High Schmidt Number Concentration in Quantum Bound Entangled States

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A deep understanding of quantum entanglement is vital for advancing quantum technologies. The strength of entanglement can be quantified by counting the degrees of freedom that are entangled, which results in a quantity called the Schmidt number. A particular challenge is to identify the strength of entanglement in quantum states that remain positive under partial transpose (PPT), otherwise recognized as undistillable states. Finding PPT states with high Schmidt numbers has become a mathematical and computational challenge. In this Letter, we introduce efficient analytical tools for calculating the Schmidt number for a class of bipartite states called grid states. Our methods improve the best-known bounds for PPT states with high Schmidt number 3 PPT state in five-dimensional systems and a family of states with a Schmidt number of (d + 1)/2 for odd *d*-dimensional systems, representing the best-known scaling of the Schmidt number in a local dimension. Additionally, these states possess intriguing geometrical properties, which we utilize to construct indecomposable entanglement witnesses.

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Introduction.—Quantum entanglement is a fundamental phenomenon of quantum theory on which the success of the rapidly advancing field of quantum technologies relies. However, in spite of the development of a complex mathematical theory of entanglement, with the primary goal to detect and quantify the entanglement present in a physical system, many fundamental questions still need to be answered. So far, no efficiently computable necessary and sufficient criterion for separability of a composite quantum state has been discovered. Generally, the problem is known to be NP-hard [1–3], and it has only been solved in qubit-qubit and qubit-qutrit cases using the famous positive partial transpose (PPT) criterion [4,5]. In higher-dimensional states, however, there is no general method to investigate entanglement.

At the same time, in recent years, high-dimensional entanglement has become experimentally feasible [6,7], demonstrating a better noise resistance in a number of applications, in comparison with low-dimensional implementations [8–11]. As a result, determining whether an experiment successfully established high-dimensional entanglement or if the experimental results can be explained by assuming low-dimensional entanglement is critical. A go-to measure that certifies that a bipartite state has been entangled across at least r degrees of freedom is called a "Schmidt number" [12], and is very challenging to estimate due to its form (see below) for general states. One typical way to determine this quantity is to construct a hermitian operator, called a "Schmidt number witness," a few examples of which can be found in the literature [13–15].

An additional challenge lies in constructing a Schmidt number witness for states with PPT (PPT states), since such Hermitian operators have to satisfy an extra mathematical property, known as being "indecomposable" [16]. Moreover, such states are known to be bound entangled, as no pure state entanglement can be ever distilled from them [17]. Because of this property, it was originally believed that PPT states are weakly entangled and cannot be used for quantum information processing tasks [18]. Yet, contrary to this perception, a family of PPT states with logarithmically increasing Schmidt numbers in the local dimension were found [19]. Later, along with discovering the potentialities of bound entangled states in quantum steering, nonlocality, and secure communication [20-22], PPT states with the Schmidt number scaling of d/4 and d/2were proposed in even-dimensional $d \times d$ systems [23,24]. At the same time, upper bounds have been derived on the amount of entanglement in bound entangled states. For example, in 3×3 no PPT state exists with Schmidt number 3 [25]. In sequences of works, high Schmidt number PPT states have been extensively investigated [13,23,24,26-28] and searched for. Despite these developments in the study of bound entanglement, only few methods, like the acclaimed Doherty-Parillo-Spedalieri (DPS) hierarchy [29] can be applied systematically. Such methods typically have a high computational cost, and do not result in an analytical solution.

In this Letter, we address precisely this problem, and for an elegant class of quantum states, so-called "grid states" [30,31], we develop a set of efficient graphical tools relying on a generalized range criterion to evaluate their exact Schmidt number. Here, we provide examples of PPT states that enjoy the highest known Schmidt number *concentration* in given local dimensions. To start with, despite the efforts, the best minimal example of a PPT bound entangled state with Schmidt number 3 was known to be in local dimensions 6×6 [24]. Here, we find a PPT state with Schmidt number 3 in 5×5 systems. We also improve other previously known bounds and derive a family of PPT states with Schmidt number scaling $(d_{\rm A}+1)/2$ in $d_{\rm A} \times d_{\rm B}$ dimensional systems, where $d_{\rm A}$ is odd and $d_A < d_B$. We find these states by resorting to tools similar to entanglement distillation, but in this case, with the goal to distill a high Schmidt number PPT state from multiple copies of low Schmidt number ones. We call this procedure Schmidt number "concentration." Similar tasks have been studied for quantum Fisher information [32] and nonlocality [33]. As a last example, using the Schmidt number concentration, we find a Schmidt number 3 state in 4×12 systems. Our findings leave as an open problem whether there exist Schmidt number 3 states in $3 \times d$, and what the smallest local dimension is in $4 \times d$ systems to accommodate such states.

Finally, our new states are not only highly entangled, but they all enjoy a striking property of being extremal in a PPT set, that is, they cannot be decomposed as a convex mixture of other PPT states. We utilize this property to obtain indecomposable entanglement witnesses for high Schmidt number states and numerically obtain such witnesses for all such states. While our findings are specifically tailored to grid states, the methods developed in this Letter can be extended to a broader range of quantum systems. This paves the way for exploring new signatures of highdimensional entanglement and bound entanglement.

Preliminaries.—Given a finite-dimensional bipartite quantum state ρ_{AB} defined over Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, and the transposition map *T* on one of the subsystems, we say that the state is positive under partial transposition, or is PPT, if

$$\rho_{\rm AB}^{T_{\rm B}} \ge 0, \quad \text{where } \rho_{\rm AB}^{T_{\rm B}} \coloneqq \mathbbm{1}_{\rm A} \otimes T_{\rm B}(\rho_{\rm AB}). \tag{1}$$

Any state that is negative under the partial transposition map is entangled and can be detected via a Hermitian operator Wof the form $W = P + Q^{T_B}$, with some $P, Q \ge 0$. Such witnesses are called "decomposable" [34,35], and, clearly, they cannot detect PPT entanglement. Instead one needs to construct an *indecomposable* witness.

An important measure of mixed state entanglement, which we focus on in this Letter, is called the "Schmidt number" (SN) of a state ρ_{AB} , and is defined as follows [12],

$$\begin{split} & \text{SN}(\rho_{\text{AB}}) \coloneqq \min \ k, \\ & \text{s.t.} \ \sum_{i} p_{i} |\psi_{i}\rangle \langle \psi_{i}| = \rho_{\text{AB}}, \\ & \text{SR}(|\psi_{i}\rangle) \leq k, \qquad p_{i} \geq 0, \quad \forall \ i. \end{split}$$

Here, the abbreviation SR means "Schmidt rank" of a pure state, and corresponds to the number of nonzero Schmidt coefficients of this state. Several SN witnesses have been derived in the literature [13–15], but determining the SN remains a difficult task, in particular for PPT states.

One method to determine the SN is through a generalized range criterion [13], which we use here. The range of ρ_{AB} is defined as the image of ρ_{AB} , $R(\rho_{AB}) \coloneqq \{\rho_{AB}|\psi\rangle||\psi\rangle \in \mathbb{C}_A \otimes \mathbb{C}_B\}$. Next, we define the Schmidt rank restricted range $R_k(\rho_{AB}) \coloneqq \{SR(|\psi\rangle) \le k||\psi\rangle \in R(\rho_{AB})\}$, and give a generalized range criterion for SN: all SN *k* states must have a complete basis in *k*-restricted range $R_k(\rho_{AB})$ to span $R(\rho_{AB})$. Then, if there is a vector $|t\rangle \in R(\rho_{AB})$, which is orthogonal to the *k*-restricted range, $|t\rangle \perp R_k(\rho_{AB})$, then SN($\rho_{AB}) > k$.

Grid states and Schmidt number criterion.—Grid states are mixed quantum states with elegant graphical representation. We explain their construction generalizing the original definition in Refs. [30,31]. We first define a two-dimensional grid in terms of its sites enumerated by two indices, $G_{AB} = \{(v_A, v_B) | 0 \le v_A < d_A, 0 \le v_B < d_B\}$. To each site in the grid, we associate a computational basis state of the bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ in the following manner $(v_A, v_B) \mapsto |v_A v_B\rangle \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$. Once we have a grid, we can define a grid state over it using a hypergraph H = (V, E). Here, E is as a collection of edges, e, containing a subset of sites of a grid, and $V \subseteq G_{AB}$ is a set of vertices given by the union of all edges. If an edge econtains k site, we call it a k edge. To $\forall e \in E$ we associate the unnormalized superposition

$$|e\rangle = \sum_{v \in e} |v\rangle = \sum_{(v_{\rm A}, v_{\rm B}) \in e} |v_{\rm A}v_{\rm B}\rangle \tag{3}$$

and call it edge representation. An unnormalized grid state ρ_H corresponding to a hypergraph *H* is then defined as the equal mixture of its edge representations:

$$\rho_H = \sum_{e \in E} |e\rangle \langle e|. \tag{4}$$

See Fig. 1 for an example. Since the normalization $1/\text{tr}(\rho_H)$ only contributes a global factor, for simplicity, it will be omitted, unless stated otherwise. Finally, a site $v \in G_{AB}$ is called "isolated," if $v \notin V$. It corresponds to a product state in the kernel of ρ_H , playing an important role later.

We are ready to give a sufficient PPT criterion for grid states. Given ρ_H , split its density matrix into the diagonal part *D* and off-diagonal part *A*. Consider *A* as an adjacency matrix defining a new graph G_H . The action of the partial transposition on ρ_H corresponds to flipping every edge $\{(v_A^1, v_B^1), (v_A^2, v_B^2)\}$ in the graph G_H to $\{(v_A^1, v_B^2), (v_A^2, v_B^1)\}$. The graph formed by these flipped edges is denoted as $G_H^{T_B}$ (See examples of taking a partial transposition in Figs. 1 and 2). Now, suppose $G_H^{T_B}$ is two-colorable. Then, we show in Supplemental Material (SM) [36] that ρ_H is PPT if and only if the degree of every

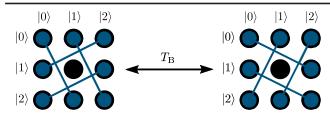


FIG. 1. Left: the crosshatch state, ρ^{CH} [30], a bound entangled grid state in 3 × 3. The sites in the grid are labeled as $\{(0,0), (0,1), (0,2), (1,0), (1,1), (1,2), (2,0), (2,1), (2,2)\}$. The crosshatch state has edges $E = \{\{(0,0), (2,1)\}, \{(0,1), (2,2)\}, \{(1,0), (0,2)\}, \{(2,0), (1,2)\}\}$. Right: partial transpose of the crosshatch state, which is also a grid state.

vertex (v_A, v_B) in $G_H^{T_B}$ is not higher than the number $\langle v_A v_B | D | v_A v_B \rangle$.

Next, we calculate the SN of grid state ρ_H . Any pure state in the range of ρ_H , $|\psi\rangle \in R(\rho_H)$ can be expressed as an arbitrary linear combination of edge representations, $|\psi\rangle = \sum_{e \in E} c_e |e\rangle$. Then according to the generalized range criterion, $SR(|\psi\rangle) \leq k$ if and only if the corresponding coefficient matrix Ψ has all of its size (k + 1) minors equal to zero [41,42], where $\{\Psi\}_{ij} \coloneqq \langle ij|\psi\rangle$, and $\{|i\rangle\}_{i=0}^{d_n-1}$ and $\{|j\rangle\}_{i=0}^{d_n-1}$ are the computational bases.

As an example, we apply this criterion to the 3×3 crosshatch state ρ^{CH} in Fig. 1. First, we give an explicit parametrization of the range of ρ^{CH} ,

$$\Psi^{\rm CH} \coloneqq \begin{pmatrix} c_{00} & c_{01} & c_{10} \\ c_{10} & 0 & c_{20} \\ c_{20} & c_{00} & c_{01} \end{pmatrix} \in R(\rho^{\rm CH}), \tag{5}$$

and show that there are no product vectors contained in its range. To that end, we first determine the one-restricted range $R_1(\rho^{\text{CH}})$ by demanding that all the 2 × 2 minors of Ψ^{CH} vanish. Four conditions of the 2 × 2 vanishing minors have a particularly simple form,

$$c_{01}c_{10} = c_{01}c_{20} = c_{00}c_{10} = c_{00}c_{20} = 0, \qquad (6)$$

admitting two nontrivial solutions, either $c_{10} = c_{20} = 0$ or $c_{00} = c_{01} = 0$. These cases are equivalent under relabeling, and assuming $c_{10} = c_{20} = 0$, we obtain another set of 2×2 minor equations $c_{00}^2 = c_{01}^2 = 0$, implying that $c_{00} = c_{01} = 0$, and, hence, $\Psi^{\text{CH}} = 0_{3\times3}$. Thus, there is no nonzero vector in the one-restricted range of ρ^{CH} , proving that the state must have $\text{SN}(\rho^{\text{CH}}) = 2$.

The form of the generalized range criterion we used here relies on having isolated sites of a grid state, as this construction translates to the powerful vanishing minor conditions in Eq. (6). In the same way, when testing a generalized range criterion for k-restricted range, if we want to keep the conditions simple, we consider states that

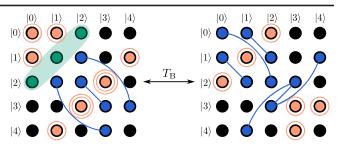


FIG. 2. Left: the smallest known Schmidt number 3 bound entangled state in 5×5 , $\rho^{5.5}$, with the multiset of edges $E = \{\{(0,0)\}, \{(0,1)\}, \{(1,0)\}, \{(2,3)\}, \{(2,3)\}, \{(3,2)\}, \{(3,2)\}, \{(1,4)\}, \{(4,1)\}, \{(2,1),(4,3)\}, \{(2,2),(3,3)\}, \{(1,2),(3,4)\}, \{(0,2),(1,1),(2,0)\}\}$. Right: the grid state corresponding to a partial transposition of $\rho^{5.5}$ has Schmidt number 2.

result in the $(k + 1) \times (k + 1)$ minor vanishing conditions having the following form, $\prod_{i=0}^{k} c_{e_i} = 0$. In this case, one of the (k + 1) coefficients shall be zero, leading to possible solution branches. We represent each branch as a grid state, with the respective edge e_i erased from the hypergraph. This procedure is repeated on all the branches and their subbranches, until no more edges can be erased in this manner. If an edge $e \in E$, with $SR(|e\rangle) = (k + 1)$, can be erased in all solution branches, then $|e\rangle \perp R_k(\rho_H)$, implying $SN(\rho_H) > k$.

We now state the first result using the construction given above and the generalized range criterion.

Result 1: A Schmidt number 3 PPT bound entangled state exists in the local dimension 5×5 .

The smallest Schmidt number 3 state was believed to be in the local dimension 6×6 [24]. See Fig. 2 for the Schmidt number 3 PPT state $\rho^{5,5}$ we found using our PPT construction and see the proof in SM [36] applying the generalized range criterion.

High Schmidt number concentration.—It is well known that no entanglement can be distilled from the PPT entangled states. Instead, here we use the tools from distillation protocols to achieve *Schmidt number concentration* in bound entanglement. The idea is to use different low Schmidt number PPT states (relative to the local dimension), act on them with local filtering operations, and obtain a single PPT state with high relative Schmidt number for the resulting local dimension. Clearly, it is important to tailor the concentration protocol to particular PPT states to ensure efficiency in calculating SN in the resulting distilled state. In what follows, we describe the procedure.

Let $\rho_{A_1B_1} = p\sigma + (1-p)|t\rangle\langle t|$, be a bipartite Schmidt number k state, $0 , and let <math>|\alpha\beta\rangle$ be a product state and $|t\rangle$ a pure state fulfilling the following conditions: $|t\rangle, |\alpha\beta\rangle \perp R(\sigma), |t\rangle \perp R_{k-1}(\rho), |t\rangle \not\perp |\alpha\beta\rangle$, then there exists a PPT preserving map Θ with its action on a bipartite state $\rho_{A_1B_1}$ defined as follows:

$$\Theta(\rho_{A_1B_1}) = (A \otimes B)\rho_{A_1B_1} \otimes \rho_{A_2B_2}^{CH}(A^{\dagger} \otimes B^{\dagger}), \quad (7)$$

where A and B are local filtering operators acting on the corresponding local Hilbert spaces. The resulting state is a bound entangled state, $\tilde{\rho}_{AB}$, with the same properties as ρ_{AB} but with the Schmidt number increased by 1, $SN(\tilde{\rho}_{AB}) = (k + 1)$, and

$$\tilde{\rho}_{\rm AB} = \tilde{p}\,\tilde{\sigma} + (1 - \tilde{p})|\tilde{t}\rangle\langle\tilde{t}|.\tag{8}$$

In SM [36], we define operations A, B, and prove that if the original state ρ_{AB} has local dimension $d_A \times d_B$, and SN k, the map Θ changes those quantities to

$$(d_{\rm A}, d_{\rm B}, k) \mapsto (d_{\rm A} + 2, d'_{\rm B}, k + 1),$$
 (9)

where $d'_{\rm B} = d_{\rm B} + \operatorname{rank}((\langle \alpha |_{\rm A} \otimes \mathbb{1}_{\rm B})\rho_{\rm AB}(|\alpha \rangle_{\rm A} \otimes \mathbb{1}_{\rm B})) + 1$. Since the resulting state shares the same properties as the starting one, we can repeatedly apply the map $\Theta^n(\rho_{\rm A_1,B_1})$, and study the Schmidt number concentration for increasing *n*. The exact values for scaled local dimensions and Schmidt numbers are derived in SM [36]. If we apply the concentration protocol to the crosshatch state $\rho^{\rm CH}$, we transform *n* copies of 3×3 crosshatch states each with Schmidt number 2 into a bound entangled grid state $\rho^{(n)} = \Theta^{(n-1)}(\rho^{\rm CH}_{\rm A,B_1})$ with properties (2n + 1, (n + 1)(n + 2)/2, n + 1), giving our second result.

Result 2: For odd values of *d*, Schmidt number (d+1)/2 PPT states exist in the local dimension $d \times [(d+1)(d+3)/8]$.

The Schmidt number scaling present in Result 2 improves on the best-known construction in evendimensional systems with the Schmidt number scaling as d/2 [24]. See SM [36] for the construction and proof of the protocol, and Fig. 3 for $\rho^{(n)}$, $n \leq 3$.

Our SN concentration technique is not limited to grid states only. To show this, we design a SN concentration protocol for a Horodecki state ρ^{Hor} in 2 × 4, the lowest dimensional bound entangled state in inhomogeneous local dimensions [40], and obtain a Schmidt number 3 bound entangled state in 4 × 12,

$$\rho^{4,12} = (\Pi_{\mathcal{A}} \otimes \mathbb{1}_{\mathcal{B}})\rho^{\mathrm{Hor}}_{\mathcal{A}_{1}\mathcal{B}_{1}} \otimes \rho^{\mathrm{CH}}_{\mathcal{A}_{2}\mathcal{B}_{2}}(\Pi_{\mathcal{A}} \otimes \mathbb{1}_{\mathcal{B}})^{\dagger}, \quad (10)$$

where $\Pi_A \coloneqq \mathbb{1}_{A_1A_2} - |1\rangle \langle 1|_{A_1} \otimes (|0\rangle \langle 0| + |2\rangle \langle 2|)_{A_2}$. See SM [36] for proof techniques and the explicit form of the states ρ^{Hor} [40] and $\rho^{4,12}$.

Extremal PPT states and indecomposable witnesses.— We call a PPT state ρ "extremal" if it cannot be decomposed into a convex mixture of a pair of distinct PPT states. This means that subtracting any PPT state with a Schmidt number less than SN(ρ) results in a matrix with negative partial transpose, a property that we use to construct SN witnesses for such states, specifically making use of the

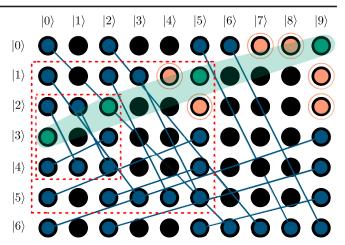


FIG. 3. Examples of $\rho^{(n)}$, for n < 4. Observe the nested structure of the examples, as indicated by the dotted rectangles. The unique Schmidt rank > 2 component is indicated as shaded shape, Schmidt rank 2 as lines, and separable as circles. The innermost rectangle contains the crosshatch state, the next one contains the first example of a SN 3 state in local dimension 5×6 , while the whole figure shows SN 4 in 7×10 .

ranges $R(\rho)$, $R(\rho^{T_{\rm B}})$. It is worth mentioning that all PPT entangled extremal states belong to the intersection of faces of the positive semidefinite set and its partial transpose, but are not extremal states of both intersected sets. Moreover, such a PPT entangled extremal state is the unique state supported on the ranges $R(\rho)$ and $R(\rho^{T_{\rm B}})$ [43]. We can directly use this result to obtain SN PPT entanglement witnesses.

Take the projectors *P* and *Q* associated to the subspaces $R(\rho)$ and $R(\rho^{T_{\rm B}})$, and add them in the following manner $W_{\rho} \coloneqq P + Q^{T_{\rm B}}$. Then $\operatorname{tr}(W_{\rho}\sigma) \leq 2$, for all PPT σ , with equality holding for $\sigma = \rho$ only. Then for every PPT extremal ρ with $\operatorname{SN}(\rho) = k + 1$, we can find μ_k such that $\mu_k \coloneqq \max_{\sigma_k} \operatorname{tr}(W_{\rho}\sigma_k) < 2$ for PPT σ_k with the Schmidt number *k*. Then $W_{\operatorname{ind},\rho} \coloneqq (\mu_k \mathbb{1} - W_{\rho})$ is a valid witness for Schmidt number (k + 1) PPT states on the PPT set. It can be easily confirmed that $W_{\operatorname{ind},\rho}$ is indeed an indecomposable witness as long as $\mu_k < 2$. More details about this construction can be found in SM [36].

We can use this technique to construct indecomposable entanglement witnesses on the PPT set, as all new normalized states ρ_i depicted in this Letter (in Figs. 1–3, and 5 in SM [36]) are extremal PPT states. For those states, we determine lower bounds on the corresponding μ_1^i using local optimization [44] and upper bounds utilizing the DPS hierarchy [29]. We report our numerical results and confidence intervals in Table I and further details in SM [36].

Discussion.—Increasing attention has been directed toward high-dimensional entanglement, primarily due to its potential advantages in robust quantum information processing. In this Letter, we explore novel classes of highly entangled bound entangled states, yielding several

TABLE I. Table contains upper and lower bounds of μ_1 for various states. Local minima were determined using a seesaw method, and upper bounds by the DPS hierarchy.

	$\rho^{\rm CH}$	$\rho^{5,5}$	$ ho^{(2)}$	$ ho^{(3)}$	$\rho^{4,12}$
$\mu_{ m L}$	≈1.8659	1.9	$(5+\sqrt{5})/4$	$(5 + \sqrt{5})/4$	$(5+2\sqrt{2})/4$
$\mu_{\rm U} - \mu_{\rm L}$	9×10^{-5}	9×10^{-4}	4×10^{-8}	3.6×10^{-2}	5×10^{-10}

technical and conceptual advancements that open a few natural research directions.

First, on the application side, interestingly nearly all our PPT Schmidt number k states enjoy the property that they can be expressed as convex mixture of a SR k maximally entangled state and its orthonormal SN 2 states. This particular property renders our states intriguing contenders as potential counterexamples to the PPT² conjecture.

The family of states presented in this Letter constitute extremal points of the PPT set. It is interesting to explore geometrical undertones for this connection, and use the states to construct indecomposable witnesses for high Schmidt number detection. To this end, a separate study needs to be done to characterize and investigate the rich structure of PPT grid states.

Next, the graphical language we developed to study the concentration protocol can be used to work with multiple copies of mixed states in an efficient manner. This tool could help compute sub- or superadditive entanglement properties of quantum states under tensor product operation.

Finally, the concentration protocol could be used to study multipartite bound entangled states, states which are PPT for any bipartite grouping of its subsystems but are genuine multipartite entangled. Only a few examples of such states exist in literature [37,38,45], and, remarkably, a tripartite grid state in the original formulation, constitutes one of the elegant representatives [30]. The grid states and the graphical concentration protocol can be used to discover more multipartite bound entangled states and investigate their entanglement properties in increasing local dimensions.

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