Characterizing generalized axisymmetric quantum states in $d \times d$ systems

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We introduce a family of highly symmetric bipartite quantum states in arbitrary dimensions. It consists of all states that are invariant under local phase rotations and local cyclic permutations of the basis. We solve the separability problem for a subspace of these states and show that a sizable part of the family is bound entangled. We also calculate some of the Schmidt numbers for the family in $d = 3$, thereby characterizing the dimensionality of entanglement. Our results allow us to estimate entanglement properties of arbitrary states, as general states can be symmetrized to the considered family by local operations.

I. INTRODUCTION

Entanglement remains one of the most significant features that distinguishes quantum theory from a classical description of our world. It also underpins a wide range of quantum information processing tasks, such as quantum key distribution [1], quantum communication [2], and quantum sensing [3], where it acts as a resource for increased performance. Detecting, characterizing, and quantifying the various forms of entanglement present in quantum states is therefore of high practical relevance as well as of fundamental interest [4], shedding light on the principles that build our physical world through the structure of possible correlations between multiple systems.

While detecting entanglement in pure states shared among two parties is trivial, there is no infallible method to decide whether an arbitrary (noisy) bipartite state is entangled [5]. Beyond detecting its presence, it is also important to identify its character. For instance, entanglement can be of high dimension, which provides additional advantages such as noise resistance in entanglement distribution protocols [6] or increased capacity of quantum communication [7]. Consequently, considerable effort is devoted to creating such high-dimensional entangled states in experiments [8].

Entanglement may also be bound, that is, a form of entanglement that cannot be distilled into its purest form of maximal dimensionality by local operations and classical communication [9], which is the resource required by most standard applications in quantum information. The observation that known bound entangled states typically lie in close proximity to the separable states has led to the belief that bound entanglement is a "weak" form of entanglement, thus useless for quantum information processing. Surprisingly though, it has been established that bound entangled states may still serve as a resource for certain tasks, e.g., for

quantum key distribution and entanglement activation [10–12]. The exact relation between distillability and dimensionality of entanglement is an actively researched open question [13–17].

In this paper we explore these two features of entanglement in families of states that obey certain symmetries. Characterizing the entanglement properties of symmetric families has two advantages: First, the reduced number of free parameters makes an otherwise daunting task easier, and second, the symmetries that generate the family provide a simple method to obtain lower bounds on the amount of entanglement (measured either quantitatively or by its dimension) of arbitrary mixed states, by "twirling" them into the family [18]. In addition, fully characterizing the set of separable states in symmetric families can even help in establishing results on entanglement theory that go beyond that subset of states. A recent example is the superadditivity of genuine multipartite entanglement [19], the proof of which relies on having a full characterization of separable isotropic states [20]. To detect the undistillability of entangled states, we resort to the positive partial transpose (PPT) criterion, as entangled states which meet the PPT criterion are known to be bound entangled [21,22]. We also look at the Schmidt numbers of the states in the family, a paradigmatic measure of entanglement dimensionality [23].

With these techniques at hand, we study a highly symmetric family of bipartite mixed states with local dimension d, introduced in Refs. [24–29], fully characterizing the set of separable states in a subset of this family and thereby providing a complete characterization of all PPT entangled states for arbitrary d. We then use fidelity-based Schmidt numbers witnesses, together with a combination of analytical and numerical methods, to further refine the characterization of the sets of states with varying Schmidt

numbers. We show explicit results for $d = 3$ and $d = 4$, although our methodology is extensible to higher local dimensions. Our results comprise an exceptional example of a rich family of states arising from symmetries where their entanglement properties can be described to a very high degree.

II. BASIC NOTIONS OF ENTANGLEMENT AND SYMMETRY

Throughout this paper we denote by ϱ a density matrix that describes a quantum state, which is shared between the two local parties Alice and Bob. We only consider scenarios where the dimensions of the local Hilbert spaces are equal and denote this dimension by d. One central question in quantum information theory is whether or not a quantum state ϱ is entangled. It is well known that for pure quantum states one can calculate the Schmidt rank to answer this question. Pure quantum states are separable if and only if they have Schmidt rank 1 and thus can be written as $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$. Otherwise they are entangled.

A. Schmidt number

In Ref. [23] the definition of the Schmidt rank is extended to mixed states and is called the Schmidt number. To determine if the Schmidt number of a state ϱ, is smaller than or equal to K, one asks for a decomposition of ϱ into pure states $|\psi_i\rangle$ where all Schmidt ranks $\mathcal{S}(|\psi_i\rangle)$ are smaller than or equal to K. To obtain the Schmidt number of ϱ we therefore need to solve

$$\mathcal{S}(\varrho) := \min_{\{p_i, |\psi_i\rangle\}} \max_i \mathcal{S}(|\psi_i\rangle), \tag{1}$$

where p_i and $|\psi_i\rangle$ give valid decompositions of ϱ. Note that if we insert a pure state $\varrho = |\psi\rangle\langle\psi|$ in the above definition we end up with the Schmidt rank $\mathcal{S}(|\psi\rangle)$ of that state. We denote the states that have Schmidt numbers equal to or less than K by S_K. The set of separable states, for example, can be denoted by S_1.

In Fig. 1 there is a schematic overview over these sets and the set of states with positive partial transpose, which we will now cover. Note that we depicted the PPT states inside the states with Schmidt number 2. This is true for dimension $d = 3$ as it was conjectured in Ref. [13] and proven in Ref. [15].

B. PPT criterion and bound entanglement

The PPT criterion to determine if a quantum state is separable was introduced in Ref. [22]. In Ref. [21] it was even shown that for (2×2)- and (2×3)-dimensional systems the criterion is sufficient and completely solves the question whether a given state of that dimension is entangled or not. In higher dimensions states can be PPT and entangled [30]. The PPT criterion states that for a separable state $\varrho = \sum_{i,j,k,l} \varrho_{i,j,k,l} |ij\rangle\langle kl|$ the partial transposition

$$\varrho^{T_B} = \sum_{i,j,k,l} \varrho_{i,l,k,j} |ij\rangle\langle kl|$$

is positive semidefinite.

Positive partial transpose entangled states are particularly interesting since they are bound entangled, i.e., one cannot distill maximally entangled, pure singlet states via local op-
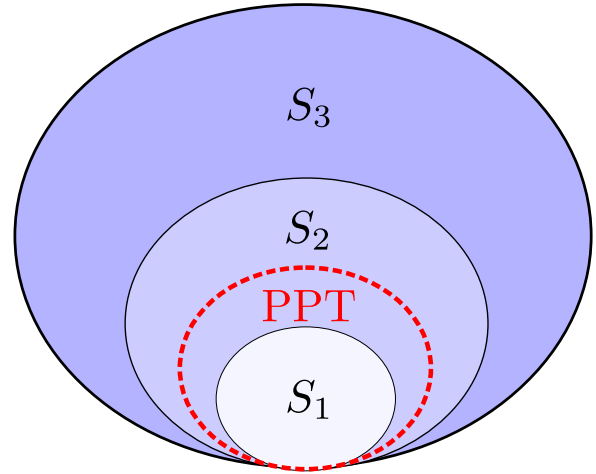

FIG. 1. Schematic view of the state space of 3×3 systems: The sets of states with Schmidt number less than or equal to K are convex. The conjecture from Ref. [13] that for dimension $d = 3$ there are no PPT states with Schmidt number 3 was proven in Ref. [15]. Here S_1 is the set of separable states.

erations and classical communication (LOCC) from them [9]. Bound entangled states were first described in Ref. [9] and even today there are a multitude of open problems about their properties. It is, for example, not known if there are bound entangled states with a negative partial transpose [31]. Furthermore, it has been researched how these states can be used in typical quantum information theory tasks. Although they cannot be directly used for quantum teleportation, it was shown in Ref. [11] that they can be *activated* and then perform these tasks in conjunction with other states.

C. Computable cross norm or realignment criterion

Another important separability criterion is the computable cross norm or realignment (CCNR) criterion [32,33]. For the set of linear operators in the local Hilbert space $\mathcal{H}_A$ there exist local orthogonal bases G_k^A. The mentioned orthogonality is with respect to the Hilbert-Schmidt scalar product, i.e.,

$$\mathrm{Tr}\big(G_k^A G_j^A\big) = \delta_{k,j} \; \forall k, j \in \{1, \dots, d^2\}, \tag{2}$$

where $d = \dim(\mathcal{H}_A)$. An example of a local orthogonal basis would be the generators of $\mathrm{SU}(d)$ appropriately normalized, together with the normalized identity matrix.

Now, by performing a singular value decomposition in operator space, any density matrix ϱ can be written as

$$\varrho = \sum_k \lambda_k G_k^A \otimes G_k^B. \tag{3}$$

The CCNR criterion states that if ϱ is separable, then $\sum_k \lambda_k \leqslant 1$.

In the formulation from Refs. [33,34] the criterion states that separable states ϱ obey

$$\mathrm{Tr}\big[\sqrt{R(\varrho)^\dagger R(\varrho)}\big] \leqslant 1, \tag{4}$$

where $R(\varrho)$ denotes the realigned matrix given by $R(\varrho) = \sum_{i,j,k,l} \varrho_{ij,kl} |ik\rangle\langle jl|$. Using this criterion, it is often possible to prove that a state is entangled although it is PPT.

D. Entanglement quantification

A frequent question in quantum information theory is how strong the entanglement between particles in a certain state is [5]. Such entanglement quantification is important, because one often thinks of entanglement as a kind of useful resource for certain tasks in quantum information processing.

Here we concentrate on the entanglement measure named linear entropy E_{lin} [35]. For pure states it is defined as

$$E_{\text{lin}}(|\psi\rangle) = 2\big[1 - \text{Tr}\big(\varrho_A^2\big)\big], \tag{5}$$

where the second term $\text{Tr}(\varrho_A^2)$ is the purity of the reduced state $\varrho_A = \text{Tr}_B(|\psi\rangle\langle\psi|)$. We extend this definition to mixed states with the convex-roof extension

$$E_{\text{lin}}(\varrho) = \inf_{\{p_k, |\psi_k\rangle\}} \sum_k p_k E_{\text{lin}}(|\psi_k\rangle\langle\psi_k|), \tag{6}$$

where the infimum is calculated over all decompositions of ϱ. A closely related entanglement measure is the concurrence, where one considers the square root of the expression in Eq. (5). For two qubits there is an analytical formula for the concurrence [36]. For larger Hilbert spaces the computation of the convex-roof expansion is often a difficult task. In Ref. [37] a method based on semidefinite programming was developed to compute these entanglement measures. This was utilized in Ref. [24] to calculate the linear entropy for a family of bound entangled qutrit states. For a pure state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ with $\psi_{jk} := \langle j\,k|\psi\rangle$ the formula

$$E_{\text{lin}} = \sum_{jklm} |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2 \tag{7}$$

was derived for the linear entropy in Refs. [38,39].

E. Symmetries

Consider maps of the form

$$\varrho \mapsto \sum_k p_k (U_k \otimes V_k)\varrho(U_k^\dagger \otimes V_k^\dagger), \tag{8}$$

where U_k and V_k are unitaries acting on the respective local Hilbert spaces. This operator defines an LOCC protocol, since the unitaries U_k and V_k act locally and with classical communication one can arrange to apply, for example, $U_j \otimes V_j$ with some probability p_j. Since this map corresponds to an LOCC protocol, we know that it only can decrease entanglement. The families of symmetric states we are interested in are states that are invariant under some of the above maps. Then if one has some insight into the entanglement properties for the family of symmetric states, one can obtain a lower bound for the entanglement of a general state. This is because the twirling map

$$\mathcal{T}(\varrho) = \int_{\mathcal{G}} dg\, g\varrho g^\dagger \tag{9}$$

maps general states to states which are invariant under the group of symmetries $\mathcal{G} \subseteq \{U \otimes V | U, V \in \mathcal{U}(\mathcal{H})\}$. Twirling

can be viewed as averaging over the symmetries $\mathcal{G}$ and behaves like the maps in Eq. (8). This discussion shows that to get insight into the entanglement of the whole state space it is a good idea to study various families of symmetric states, where each family is determined by a group of symmetries $\mathcal{G}$. Multiple families of symmetric states have already been researched. The Werner states [40] and the isotropic states [20] are well known examples of such families. Other families that fulfill this property and have been extensively studied include the graph-diagonal states [41–43] and the Greenberger-Horne-Zeilinger diagonal states [44–48].

III. INTRODUCTION OF THE FAMILY OF STATES EXPLORED

Now we consider states with the following symmetries.

(a) First are simultaneous cyclic permutations of the basis elements of both parties, i.e., $|ij\rangle\langle kl| \mapsto |i \oplus n, j \oplus n\rangle\langle k \oplus n, l \oplus n|$ with $n \in \{1, \ldots, d-1\}$. For dimension $d = 3$, exemplary matrices U_k and V_k from Eq. (8) that correspond to this symmetry are

$$U_1 \otimes V_1 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{10}$$

(b) Second are simultaneous local phase rotations of the form $S(\varphi_1, \varphi_2, \ldots, \varphi_{d-1}) = \exp(i \sum_j \varphi_j \mathfrak{g}_j) \otimes \exp(-i \sum_j \varphi_j \mathfrak{g}_j)$, where $\varphi_1, \ldots, \varphi_{d-1}$ are real parameters and $\mathfrak{g}_j$ are the generators of SU(d) that are diagonal matrices. For $d = 3$ this yields

$$U(\phi_1, \phi_2) \otimes V(\phi_1, \phi_2) = \begin{pmatrix} e^{2\pi i\phi_1} & 0 & 0 \\ 0 & e^{2\pi i\phi_2} & 0 \\ 0 & 0 & e^{-2\pi i(\phi_1+\phi_2)} \end{pmatrix} \tag{11}$$

$$\otimes \begin{pmatrix} e^{-2\pi i\phi_1} & 0 & 0 \\ 0 & e^{-2\pi i\phi_2} & 0 \\ 0 & 0 & e^{2\pi i(\phi_1+\phi_2)} \end{pmatrix}, \tag{12}$$

with real phases $\phi_1, \phi_2 \in \mathbb{R}$. The last diagonal entry is chosen in a way that the determinant is 1. This can be done, since global phases have no physical meaning.

These states were introduced in Ref. [24] and mainly studied for dimension $d = 3$. For a subfamiliy Sentís *et al.* [24] explicitly calculated the convex-roof extension of the linear entropy as well as the concurrence. This is particularly interesting, because the family contains a sizable part of bound entangled states. The family is obtained by relaxing the symmetries from the axisymmetric states in Ref. [49]. The 3×3 family of bound entangled states from Horodecki *et al.* [11] is also contained in the family.

To address the components of the density matrices $\varrho^\diamond$ that are invariant under these symmetries we use the variables

$$\varrho^\diamond_{kj,kj} =: x_{(j-k \bmod d)+1}, \tag{13}$$

and for $k \neq j$,

$$\varrho^\diamond_{kk,jj} =: y_{(k-j \bmod d)}. \tag{14}$$

For $d = 3$ we have the matrix

$$
\varrho^\diamond =
\begin{pmatrix}
x_1 & & & \vdots & & y_2 & & \vdots & & & y_1 \\
& x_2 & & \vdots & & & & \vdots & & & \\
& & x_3 & \vdots & & & & \vdots & & & \\
\hdashline
& & & \vdots & x_3 & & & \vdots & & & \\
y_1 & & & \vdots & & x_1 & & \vdots & & y_2 & \\
& & & \vdots & & & x_2 & \vdots & & & \\
\hdashline
& & & \vdots & & & & \vdots & x_2 & & \\
& & & \vdots & & & & \vdots & & x_3 & \\
y_2 & & & \vdots & y_1 & & & \vdots & & & x_1
\end{pmatrix} . \quad (15)
$$

In the Appendix, Sec. 1, there is a depiction of the matrix for arbitrary dimension.

The matrix has to be Hermitian in order to still be a density matrix. Therefore, the parameters y_i need to fulfill $y_i = y_{d-i}^*$. From the positive semidefiniteness it follows directly that $x_i \geqslant 0$.

We want to find further conditions for the off-diagonal parameters so that $\varrho^\diamond$ is positive semidefinite. For this we change the order of the basis vectors so that the resulting matrix has a circulant block in the upper left corner and the rest of the matrix is diagonal. For $d = 3$ we obtain

$$
\varrho^\diamond =
\begin{pmatrix}
x_1 & y_2 & y_1 & \vdots & & & \vdots & & & \\
y_1 & x_1 & y_2 & \vdots & & & \vdots & & & \\
y_2 & y_1 & x_1 & \vdots & & & \vdots & & & \\
\hdashline
& & & \vdots & x_2 & & \vdots & & & \\
& & & \vdots & & x_2 & \vdots & & & \\
& & & \vdots & & & x_2 & \vdots & & \\
\hdashline
& & & \vdots & & & \vdots & x_3 & & \\
& & & \vdots & & & \vdots & & x_3 & \\
& & & \vdots & & & \vdots & & & x_3
\end{pmatrix} . \quad (16)
$$

In the upper left corner there is a circulant matrix. Its eigenvalues are given by [50] $\lambda_j = x_1 + \sum_{k=1}^{d-1} y_k \omega^{jk} y_k$, where $\omega = e^{2\pi/\mathrm{i}d}$ is the dth root of unity. Therefore, since $\lambda_j \geqslant 0$ the parameters for the off-diagonal elements need to fulfill the inequality

$$
\lambda_j = x_1 + \sum_{k=1}^{d-1} e^{2/\pi ijk/d} y_k \geqslant 0 \; \forall j \in \{0, \ldots, d-1\}. \quad (17)
$$

In the following, we show that the physical states obeying the symmetries form a polytope in the sense that every state that is contained in it can be written as convex combination of a finite set of extremal states. These extremal states cannot be written as a nontrivial convex combination of other states in the family. We begin by searching for these extremal points or vertices.

First we note that states where for a $k \in \{2, \ldots, d\}$ the parameter $x_k = \frac{1}{d}$ and all the other parameters are zero are

extremal. To find all vertices with $x_1 \neq 0$ we have a closer look at the eigenvalues of the circulant block.

With the convention $y_0 := x_1$ we have

$$
\sum_{k=0}^{d-1} e^{2\pi ijk/d} y_k = \lambda_j \geqslant 0, \quad \sum_{j=0}^{d-1} \lambda_j = dy_0. \quad (18)
$$

Therefore, we have a polytope in the space of the possible eigenvalues. Now we can apply the reverse discrete Fourier transform

$$
y_k = \frac{1}{d} \sum_{j=0}^{d-1} \lambda_j e^{-2\pi ijk/d} \quad (19)
$$

to obtain the off-diagonal parameters of our family again. Since the reverse discrete Fourier transform is just a linear operation, we conclude that we have a polytope with a finite set of vertices. For these new vertices we have $\lambda_j = dy_0 = 1$ for only one $j \in \{0, \ldots, d-1\}$ and the other λ_k are zero. In total we have $d + d - 1 = 2d - 1$ vertices. Because we have to enforce the normalization condition, every state is determined by $2(d-1)$ real parameters. This is due to the fact that all introduced vertices are already Hermitian.

One particular vertex corresponds to the maximally entangled state $|\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_i |ii\rangle$. There λ_0 is maximal and the other eigenvalues are zero. The values of the off-diagonal parameters y_j are equal to $x_1 = \frac{1}{d}$ and the other x_k are zero. In later sections we will restrict ourselves to the facet where $|\phi_d^+\rangle\langle\phi_d^+|$ is the only nondiagonal vertex.

PPT and CCNR criteria for the family

To investigate the entanglement properties of the family $\varrho^\diamond$ we apply the CCNR and the PPT criterion. The partial transpose of a matrix like $\varrho^\diamond$ is block diagonal with 2×2 blocks after changing the order of the basis. The PPT criterion states that the determinant of these blocks is, for all j and k, positive for separable states. So PPT states need to fulfill

$$
x_{j-k+1} \times x_{k-j+d+1} - |y_{j-k}|^2 \geqslant 0 \; \forall j, k \in \{1, \ldots, d\}, \; j > k \quad (20)
$$

$$
\Leftrightarrow \sqrt{x_{j-k+1} \times x_{k-j+d+1}} \geqslant |y_{j-k}| \; \forall j, k \in \{1, \ldots, d\}, \; j > k \quad (21)
$$

$$
\Leftrightarrow \sqrt{x_{i+1} \times x_{d+1-i}} \geqslant |y_i| \; \forall i \in \{1, \ldots, d-1\}. \quad (22)
$$

To search for PPT entangled states, we also calculate the CCNR criterion to detect entanglement. The realigned matrix has nonzero entries at the same places as the original density matrix $\varrho^\diamond$. To calculate its eigenvalues we consider again a matrix where the basis vectors are ordered such that in the upper left corner there is a circulant matrix, for which we have formulas for the eigenvalues. The sum of the absolute value of all the eigenvalues is

$$
\sum_i |\eta_i| = d \sum_j |y_j| + \sum_{j=0}^{d-1} \left| \sum_{k=0}^{d-1} x_{k+1} e^{2\pi ikj/d} \right| \quad (23)
$$

and the CCNR criterion states that for separable states $\sum_i |\eta_i| \leqslant 1$. In order to obtain explicit results from Eqs. (22) and (23) we only consider certain facets of the polytope.

IV. BLOCH REPRESENTATION OF THE STATES IN THE FAMILY

The goal of this section is twofold. On the one hand, we elucidate the relation between the magic simplex [25,28] and the family of axisymmetric states as well as the facet of the relaxed axisymmetric states that we will study in detail. On the other hand, we show that there exists a straightforward operator decomposition for these states, which is important for entanglement detection by means of the CCNR criterion.

A. Axisymmetric states as a subset of the magic simplex

The main ingredient needed to discuss the magic simplex is a basis of maximally entangled states in the $(d \times d)$-dimensional Hilbert space. Such bases can always be constructed [51] (discussed below). The magic simplex then is the set of all convex combinations of these basis states. It is characterized by $d^2 - 1$ real parameters, in contrast to the full state space with $d^4 - 1$ parameters.

A basis of maximally entangled states can be found by starting from the standard Bell state in $d \times d$ dimensions,

$$|\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |jj\rangle. \tag{24}$$

By applying local unitaries to $|\phi_d^+\rangle$ we can achieve a complete basis. To this end, we introduce the unitary Weyl matrices Z and X (see, e.g., Refs. [52,53]) that act on d-dimensional Hilbert spaces and have the properties $Z|j\rangle = \omega^j|j\rangle$ and $X|j\rangle = |j \oplus 1\rangle$. As mentioned before, $\omega = e^{2\pi i/d}$ and the addition has to be understood modulo d. Then a full orthonormal basis $\{|\phi_{kl}\rangle\}$ of maximally entangled states is obtained by defining

$$|\phi_{kl}\rangle = Z^k \otimes X^l |\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \omega^{jk} |j(j \oplus l)\rangle, \tag{25}$$

where $0 \leqslant k, l \leqslant d - 1$. For $k = l = 0$ we have $|\phi_{00}\rangle \equiv |\phi_d^+\rangle$.

The magic simplex, i.e., the convex combinations $\sum_{kl} c_{kl} |\phi_{kl}\rangle\langle\phi_{kl}|$ with $0 \leqslant c_{kl} \leqslant 1$ and $\sum_{kl} c_{kl} = 1$, is still a rather complicated object. Therefore, one may consider peculiar families of highly symmetric states that are subsets of the magic simplex, but are described by fewer parameters. The first family we consider here are the axisymmetric states [54] that generalize the isotropic states [20],

$$\varrho_{\text{axi}} = p|\phi_d^+\rangle\langle\phi_d^+| + q\varrho_0 + (1 - p - q)\varrho_{(1)} \tag{26}$$

with $0 \leqslant p, q \leqslant 1$, where

$$\varrho_0 = \frac{1}{d-1} \sum_{k=1}^{d-1} |\phi_{k0}\rangle\langle\phi_{k0}|$$

$$= \frac{1}{d-1} \sum_{k=1}^{d-1} |kk\rangle\langle kk| - \frac{1}{d(d-1)} \sum_{k \neq l} |kk\rangle\langle ll| \tag{27}$$

and

$$\varrho_{(1)} = \frac{1}{d(d-1)} \sum_{k=0, l=1}^{d-1} |\phi_{kl}\rangle\langle\phi_{kl}|$$

$$= \frac{1}{d-1} \sum_{l=1}^{d-1} \frac{1}{d} \sum_{k=0}^{d-1} |k(k \oplus l)\rangle\langle k(k \oplus l)|. \tag{28}$$

The axisymmetric states are all the mixed states that share the symmetries of the Bell state $|\phi_d^+\rangle$ (simultaneous local phase rotations with opposite sign for the two parties, simultaneously exchanging the labels of the levels of the local d-state systems). They are convex combinations of the three states given above for all local dimensions d. Evidently, this family is a subset of the magic simplex. It was shown [54] that there are no bound entangled axisymmetric states, so in order to have such states in the family we have to lower the degree of symmetry.

It turns out that it is sufficient to relax the symmetry under arbitrary simultaneous level permutations of the two parties into a cyclic permutation symmetry in order to allow for bound entanglement. One consequence of this modification compared to the axisymmetric states is that the state $\varrho_{(1)}$ in Eq. (28) splits up into $d - 1$ states ϱ_l, $l = 1, \ldots, d - 1$. Another consequence of the symmetry relaxation is that the off-diagonal elements may have different moduli as well as complex phases, as we explained in the preceding section. We restrict our attention to a subfamily of the relaxed axisymmetric states that evidently lies within the magic simplex. The peculiar facet that we consider here is the convex hull of the standard Bell state $|\phi_d^+\rangle$ and the states ϱ_l that result from splitting up $\varrho_{(1)}$,

$$\varrho_{\text{facet}}^{\diamond} = p|\phi_d^+\rangle\langle\phi_d^+| + \sum_{l=1}^{d-1} q_l \varrho_l, \tag{29}$$

where $p + \sum_l q_l = 1$ and

$$\varrho_l = \frac{1}{d} \sum_{k=0}^{d-1} |\phi_{kl}\rangle\langle\phi_{kl}|$$

$$= \frac{1}{d} \sum_{k=0}^{d-1} |k(k \oplus l)\rangle\langle k(k \oplus l)|, \ l = 1, \ldots, d - 1. \tag{30}$$

B. Bloch representation for a facet of the relaxed axisymmetric states

Because of their high symmetry it is *per se* interesting to study what this means for the Bloch representation of the states in the family. It will turn out particularly useful for the application of the CCNR criterion.

As a matrix basis for the Bloch representation we will choose the (unitary) displacement operators D_{jk} with their standard definition [53]

$$D_{jk} = Z^j X^k \omega^{-jk/2}. \tag{31}$$

An important rule for calculations is $X^k Z^j = Z^j X^k \omega^{-jk}$. Again we start with the standard Bell state whose Bloch

representation is given by

$$|\phi_d^+\rangle\langle\phi_d^+| = \frac{1}{d^2}\sum_{a,b=0}^{d-1} D_{ab} \otimes D_{ab}^*. \tag{32}$$

The validity of this equation is readily seen from the general representation of the SWAP operator valid for any orthonormal matrix basis $\{G_j\}$, $j = 1 \ldots d^2$, $\mathrm{Tr}(G_j^\dagger G_k) = d\delta_{jk}$, that is, SWAP $= \frac{1}{d}\sum_j G_j \otimes G_j^\dagger$, and the well-known relation SWAP $= d|\phi_d^+\rangle\langle\phi_d^+|^{T_B}$ (cf. Ref. [55]). With the definition (25) we obtain also the Bloch representations of the other states of the basis $\{|\phi_{kl}\rangle\}$,

$$|\phi_{kl}\rangle\langle\phi_{kl}| = \frac{1}{d^2}\sum_{a,b=0}^{d-1} D_{ab} \otimes D_{ab}^* \omega^{al+bk}. \tag{33}$$

It is now straightforward to determine the Bloch decomposition of the remaining extremal states of the facet, Eq. (29). We find

$$\varrho_l = \frac{1}{d^2}\sum_{a=0}^{d-1} D_{a0} \otimes D_{a0}^* \omega^{al}, \quad l = 1, \ldots, d-1. \tag{34}$$

These results are remarkable because of their simplicity. The most important property is that the Bloch decomposition of the axisymmetric states is diagonal in the Weyl basis, which facilitates direct application of the CCNR criterion: It suffices to use the absolute values of the Bloch coefficients instead of the singular values of the operator Schmidt decomposition (see Sec. II).

V. ENTANGLEMENT ANALYSIS FOR A CERTAIN FACET

We will fully characterize the set of separable states in a subfamily of $\varrho^\diamond$ corresponding to a facet of the polytope. By adapting the state parameters to those of Sec. III, we obtain for the states in the facet of the polytope

$$\varrho_{\mathrm{facet}}^\diamond := dx_1|\phi_d^+\rangle\langle\phi_d^+| + \sum_{k=1}^{d-1} x_{k+1} \sum_{j=0}^{d-1} |j(j \oplus k)\rangle\langle j(j \oplus k)|, \tag{35}$$

which are determined by $d-1$ real parameters. A schematic overview of the facet can be seen in Fig. 2. How one obtains results for the Schmidt numbers will be discussed in Sec. VI A.

The previously defined off-diagonal parameters y_k are all set to $y_k = x_1$. The normalization relation is still the same:

$$d\sum_{k=1}^{d} x_k = 1. \tag{36}$$

We want to show that in this facet all separable states are convex combinations of $\varrho_k := \frac{1}{d}\sum_{j=0}^{d-1} |j(j \oplus k)\rangle\langle j(j \oplus k)|$ and the state ϱ_{sep}, which is defined such that $\frac{1}{d^2} = x_j = y_j \, \forall j \in \{1, \ldots, d\}$. The state ϱ_{sep} is part of the family of axisymmetric states in Ref. [49]. There it was shown to be separable. Another proof is given in Ref. [56] [see Eq. (B5) therein]. Additionally, we show a decomposition into separable states of ϱ_{sep} in the Appendix, Sec. 2.
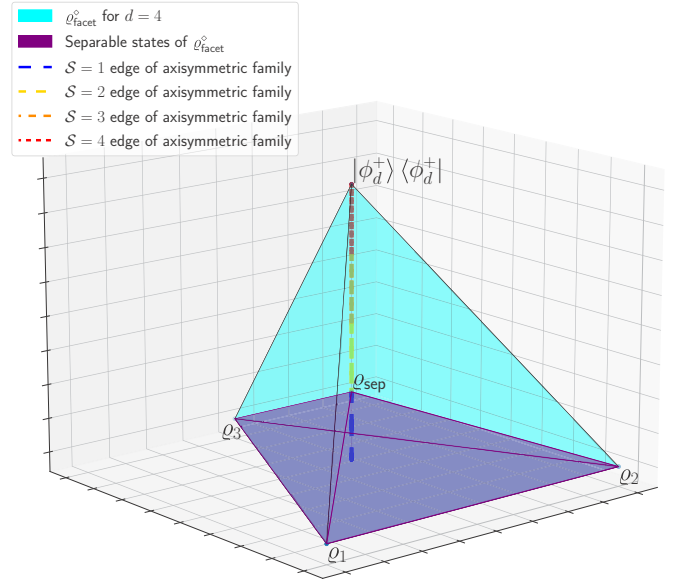

FIG. 2. Facet for $d = 4$. If $x_2 = x_3 = x_4$ we arrive at an edge from the axisymmetric states from Ref. [49]. We will prove that all separable states lie in the purple (dark gray) polytope.

A. Linear entropy as an entanglement criterion

In Ref. [24] a method was described to calculate the linear entropy of states that are invariant under an entanglement preserving symmetry. It can be applied as follows. The set $\{|\phi_d^+\rangle\langle\phi_d^+|, \varrho_1, \ldots, \varrho_{d-1}\}$ consists of states that span the facet we are interested in. They are invariant under the symmetries, which were used to construct these states. We can parametrize an arbitrary state as follows:

$$\mathrm{Tr}(\varrho\varrho_k) = x_{k+1} \, \forall k \in \{1, \ldots, d-1\}$$
$$\wedge \, \mathrm{Tr}(\varrho|\phi_d^+\rangle\langle\phi_d^+|) = dx_1. \tag{37}$$

A state in the facet $\sigma_{x_1,\ldots,x_d}$ is uniquely determined by the parameters $x_1, \ldots, x_d$. With the theorem from Ref. [24] we can get a formula for the linear entropy. Explicitly, we have to do the following steps.

(i) Find a parametrization for all pure states in the span of σ dependent on the facet parameters $x_1, \ldots, x_d$ and other parameters ξ. Denote these pure states by $|\psi_\sigma\rangle$. It follows that every decomposition of a state σ only uses pure states from $|\psi_\sigma\rangle$.

(ii) Compute the function $\tilde{E}_{\mathrm{lin}}(x_1, \ldots, x_d) = \min_\xi E_{\mathrm{lin}}(|\psi_\sigma(x_1, \ldots, x_d, \xi)\rangle)$, where ξ are the parameters of $|\psi_\sigma\rangle$ that are not facet parameters.

(iii) The function $\tilde{E}_{\mathrm{lin}}(x_1, \ldots, x_d)$ is not necessarily convex. Compute its convexification $\tilde{E}_{\mathrm{lin}}^c(x_1, \ldots, x_d)$.

(iv) Then the identity $\tilde{E}_{\mathrm{lin}}^c(x_1, \ldots, x_d) = E_{\mathrm{lin}}(\sigma_{x_1,\ldots,x_d})$ holds.

In the following we construct a subset $\mathcal{K}$ of the facet that includes all separable states. This property would be fulfilled

if the following were true:

$$\tilde{E}_{\text{lin}}^c(x_1, \dots, x_d) = 0 \implies \sigma_{x_1, \dots, x_d} \in \mathcal{K}. \tag{38}$$

We know that the zero set of the convexified function $\tilde{E}_{\text{lin}}^c(x_1, \dots, x_d)$ is just the convexification of the zero set of the initial function $\tilde{E}_{\text{lin}}(x_1, \dots, x_d)$:

$$\{x_1, \dots, x_d | \tilde{E}_{\text{lin}}^c(x_1, \dots, x_d) = 0\}$$
$$= \{x_1, \dots, x_d | \tilde{E}_{\text{lin}}(x_1, \dots, x_d) = 0\}^c. \tag{39}$$

For now we search for a set that includes all states where $\tilde{E}_{\text{lin}}(x_1, \dots, x_d) = 0$. This can be achieved by finding the states where $\tilde{E}_{\text{lin}}(x_1, \dots, x_d) > 0$ and considering all other states.

Pure states that build a decomposition of a state in the facet are of the form

$$|\psi_\sigma\rangle = \sqrt{dx_1}|\phi_d^+\rangle + \sum_{k=1}^{d-1} \sqrt{dx_{k+1}} \sum_{j=0}^{d-1} \xi_{k,j} |j\ (j \oplus k)\rangle, \quad (40)$$

where $\sum_{j=0}^{d-1} |\xi_{k,j}|^2 = 1$ and $\xi_{j,k} \in \mathbb{C}$ for all $k \in \{1, \dots, d-1\}$.

Now by using Eq. (7) we get the formula

$$\tilde{E}_{\text{lin}}(x_1, \dots, x_d) = \min_\xi \sum_{jklm} |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2, \tag{41}$$

where $\psi_{lm} := |\psi(x_1, \dots, x_d, \xi)\rangle_{lm}$. The minimization over the complex phases is simple. For two complex numbers $r_1 e^{i\phi_1}$ and $r_2 e^{i\phi_2}$, the minimum of $|r_1 e^{i\phi_1} + r_2 e^{i\phi_2}|^2$ is achieved for $\phi_1 = \phi_2 + \pi$. Therefore, our minimization problem yields the same value if we assume all coefficients $\xi_{k,j}$ to be real. This allows us to conclude that, for $\tilde{E}_{\text{lin}}(x_1, \dots, x_d)$ to be zero, there has to exist a ξ so that

$$|\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2 = 0 \,\forall j, k, l, m \in \{0, \dots, d-1\}$$
$$\Leftrightarrow \psi_{jk}\psi_{lm} = \psi_{jm}\psi_{lk} \,\forall j, k, l, m \in \{0, \dots, d-1\}. \tag{42}$$

An implication of Eq. (42) is the following:

$$\prod_{l=1}^{d} \psi_{ll} = \prod_{l=1}^{d} \psi_{l\,l\oplus m} \,\forall m \in \{0, \dots, d-1\}. \tag{43}$$

For example, for $d = 3$, $\psi_{00}\psi_{11}\psi_{22} = \psi_{01}\psi_{10}\psi_{22} = \psi_{01}\psi_{12}\psi_{20}$. Inserting the state coefficients from Eq. (40), we obtain

$$(\sqrt{x_1})^d = (\sqrt{dx_{k+1}})^d \prod_{j=0}^{d-1} \xi_{k,j} \leqslant (\sqrt{x_{k+1}})^d. \tag{44}$$

Here the inequality $\prod_{j=0}^{d-1} \xi_{k,j} \leqslant (\frac{1}{\sqrt{d}})^d$ was used.[1]

Since squaring and taking the dth power are both monotonic operations, the inequalities (44) cannot be true (regardless of ξ) if for some $k \in \{2, \dots, d\}$, $x_1 > x_k$. However, since

---

[1]Consider the optimization problem $\max_{(a_1, \dots, a_d) \in \mathbb{R}_+^d} \prod_{i=1}^{d} a_i$ subject to $\sum_i a_i^2 = 1$. For $d = 2$ the solution is straightforward. For higher dimensions one can solve this iteratively. The geometric interpretation is that the hyperrectangle with the largest volume that is contained in a hypersphere is a hypersquare.

the inequalities (44) are an implication of $\tilde{E}_{\text{lin}}(x_1, \dots, x_d) = 0$, we get the true statement

$$\tilde{E}_{\text{lin}}(x_1, \dots, x_d) = 0 \Rightarrow x_1 \leqslant x_k \,\forall k \in \{2, \dots, d\}. \tag{45}$$

Therefore, we know that the set of states where the coefficients have the property $x_1 \leqslant x_r \,\forall r \in \{2, \dots, d\}$ includes all the states with facet parameters so that $\tilde{E}_{\text{lin}}(x_1, \dots, x_d) = 0$. It is easy to see that the set of states with coefficients obeying $x_1 \leqslant x_k \,\forall k \in \{2, \dots, d\}$ coincides with the polytope spanned by $\varrho_{\text{sep}}, \varrho_1, \dots, \varrho_{d-1}$. According to Eq. (39), the convexification of this subset yields a set that includes all states where the linear entropy is zero. Since our subset is already convex, the convexification leaves it invariant. This shows that all separable states in the facet are convex combinations of $\varrho_{\text{sep}}, \varrho_1, \dots, \varrho_{d-1}$. However, since we showed at the beginning that ϱ_{sep} is separable, the converse is also true and we know that all states in the polytope spanned by $\varrho_{\text{sep}}, \varrho_1, \dots, \varrho_{d-1}$ are separable.

B. PPT and CCNR criteria for the facet

From Eq. (22) we can directly state the PPT criterion for the facet

$$\sqrt{x_{i+1} \times x_{d+1-i}} \geqslant |x_1| \,\forall i \in \{1, \dots, d-1\}. \tag{46}$$

Next we look at the CCNR criterion given in Eq. (23) for the facet

$$\sum_i |\lambda_i| = d(d-1)x_1 + \sum_{j=0}^{d-1} \left| \sum_{k=0}^{d-1} x_{k+1} e^{2\pi ikj/d} \right|. \tag{47}$$

Applying the triangle inequality yields

$$\sum_i |\lambda_i| \geqslant d(d-1)x_1 + \left| \sum_{j=0}^{d-1} \sum_{k=0}^{d-1} x_{k+1} e^{2\pi ikj/d} \right|$$
$$= d(d-1)x_1 + \left| dx_1 + \sum_{k=1}^{d-1} x_{k+1} \frac{1 - e^{2\pi ikd/d}}{1 - e^{2\pi ik/d}} \right|$$
$$= d(d-1)x_1 + \left| dx_1 + \sum_{k=1}^{d-1} x_{k+1} \frac{1 - 1}{1 - e^{2\pi ik/d}} \right|$$
$$= d(d-1)x_1 + |dx_1|$$
$$= d^2 x_1. \tag{48}$$

Therefore, we know that if $x_1 > \frac{1}{d^2}$ the state is entangled according to the CCNR criterion. By its negation, separability implies that $x_1 \leqslant \frac{1}{d^2}$, which is in accordance with our result from the preceding section. We now give an example for some

PPT entangled states with

$$x_1 \leqslant \frac{1}{d^2}, \quad \beta \in [0, x_1], \quad l \in \left\{ 2, \ldots, \left\lfloor \frac{d}{2} \right\rfloor \right\} \forall k \in \{2, \ldots, d\} \setminus \{l, d-l+2\}$$

$$x_k = x_1, \quad x_l = x_1 - \beta, \quad x_{d+2-l} = \frac{1}{d} - (d-1)x_1 + \beta. \tag{49}$$

We calculate the CCNR criterion for these states,

$$\begin{aligned}
\sum |\eta_i| &= d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| \sum_{k=0}^{d-1} x_k e^{2\pi i jk/d} \right| \\
&= d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| -\beta e^{2\pi i jl/d} + \left(\frac{1}{d} - dx_1 + \beta \right) e^{2\pi i j(d+2-l)/d} \right| \\
&= d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| e^{4\pi i j(1-l)/d} \left(\frac{1}{d} - dx_1 + \beta \right) - \beta \right| \\
&\geqslant d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| \left| e^{4\pi i j(1-l)/d} \left(\frac{1}{d} - dx_1 + \beta \right) \right| - \beta \right| \\
&= d(d-1)x_1 + \frac{1}{d} + (d-1) \left[\left(\frac{1}{d} - dx_1 + \beta \right) - \beta \right] \\
&= d(d-1)x_1 + \frac{1}{d} + (d-1) \left(\frac{1}{d} - dx_1 \right) = 1, \tag{50}
\end{aligned}$$

where we applied the reverse triangle inequality. Since $e^{4\pi i j(1-l)/d}$ is not equal to 1 for all j, the inequality is not tight and thus we know that the state is entangled. Next we calculate for which values of β the states are PPT. For the states described in Eq. (49), the inequality (22) reads

$$\begin{aligned}
x_1 &\leqslant \sqrt{(x_1 - \beta) \left(\frac{1}{d} - (d-1)x_1 + \beta \right)} \\
&= \sqrt{(x_1 - \beta) \left(\frac{1}{d} - dx_1 \right) + x_1^2 - \beta^2}
\end{aligned}$$

$$\Leftrightarrow 0 \leqslant (x_1 - \beta) \left(\frac{1}{d} - dx_1 \right) - \beta^2$$

$$\Leftrightarrow 0 \geqslant \beta^2 + \left(\frac{1}{d} - dx_1 \right) \beta - \left(\frac{1}{d} - dx_1 \right) x_1. \tag{51}$$

We check for which β the equality is fulfilled:

$$\beta_{\pm} = -\frac{\frac{1}{d} - dx_1}{2} \pm \sqrt{\frac{\left(\frac{1}{d} - dx_1 \right)^2}{4} + \left(\frac{1}{d} - dx_1 \right) x_1}. \tag{52}$$

For the case that there is a plus sign the solution is positive (β_+) and the state is PPT entangled for $\beta \in [0, \beta_+]$. The states can be seen in Fig. 3 for a cross section in $d = 4$.

In this section we restricted our analysis of entanglement properties to a facet of the state polytope. We proved that the state ϱ_{sep}, where all matrix elements have the same value, is separable. Moreover, we proved that all separable states are in the polytope spanned by ϱ_{sep} and the vertices that correspond to states with diagonal density matrices. Since the PPT

criterion is easy to compute, we have a full characterization of the PPT entangled states in the facet.

In the Appendix, Sec. 3, we also give an example of an entangled state that is not detected by the CCNR criterion.

VI. CHARACTERIZING THE DIMENSIONALITY OF ENTANGLEMENT

A. Calculation of Schmidt numbers

To get some insight into the dimensionality of entanglement of our states we want to calculate their Schmidt numbers.
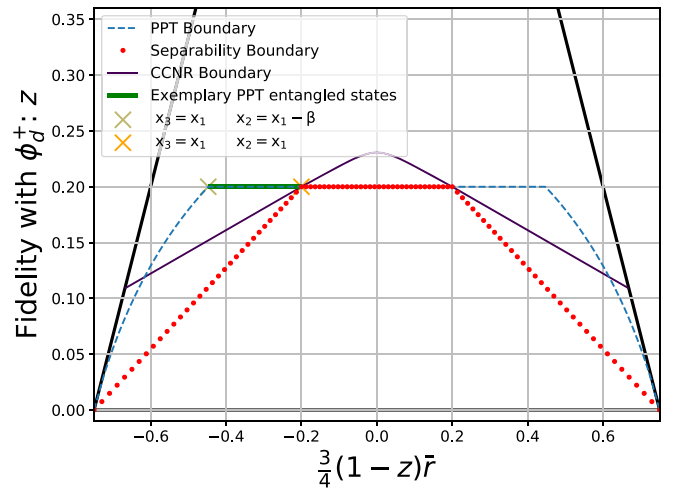

FIG. 3. Cross section of the facet in $d = 4$ in $x_3 = \frac{1}{4d}(1-z)$ and $x_{2,4} = \frac{3}{4d}(1-z)\frac{1 \pm \bar{r}}{2}$, where z and $\bar{r}$ are fidelity parameters analogous to those defined in Eqs. (58)–(60).

In analogy to entanglement witnesses, Schmidt number witnesses play an important role in calculating Schmidt numbers. In Ref. [23] Schmidt number witnesses were introduced. An observable W is called a Schmidt witness of class $K \in \mathbb{N}$ if and only iff $\mathrm{Tr}(W\rho) \geqslant 0$ for all ρ with Schmidt number smaller than K. One also requires that at least one state with Schmidt number K is detected, i.e., fulfills $\mathrm{Tr}(W\rho) < 0$. A K Schmidt witness W_1 is called finer than a K Schmidt witness W_2 if W_1 detects the same states as W_2 and some states in addition.

It was proven in Ref. [23] that $W = \frac{K-1}{d}\mathbb{I} - |\phi_d^+\rangle\langle\phi_d^+|$ is an optimal K Schmidt witness. We calculate the states in the facet that are detected by this witness:

$$
\begin{aligned}
\mathrm{Tr}(W\varrho) &= \mathrm{Tr}\Bigg[\left(\frac{K-1}{d}\mathbb{I} - |\phi_d^+\rangle\langle\phi_d^+|\right)\left(a|\phi_d^+\rangle\langle\phi_d^+|\right. \\
&\quad \left. + \sum_{k=1}^{d-1} b_k \sum_{j=0}^{d-1} |j(j \oplus k)\rangle\langle j(j \oplus k)|\right)\Bigg] \\
&= \frac{K-1}{d} - \mathrm{Tr}(a|\phi_d^+\rangle\langle\phi_d^+|) \\
&= \frac{K-1}{d} - a.
\end{aligned} \tag{53}
$$

Since we are interested in the separable states, which have Schmidt number 1, we look at the case $K = 2$. This yields

$$
\begin{aligned}
\mathrm{Tr}(W\varrho) \geqslant 0 &\Leftrightarrow \frac{1}{d} - a \geqslant 0 \\
&\Leftrightarrow \frac{1}{d} \geqslant dx_1 \Leftrightarrow \frac{1}{d^2} \geqslant x_1,
\end{aligned} \tag{54}
$$

which is the same bound as the one we already derived above in Eq. (48).

We will now describe a strategy to approximate the border between states with maximal Schmidt number and states with less than maximal Schmidt number. First one searches pure states that do not have full Schmidt rank and are twirled to the facet. Then the resulting states after the twirling operation cannot have full Schmidt number either since twirling is an LOCC map.

Therefore, we start by looking at the full Hilbert space $\mathcal{H} \otimes \mathcal{H}$ and consider how the pure states are mapped by the twirling operator. Let $\sigma \in \mathcal{H} \otimes \mathcal{H}$ and $\mathcal{T}\sigma = \varrho$. Then

$$
\varrho_{i;i\oplus j,i;i\oplus j} = \frac{1}{d}\sum_k \sigma_{k;k\oplus j,k;k\oplus j} \; \forall i,j \in \{0,\dots,d-1\},
$$

$$
\tag{55}
$$

$$
\varrho_{i;i,i\oplus j;i\oplus j} = \frac{1}{2d}\sum_k (\sigma_{k;k,k\oplus j;k\oplus j} + \sigma_{k\oplus j;k\oplus j,k;k}). \tag{56}
$$

If the twirling operator maps the state σ to the state ϱ, then we know that the Schmidt number of σ is greater than or equal to the Schmidt number of ϱ, since twirling is an LOCC map. For simplicity, we investigate the problem for dimension $d = 3$. In Ref. [24] we have the following parametrization of the pure
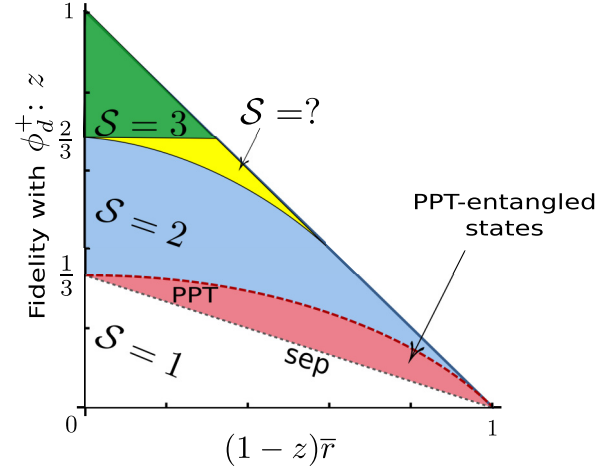

FIG. 4. Progress in calculating the Schmidt numbers $\mathcal{S}$ of the states in the facet for $d = 3$. While witnesses can give a lower bound on the Schmidt number, showing that a state with nonfull Schmidt rank is twirled to a state in the facet can give an upper bound.

states that are mapped in the span of $\rho^\diamond$:

$$
\begin{aligned}
|\psi_\sigma\rangle = \sqrt{z}|\phi_d^+\rangle + \sqrt{1-z}&\Bigg(\sqrt{\frac{1+\bar{r}}{2}}(a|01\rangle + b|12\rangle \\
&+ c|20\rangle) + \sqrt{\frac{1-\bar{r}}{2}}(e|02\rangle + f|10\rangle + g|21\rangle)\Bigg).
\end{aligned} \tag{57}
$$

Here z is a facet parameter with respect to $|\phi_d^+\rangle$, $\bar{r} \in [-1, 1]$, and the complex parameters a, b, c, e, f, and g fulfill the normalization conditions $|a|^2 + |b|^2 + |c|^2 = 1$ and $|e|^2 + |f|^2 + |g|^2 = 1$. The connection to the previously used parametrization is

$$
x_1 = \frac{z}{3}, \tag{58}
$$

$$
x_2 = \frac{(1-z)(1+\bar{r})}{6}, \tag{59}
$$

$$
x_3 = \frac{(1-z)(1-\bar{r})}{6}. \tag{60}
$$

In the Appendix, Sec. 4, we calculated some upper bounds for several values of $\bar{r}$ by choosing the parameters $a, \dots, g$ so that the coefficient matrix becomes circulant.

The obtained results for the Schmidt numbers in the facet for dimension $d = 3$ are schematically summarized in Fig. 4. For states in the yellow area we still do not know if they have Schmidt number 2 or 3. The curve between the yellow and the blue area is given by Eq. (A8) in the Appendix, Sec. 4.

For higher dimensions one can also obtain upper bounds for the Schmidt number by twirling of pure states without full Schmidt rank. We start from the parametrization of an arbitrary pure state that is twirled to the facet, which can be seen in Eq. (40). We choose $a_{k,j} = -\frac{1}{\sqrt{d}}$ so that the coefficient matrix becomes circulant. Because of this simplification, we will not find all states with maximal Schmidt number. We again set the eigenvalue that is a sum of the distinct matrix
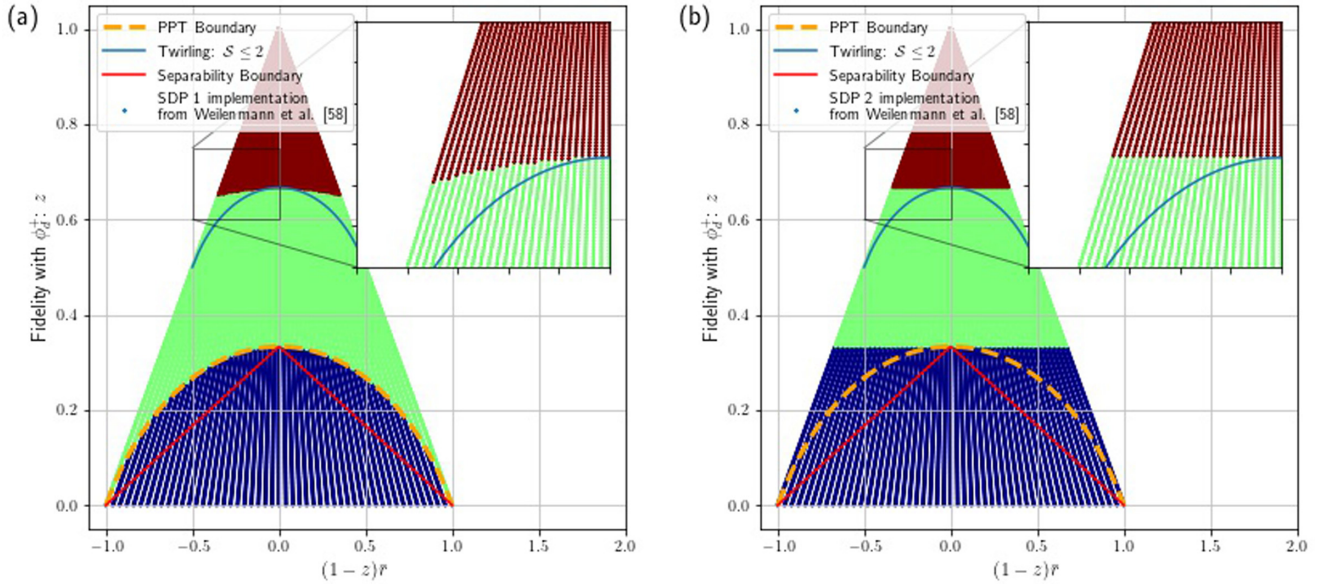
FIG. 5. Calculation of the Schmidt numbers $\mathcal{S}$ of the states in the facet for $d = 3$: (a) states with at least Schmidt number 1 (blue, bottom), 2 (green, middle), and 3 (red, top) ad (b) the blue states in the region at the bottom are 2-unfaithful, while the green ones in the middle are 3-unfaithful. The parametrization is analogous to that in [24]. For 500×50 states we calculated (a) SDP1 and (b) SDP2 from Ref. [58].

entries to zero:

$$\sqrt{x_1} = \sum_{k=1}^{d-1} \sqrt{x_{k+1}}. \tag{61}$$

In the Appendix, Sec. 5, we solve this equation for x_1.

With this equation we certified for some states that they do not have full Schmidt rank. For $d = 3$, we show the resulting upper bound for Schmidt number 2 states in Fig. 5. Note that applying Schmidt witnesses, on the other hand, gives lower bounds on the Schmidt number of the respective states.

Another idea to get insight into the Schmidt numbers is by calculating the K concurrence from Ref. [57] using the convex characteristic curve method. If the K concurrence then vanishes for a particular state we know that its Schmidt number is smaller than K. However, we realized that this idea is impractical, since in the analogous formulas like Eq. (41) for $K > 2$ one cannot eliminate the complex phases.

B. Computation of semidefinite programming hierarchy

In Ref. [58] a method was presented to estimate Schmidt numbers that cannot be calculated from pure fidelity Schmidt witnesses. Pure fidelity Schmidt witnesses can be written as a linear combination of the identity and a projection onto a pure entangled state. In Fig. 5 we computed the first semidefinite programming (SDP) hierarchy. This computation can give a lower bound on the Schmidt number of a mixed state, whereas the second SDP hierarchy proposed in Ref. [58] can prove for a state that its Schmidt number cannot be detected with a fidelity witness.

As shown in Fig. 5, bound entangled states are not detectable as entangled by the first SDP hierarchy. On the other hand, the hierarchy detects states as having Schmidt number 3 beyond those detectable by a pure fidelity Schmidt witness (insets of Fig. 5).

VII. CONCLUSION

In summary, we have discussed the entanglement properties of a family of highly symmetric, bipartite, mixed quantum states in arbitrary dimensions, which can be seen as a generalization of axisymmetric states. We were able to solve the separability problem for a subfamily, including the characterization of bound entanglement, and characterized also the dimensionality of entanglement for some cases.

There are several directions in which our work may be extended. First, one may study bipartite quantum states with the given symmetry further. Here it would be desirable to find bound entangled states far away from the border of separability or to determine entanglement monotones, such as the entanglement of formation for the considered family of states. In addition, the symmetric bound entangled states in our family, defined in arbitrary dimensions, comprise a promising test bed for finding simpler counterexamples to the Peres conjecture, which stated that bound entangled states cannot display nonlocality. The known counterexamples to date [59–61] are constructed *ad hoc* and are not defined through symmetries. Finding counterexamples that arise more naturally, as our family of states, could shed more light on whether the original statement by Peres is true except for specially handcrafted examples or it is more generally false. Finally, one may consider the multipartite scenario, where states with the given symmetries can also be defined in a straightforward manner. Then it would be useful to discuss the different classes of multiparticle entanglement in this scenario.

ACKNOWLEDGMENTS

APPENDIX: PROOFS AND CALCULATIONS

1. Form of the density matrix $\varrho^\diamond$

The density matrices $\varrho^\diamond$ of states that are invariant under these symmetries can be written in the form

$$
\varrho^\diamond =
\begin{pmatrix}
x_1 & 0 & 0 & & & y_{d-1} & & & & y_2 & \cdots & y_1 \\
0 & x_2 & 0 & & & & & & & & & \\
0 & 0 & x_3 & & & & & & & & & \\
& & & \ddots & & & & & & & \ddots & \\
& & & & x_d & & & & & & & \\
\hline
& & & & & x_d & & & & & & \cdots \\
y_1 & & & & & & x_1 & & & y_{d-1} & & \\
& & & & & & & x_2 & & & & \\
& & & & & & & & \ddots & & & \\
& & & & & & & & & x_{d-1} & & \\
\hline
& & & & & & & & & & x_{d-1} & \cdots \\
& & & & & & & & & & & x_d \\
y_2 & & & & y_1 & & & & & & & x_1 \\
\vdots & \ddots & & \vdots & & \ddots & & \vdots & & & & x_2 & \ddots \\
y_{d-1} & & & & & & & & & & & & x_1
\end{pmatrix}.
\tag{A1}
$$

2. Decomposition into separable states for ϱ_{sep}

To prove that ϱ_{sep} is indeed separable we give a decomposition into separable states. First we define 2^d states of the following form:

$$
|\varphi_b\rangle := \frac{1}{d} \sum_{k=0}^{d-1} (-1)^{b_k} e^{i\omega k} |k\rangle \; \forall b \in \{0,1\}^d.
\tag{A2}
$$

We consider states of the form $|\varphi_b\rangle \otimes |\varphi_b^*\rangle$ to decompose ϱ_{sep} into separable states. The following calculation shows the decomposition:

$$
\frac{1}{2\pi 2^d} \int d\omega \sum_{b \in \{0,1\}^d} |\varphi_b\rangle \otimes |\varphi_b^*\rangle \langle \varphi_b| \otimes \langle \varphi_b^*|
$$

$$
= \frac{1}{2\pi 2^d d^2} \int d\omega \sum_{b \in \{0,1\}^d} \sum_{j,k,l,m} (-1)^{b_j+b_k+b_l+b_m} e^{i\omega(j-k-l+m)} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m|
$$

$$
= \frac{1}{2^d d^2} \sum_{b \in \{0,1\}^d} \sum_{j,k,l,m} (-1)^{b_j+b_k+b_l+b_m} \delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m|
$$

$$
= \frac{1}{d^2} \sum_{j,k,l,m} [(\delta_{j,k}\delta_{l,m} + \delta_{j,m}\delta_{l,k})(1 - \delta_{j,l}) + \delta_{j,l}\delta_{k,m}] \delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m|
$$

$$
= \frac{1}{d^2} \sum_{j,k,l,m} [\delta_{j,k}\delta_{l,m}(1 - \delta_{j,m}) + \delta_{j,l}\delta_{k,m}] \delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m|
$$

$$= \frac{1}{d^2} \sum_{j,k,l,m} [\delta_{j,k}\delta_{l,m}(1 - \delta_{j,m}) + \delta_{j,l}\delta_{k,m}]|j\rangle \otimes |k\rangle\langle l| \otimes \langle m|$$

$$= \frac{1}{d^2} \sum_{j,l} \sum_{j \neq l} |jj\rangle\langle ll| + \frac{1}{d^2} \sum_{j,k} |jk\rangle\langle jk| = \varrho_{\text{sep}}. \tag{A3}$$

3. Example of an entangled state that is not detected by CCNR

Consider the state with

$$x_1 = \tfrac{1}{80}, \quad x_2 = x_3 = \tfrac{19}{160}. \tag{A4}$$

Since $x_3 = 0 < x_1$ this state is entangled according to the above considerations. However, calculating the formula (23) yields a value smaller than 1.

4. Determining upper bounds for Schmidt coefficients by looking at pure states with a circulant coefficient matrix

For the general case in Eq. (57) it is difficult to calculate the number of nonvanishing singular values of the coefficient matrix analytically. Although it is possible to obtain the Schmidt rank numerically (uniformly), randomly sampling the pure states will almost certainly lead to a state with full Schmidt rank.

However, if we consider states with $a = b = c$ and $e = f = g$, the coefficient matrix is circulant and one can easily calculate the eigenvalues. We get a particular easy example if we set $\frac{1}{\sqrt{3}} = a = b = c = e = f = g$. For the case $\bar{r} = 0$ we obtain that all coefficients are equal:

$$\sqrt{\frac{z}{3}} = \sqrt{\frac{1-z}{6}} \Rightarrow z = \frac{1-z}{2} \Rightarrow z = \frac{1}{3}. \tag{A5}$$

Since all entries of the coefficient matrix are equal, the matrix has only one eigenvalue and therefore Schmidt number 1. Further, the state is indeed twirled to ϱ_{sep}, which was shown to be separable above. Another state we can construct has the parameters $\frac{-1}{\sqrt{3}} = a = b = c = e = f = g$. Since the coefficient matrix is circulant, one of the three eigenvalues is simply the sum over all different entries of the matrix. To get an upper bound of the Schmidt number of the state σ, we set this particular eigenvalue to zero for $\bar{r} = 0$:

$$0 = \sqrt{\frac{z}{3}} - 2\sqrt{\frac{1-z}{6}} \Rightarrow z = 2(1-z) \Rightarrow z = \frac{2}{3}. \tag{A6}$$

This result is in agreement with the first Schmidt number witness W_2 in Eq. (53) that we applied, because the Schmidt witness is tangent to the state. Another state we can investigate is at $\bar{r} = 1$. We again set the same eigenvalue equal to zero and keep in mind that the coefficients with $\sqrt{1-r}$ vanish:

$$0 = \sqrt{\frac{z}{3}} - \sqrt{2}\sqrt{\frac{1-z}{6}} \Rightarrow z = (1-z) \Rightarrow z = \frac{1}{2}. \tag{A7}$$

For the $\bar{r}$ values in between we still can look at a circulant coefficient matrix and set one eigenvalue equal to zero,

$$0 = \sqrt{\frac{z}{3}} - \sqrt{1-z}\left(\sqrt{\frac{1+\bar{r}}{6}} + \sqrt{\frac{1-\bar{r}}{6}}\right) \Leftrightarrow \sqrt{x_1} = \sqrt{x_2} + \sqrt{x_3} \Rightarrow x_1 = x_2 + x_3 + 2\sqrt{x_2 x_3} \Rightarrow 2x_1 = \tfrac{1}{3} + 2\sqrt{x_2 x_3}$$

$$\Rightarrow x_1 = \tfrac{1}{6}\left(1 - 3x_2 \pm \sqrt{3}\sqrt{2x_2 - 9x_2^2}\right), \tag{A8}$$

where we used the normalization condition $x_1 + x_2 + x_3 = \frac{1}{3}$.

5. States with Schmidt rank less than d

We saw that some states with Schmidt rank smaller than d are characterized by

$$\sqrt{x_1} = \sum_{k=1}^{d-1} \sqrt{x_{k+1}}. \tag{A9}$$

With the normalization condition $\frac{1}{d} = \sum_{k=1}^{d} x_k$ we get $\sqrt{x_1} = \sqrt{\frac{1}{d} - x_1 - \sum_{m=3}^{d} x_m + \sum_{k=3}^{d} \sqrt{x_k}}. \tag{A10}$

To solve this for x_1 one has to essentially solve some quadratic equation. The solution is

$$x_1 = \frac{1}{2}\left[\frac{1}{d} - \sum_{k=3}^{d} x_k - \left(\sum_{k=3}^{d}\sqrt{x_k}\right)\sqrt{4\left(\frac{1}{d} - \sum_{m=3}^{d} x_m\right) + \left(\sum_{m=3}^{d}\sqrt{x_m}\right)^2}\right], \tag{A11}$$

which is the generalization of (A8) to higher dimensions.

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[1] M. Curty, M. Lewenstein, and N. Lütkenhaus, Entanglement as a Precondition for Secure Quantum Key Distribution, Phys. Rev. Lett. **92**, 217903 (2004).

[2] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Quantum entanglement, Rev. Mod. Phys. **81**, 865 (2009).

[3] L. Pezzé and A. Smerzi, Entanglement, Nonlinear Dynamics, and the Heisenberg Limit, Phys. Rev. Lett. **102**, 100401 (2009).

[4] A. C. Dada, J. Leach, G. S. Buller, M. J. Padgett, and E. Andersson, Experimental high-dimensional two-photon entanglement and violations of generalized Bell inequalities, Nat. Phys. **7**, 677 (2011).

[5] O. Gühne and G. Tóth, Entanglement detection, Phys. Rep. **474**, 1 (2009).

[6] S. Ecker, F. Bouchard, L. Bulla, F. Brandt, O. Kohout, F. Steinlechner, R. Fickler, M. Malik, Y. Guryanova, R. Ursin, and M. Huber, Overcoming Noise in Entanglement Distribution, Phys. Rev. X **9**, 041042 (2019).

[7] M. Mirhosseini, O. S. Magaña-Loaiza, M. N. O'Sullivan, B. Rodenburg, M. Malik, M. P. J. Lavery, M. J. Padgett, D. J. Gauthier, and R. W. Boyd, High-dimensional quantum cryptography with twisted light, New J. Phys. **17**, 033033 (2015).

[8] M. Erhard, M. Krenn, and A. Zeilinger, Advances in high-dimensional quantum entanglement, Nat. Phys. **2**, 365 (2020).

[9] M. Horodecki, P. Horodecki, and R. Horodecki, Mixed-State Entanglement and Distillation: Is there a "Bound" Entanglement in Nature? Phys. Rev. Lett. **80**, 5239 (1998).

[10] K. Horodecki, M. Horodecki, P. Horodecki, and J. Oppenheim, Secure Key from Bound Entanglement, Phys. Rev. Lett. **94**, 160502 (2005).

[11] P. Horodecki, M. Horodecki, and R. Horodecki, Bound Entanglement Can Be Activated, Phys. Rev. Lett. **82**, 1056 (1999).

[12] L. Masanes, All Bipartite Entangled States Are Useful for Information Processing, Phys. Rev. Lett. **96**, 150501 (2006).

[13] A. Sanpera, D. Bruß, and M. Lewenstein, Schmidt-number witnesses and bound entanglement, Phys. Rev. A **63**, 050301(R) (2001).

[14] S. J. Szarek, E. Werner, and K. Życzkowski, How often is a random quantum state k-entangled? J. Phys. A: Math. Theor. **44**, 045303 (2011).

[15] Y. Yang, D. H. Leung, and W.-S. Tang, All 2-positive linear maps from $M_3(\mathbb{C})$ to $M_3(\mathbb{C})$ are decomposable, Linear Algebra Appl. **503**, 233 (2016).

[16] L. Chen, Y. Yang, and W.-S. Tang, Schmidt number of bipartite and multipartite states under local projections, Quantum Inf. Process. **16**, 75 (2017).

[17] M. Huber, L. Lami, C. Lancien, and A. Müller-Hermes, High-Dimensional Entanglement in States with Positive Partial Transposition, Phys. Rev. Lett. **121**, 200503 (2018).

[18] G. Sentís, C. Eltschka, O. Gühne, M. Huber, and J. Siewert, Quantifying Entanglement of Maximal Dimension in Bipartite Mixed States, Phys. Rev. Lett. **117**, 190502 (2016).

[19] C. Palazuelos and J. I. de Vicente, Genuine multipartite entanglement of quantum states in the multiple-copy scenario, Quantum **6**, 735 (2022).

[20] M. Horodecki and P. Horodecki, Reduction criterion of separability and limits for a class of distillation protocols, Phys. Rev. A **59**, 4206 (1999).

[21] M. Horodecki, P. Horodecki, and R. Horodecki, Separability of mixed states: Necessary and sufficient conditions, Phys. Lett. A **223**, 1 (1996).

[22] A. Peres, Separability Criterion for Density Matrices, Phys. Rev. Lett. **77**, 1413 (1996).

[23] B. M. Terhal and P. Horodecki, Schmidt number for density matrices, Phys. Rev. A **61**, 040301(R) (2000).

[24] G. Sentís, C. Eltschka, and J. Siewert, Quantitative bound entanglement in two-qutrit states, Phys. Rev. A **94**, 020302(R) (2016).

[25] B. Baumgartner, B. C. Hiesmayr, and H. Narnhofer, State space for two qutrits has a phase space structure in its core, Phys. Rev. A **74**, 032327 (2006).

[26] R. A. Bertlmann and P. Krammer, Bloch vectors for qudits, J. Phys. A: Math. Theor. **41**, 235303 (2008).

[27] R. A. Bertlmann and P. Krammer, Bound entanglement in the set of Bell-state mixtures of two-qutrits, Phys. Rev. A **78**, 014303 (2008).

[28] R. A. Bertlmann and P. Krammer, Geometric entanglement witnesses and bound entanglement, Phys. Rev. A **77**, 024303 (2008).

[29] R. A. Bertlmann and P. Krammer, Entanglement witnesses and geometry of entanglement of two-qutrit states, Ann. Phys. (NY) **324**, 1388 (2009).

[30] P. Horodecki, Separability criterion and inseparable mixed states with positive partial transposition, Phys. Lett. A **232**, 333 (1997).

[31] P. Horodecki, Ł. Rudnicki, and K. Życzkowski, Five open problems in quantum information theory, PRX Quantum **3**, 010101 (2022); O. Krueger and R. F. Werner, Some open problems in quantum information theory, arXiv:quant-ph/0504166.

[32] O. Rudolph, Further results on the cross norm criterion for separability, Quantum Inf. Process. **4**, 219 (2005).

[33] K. Chen and L.-A. Wu, A matrix realignment method for recognizing entanglement, Quantum Inf. Comput. **3**, 193 (2003).

[34] C.-K. Li, Y. Poon, and N.-S. Sze, A note on the realignment criterion, J. Phys. A: Math. Theor. **44**, 315304 (2011).

[35] P. Rungta, V. Bužek, C. M. Caves, M. Hillery, and G. J. Milburn, Universal state inversion and concurrence in arbitrary dimensions, Phys. Rev. A **64**, 042315 (2001).

[36] W. K. Wootters, Entanglement of Formation of an Arbitrary State of Two Qubits, Phys. Rev. Lett. **80**, 2245 (1998).

[37] G. Tóth, T. Moroder, and O. Gühne, Evaluating Convex Roof Entanglement Measures, Phys. Rev. Lett. **114**, 160501 (2015).

[38] S. Albeverio and S.-M. Fei, A note on invariants and entanglements, J. Opt. B **3**, 223 (2001).

[39] P. Badziag, P. Deuar, M. Horodecki, P. Horodecki, and R. Horodecki, Concurrence in arbitrary dimensions, J. Mod. Opt. **49**, 1289 (2002).

[40] R. F. Werner, Quantum states with Einstein-Podolsky-Rosen correlations admitting a hidden-variable model, Phys. Rev. A **40**, 4277 (1989).

[41] M. Hein, J. Eisert, and H. J. Briegel, Multiparty entanglement in graph states, Phys. Rev. A **69**, 062311 (2004).

[42] A. Kay, Bound entanglement in tree graphs, J. Phys. A: Math. Theor. **43**, 495301 (2010).

[43] O. Gühne, Entanglement criteria and full separability of multiqubit quantum states, Phys. Lett. A **375**, 406 (2011).

[44] W. Dür and J. I. Cirac, Classification of multiqubit mixed states: Separability and distillability properties, Phys. Rev. A **61**, 042314 (2000).

[45] A. O. Pittenger and M. H. Rubin, Complete separability and Fourier representations of *n*-qubit states, Phys. Rev. A **62**, 042306 (2000).

[46] O. Gühne and M. Seevinck, Separability criteria for genuine multiparticle entanglement, New J. Phys. **12**, 053002 (2010).

[47] K. Nagata, Necessary and sufficient condition for Greenberger-Horne-Zeilinger diagonal states to be full *N*-partite entangled, Int. J. Theor. Phys. **48**, 3358 (2009).

[48] L. E. Buchholz, T. Moroder, and O. Gühne, Evaluating the geometric measure of multiparticle entanglement, Ann. Phys. (Berlin) **528**, 278 (2016).

[49] C. Eltschka and J. Siewert, Negativity as an Estimator of Entanglement Dimension, Phys. Rev. Lett. **111**, 100503 (2013).

[50] R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge University Press, Cambridge, 2012).

[51] K. Vollbrecht and R. Werner, Why two qubits are special, J. Math. Phys. **41**, 6772 (2000).

[52] H. Weyl, Quantenmechanik und Gruppentheorie, Z. Phys. **46**, 1 (1927).

[53] A. Vourdas, Quantum systems with finite Hilbert space, Rep. Prog. Phys. **67**, 267 (2004).

[54] C. Eltschka, G. Tóth, and J. Siewert, Partial transposition as a direct link between concurrence and negativity, Phys. Rev. A **91**, 032327 (2015).

[55] M. M. Wolf, Quantum channels & operations: A guided tour, available at http://www-m5.ma.tum.de/foswiki/pub/M5/Allgemeines/MichaelWolf/QChannelLecture.pdf (unpublished).

[56] G. Vidal and R. Tarrach, Robustness of entanglement, Phys. Rev. A **59**, 141 (1999).

[57] G. Gour, Family of concurrence monotones and its applications, Phys. Rev. A **71**, 012318 (2005).

[58] M. Weilenmann, B. Dive, D. Trillo, E. A. Aguilar, and M. Navascués, Entanglement Detection beyond Measuring Fidelities, Phys. Rev. Lett. **124**, 200502 (2020).

[59] T. Vértesi and N. Brunner, Disproving the Peres conjecture by showing Bell nonlocality from bound entanglement, Nat. Commun. **5**, 5297 (2014).

[60] T. Moroder, O. Gittsovich, M. Huber, and O. Gühne, Steering Bound Entangled States: A Counterexample to the Stronger Peres Conjecture, Phys. Rev. Lett. **113**, 050404 (2014).

[61] S. Yu and C. H. Oh, Family of nonlocal bound entangled states, Phys. Rev. A **95**, 032111 (2017).