both cases, we prove the inequality

$$\left\lfloor \frac{\sum_{m=1}^3 \frac{D}{d_m} - 2}{N-1} \right\rfloor + 1 \geqslant d_1 + \frac{D}{d_1} + 1. \tag{B3}$$

When $(d_1, d_2, d_3) = (2p, 2p, 3p-1)$ with integer $p \geqslant 2$, we have

$$\left\lfloor \frac{\sum_{m=1}^3 \frac{D}{d_m} - 2}{N-1} \right\rfloor + 1 = 8p^2 - 2p$$

and

$$d_1 + \frac{D}{d_1} + 1 = 6p^2 + 1.$$

Hence the inequality (B3) is equivalent to

$$2p^2 - 2p - 1 \geqslant 0. \tag{B4}$$

Note that Eq. (B4) holds for any $p \geqslant 2$. Hence the bound (2) is nontrivial for every $p \geqslant 2$.

Let us now consider the case where $(d_1, d_2, d_3) = (2p-1, \tilde{d}, 3p-2)$ for some integer $p \geqslant 2$ and some integer $\tilde{d}$ satisfying $2p-1 \leqslant \tilde{d} \leqslant 3p-2$. In this case, we have

$$\left\lfloor \frac{\sum_{m=1}^{3} \frac{D}{d_m} - 2}{N-1} \right\rfloor + 1 = \left\lfloor \frac{\tilde{d}(5p-3) + 6p^2 - 7p}{2} \right\rfloor + 1$$

and

$$d_1 + \frac{D}{d_1} + 1 = 2p + \tilde{d}(3p-2),$$

and the inequality (B3) is equivalent to

$$\left\lceil \frac{\tilde{d}(p-1) - 6p^2 + 11p - 2}{2} \right\rceil \leqslant 0. \tag{B5}$$

Notice that if Eq. (B5) holds for $\tilde{d} = 3p-2$, then it holds for any $2p-1 \leqslant \tilde{d} \leqslant 3p-2$. Since

$$(3p-2)(p-1) - 6p^2 + 11p - 2 = -3p^2 + 6p \leqslant 0 \tag{B6}$$

for any $p \geqslant 2$, then Eq. (B5) holds for any $p \geqslant 2$ and $2p-1 \leqslant \tilde{d} \leqslant 3p-2$. Therefore, Eq. (B3) holds for any $p \geqslant 2$ and $2p-1 \leqslant \tilde{d} \leqslant 3p-2$, meaning that the bound (2) is nontrivial for these values. ∎

We now provide the proofs of Propositions 4 and 5. The proofs are presented in inverted order, because the proof of Proposition 4 uses Proposition 5 as an intermediate step.

*Proposition 5.* For a minimal GUPB saturating the bound (2), the orthogonality graph $G_m$ is a $(k - \frac{D}{d_m})$-regular graph for every $m \in \{1, \dots, N\}$.

*Proof.* For the bound (2) to be saturated, we must have $k = \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N-1}$ or, equivalently,

$$(N-1)k = \sum_{m=1}^{N} \frac{D}{d_m} - 1. \tag{B7}$$

Since $\{|\varphi_1^{(i)}\rangle_{A_1} |\varphi_2^{(i)}\rangle_{A_2} \cdots |\varphi_N^{(i)}\rangle_{A_N}\}_{i=1}^{k}$ is still a UPB in the bipartition $A_m \mid \{A_1 A_2 \cdots A_N\} \setminus \{A_m\}$ for $1 \leqslant m \leqslant N$, then by Lemma 3, the degree of every vertex $v_i$ of $G_m$ satisfies

$$\deg_{G_m}(v_i) \leqslant k - \frac{D}{d_m}. \tag{B8}$$

On the other hand, the minimality condition (B7) implies

$$\sum_{m=1}^{N} \left( k - \frac{D}{d_m} \right) = k - 1 \leqslant \sum_{m=1}^{N} \deg_{G_m}(v_i), \tag{B9}$$

where the inequality comes from $\bigcup_{m=1}^{N} G_m = K_k$. Combining the two inequalities above, we obtain $\deg_{G_m}(v_i) = k - \frac{D}{d_m}$ for $1 \leqslant m \leqslant N$. ∎

*Proposition 4.* If at least one of the local dimensions $(d_m)_{m=1}^{N}$ is even and the sum $\sum_{m=1}^{N} \frac{D}{d_m} - 1$ is an odd multiple of $N-1$, then the size of any GUPB in $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \cdots \otimes \mathbb{C}^{d_N}$ is lower bounded as

$$k \geqslant \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N-1} + 1. \tag{B10}$$

*Proof.* We prove that, when the local dimensions satisfy the above conditions, the bound (2) cannot hold with the equality sign. If a GUPB saturated the bound (2), its size should be $k' = \frac{\sum_{m=1}^{N} \frac{D}{d_m} - 1}{N-1}$ and $k'$ is odd. This means that each orthogonality graph $G_m$ is a $(k' - \frac{D}{d_m})$-regular graph with $k'$ vertices by Proposition 5. By Handshaking Lemma [64], $k'(k' - \frac{D}{d_m})$ must be even for each $1 \leqslant m \leqslant N$. Assume $d_m$ is even, then $\frac{D}{d_{m'}}$ is even for $m' \neq m$. In this case, $k'(k' - \frac{D}{d_{m'}})$ is odd and this is impossible. Thus a GUPB of size $k'$ does not exist. This completes the proof. ∎

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