The structure of multidimensional entanglement in multipartite systems

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We explore the structure of multipartite quantum systems which are entangled in multiple degrees of freedom. We find necessary and sufficient conditions for the characterization of tripartite systems and necessary conditions for any number of parties. Furthermore we develop a framework of multi-level witnesses for efficient discrimination and quantification of multidimensional entanglement that is applicable for an arbitrary number of systems and dimensions.

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ψ be a pure bipartite state and let ρA and ρB be its corresponding reductions. The Schmidt rank of ψ is defined as dψ := rank(ρA) = rank(ρB). Since dψ is the minimal number of terms one needs to write the state in a biorthogonal product basis (i.e., Schmidt decomposition), this number clearly gives the minimal local dimensions for subsystems A and B. Thus, ψ is effectively a two-qudit state. The generalization to mixed states ρ is given by the Schmidt number \[ d_\rho = \min \max_{\mathcal{D}(\rho)} d_\psi, \] where the minimization is over all ensemble decompositions of ρ, \( \mathcal{D}(\rho) = \{ p_i, |\psi_i\rangle : \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i | \} \). This is a very natural definition as this means that ρ cannot be obtained by mixing pure states of Schmidt rank lower than \( d_\rho \), and that there exists a way to prepare the state by mixing states with Schmidt rank at most \( d_\rho \). Moreover, the Schmidt number is an entanglement monotone and can thus be used to quantify the degree of entanglement \( d_\rho \) and, also, it can be operationally interpreted as the zero-error entanglement cost in the protocol of one-shot entanglement dilution \[ [22] \]. Notice that although in general the computation of the Schmidt number is involved, there exists ways to obtain lower bounds for this measure. In particular, one can define the set of states with Schmidt number at most \( d \), \( S_d \), which induces a Russian doll structure of convex sets (i.e., \( S_d \subset S_{d+1} \)) and Schmidt number witnesses can be defined \[ [23] \].

Let us now move to the multipartite case. For the sake of readability we will discuss the tripartite case in detail, as the generalization to even higher numbers of parties follows in a straightforward way. A tripartite pure state has three single-particle marginals of inequivalent rank (which we will from now on abbreviate via rank(ρM) := rM), i.e., for |ψ⟩ ∈ \( \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \) we can look at reduced states \( p_i := \text{Tr}_i (|\psi\rangle \langle \psi |) \). Three of the six possible reductions are sufficient as of course \( r_A = r_{BC}, r_B = r_{AC} \) and \( r_C = r_{AB} \) holds. Thus in order to characterize tripartite states three numbers are enough, i.e., \( (r_A, r_{AB}, r_{AC}) \). Although these three ranks can potentially be different not every combination of integers can actually be achieved by a physical quantum state. One can show that the subadditivity of the Rényi 0-entropy, which translates as the submultiplicativity of the ranks is actually a necessary and sufficient constraint on the three numbers, i.e., let without loss of generality \( r_A \geq r_B, r_C \) be fulfilled, then for every set of numbers fulfilling \( r_A \leq r_{BC} \) there exists a pure state realizing exactly this combination \[ [31] \]. For a higher number of parties this is not sufficient anymore \[ [32] \], which could be solved via introducing the following conjecture for tripartite reductions of 4-partite pure states \( r_{AB} r_{AC} r_{BC} \geq r_{A} r_{B} r_{C} \) \[ [33] \].

Focusing again on tripartite systems we arrange \( r_A, r_B \) and \( r_C \) in non-increasing order to form the vector \( (r_1, r_2, r_3) \). Given a pure state |ψ⟩, its entanglement dimensionality vector (or Schmidt rank vector) is defined as \( d_\psi := (r_1^\psi, r_2^\psi, r_3^\psi) \). The extension of this definition to mixed states is not completely straightforward because, contrary to the bipartite case, if one consider states of entanglement dimensionality \( r_1 \) or less, \( r_2 \) or less and \( r_3 \) or less, this just defines a partial ordering and, as a consequence, one cannot trivially obtain a structure of sets in which, given any two subsets, one is always embedded in the other. This can be seen by considering the example of a state with Schmidt vector \( (4, 2, 2) \) and a state of Schmidt vector \( (3, 3, 2) \). In order to resolve this ambiguity, to obtain a well-defined mathematical structure and to impose a physically-meaningful classification we propose the following definition for entanglement dimensionality vectors (or Schmidt number vectors) for mixed states: A state \( \rho \) has Schmidt number vector \( d_\rho = (r_1, r_2, r_3) \) iff

\[ r_j = \min \max_{\mathcal{D}(\rho)} r_\psi. \] That is, for all ensemble decompositions of \( \rho, \mathcal{D}(\rho) = \{ p_i, |\psi_i\rangle : \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i | \} \), there exists a \( |\psi_i\rangle \) with \( r_j^\psi \) at least \( r_j \) and there exists a particular ensemble decomposition in which all \( |\psi_i\rangle \) satisfy \( r_j^\psi \leq r_j \forall i \).

The structure of sets of states induced by this definition is depicted in Fig. 4 where in a slight abuse of notation we denote by \( (r_1, r_2, r_3) \) the set of all states with Schmidt number vector with entries at most \( r_1 \), at most \( r_2 \) and at most \( r_3 \). Some comments are in order. First, notice that each entry \( r_j \) of the Schmidt number vector is an entanglement monotone. This is straightforward as the local rank of each \( |\psi_i\rangle \) in an ensemble decomposition of \( \rho \) cannot be increased by LOCC \[ [24] \]. However, this is just a partial order as there exist incomparable states according to this measure, e.g., those in the subsets \( (r_1, r_2, r_3) \) and \( (r_1', r_2', r_3') \) when \( r_1 > r_1' \) but \( r_2 < r_2' \), which is very natural since the states in these subsets are LOCC incomparable. This is reflected in the structure of the set of states by the fact that there are subsets in which neither is included in the other like in the case of \( (4, 2, 2) \) and \( (3, 3, 2) \) as schematically shown in Fig. 4. Second, it should be noticed that \( d_\rho = (r_1, r_2, r_3) \) does not imply that \( \rho \) has an optimal ensemble decomposition with one \( |\psi_i\rangle \) such that \( d_\psi = (r_1, r_2, r_3) \) but rather that the state cannot be written solely as mixture of states which are all contained in a set which is lower in the hierarchy induced by the Schmidt number vector to \( (r_1, r_2, r_3) \). Consider for instance the qudit \( (d = 7) \) state \( \rho = p|332\rangle \langle 332| + (1 - p)|422\rangle \langle 422| \).
with \(0 < p < 1\) and
\[
|\psi_{332}\rangle = \frac{1}{\sqrt{3}}(|000\rangle + |111\rangle + |122\rangle),
\]
\[
|\psi_{422}\rangle = \frac{1}{2}(|333\rangle + |344\rangle + |435\rangle + |446\rangle).
\]

This decomposition is clearly optimal as \(|\psi_{332}\rangle\langle\psi_{332}|\) and \(|\psi_{422}\rangle\langle\psi_{422}|\) are supported on orthogonal subspaces. Therefore, \(d_p = (4, 3, 2)\) although it is a mixture of \((3, 3, 2)\) and \((4, 2, 2)\) states and does not contain any \((4, 3, 2)\) state in its support. However, this convention turns out to be very natural from the physical point of view when interpreting the Schmidt number vector as an indication of the number of levels one has to be able to effectively entangle to prepare the state. Despite it is not necessary to mix \((4, 3, 2)\) pure states to prepare \(\rho\), this state cannot be obtained in an experiment without the ability to effectively access 4 quantum levels for one subsystem, 3 for another and 2 for the remaining one \[^{34}\]. Third last, one cannot exclude the possibility of a state that admits two different ensemble decompositions, each of which with states in incomparable subsets like \((3, 3, 2)\) and \((4, 2, 2)\). According to our definition such a state would have entanglement dimensionality \((3, 2, 2)\). This is again physically reasonable taking into account the entanglement monotonicity of each \(r_j\). Moreover, this quantifies the least number of levels one must be able to effectively entangle.

\[
\text{FIG. 1: Schematic representation of a few sets of states}
\]

\[
\text{with a given Schmidt number vector.}
\]

We consider now how to derive conditions to discriminate the entanglement dimensionality of a given mixed state of \(N\) parties. Notice that, contrary to the bipartite case, although Schmidt number vector witnesses can be defined, a single one of them cannot fully identify certain states due to the lack of a Russian doll structure of convex sets. This can be seen by considering the states in \((4, 3, 2)\) which lie in the convex hull of \((3, 3, 2)\) and \((4, 2, 2)\). This problem can be overcome in principle by considering several entanglement witnesses or by defining nonlinear witnesses. We will follow this second approach by introducing the measures
\[
E_k := \inf_{D(\rho)} \sum_i p_i S_k(\psi_i) \quad (k = 1, 2, \ldots, N).
\]

Here, \(S_k(\psi)\) are the entries arranged in non-increasing order of the vector given by the entropies of the single-particle reduced density matrices. For the sake of mathematical convenience we use the linear entropy, i.e. \(S(\rho_A) = \sqrt{2(1 - \text{Tr}(\rho_A^2))}\). We will denote by \(\rho_{s_1}, \ldots, \rho_{s_k}\) the different single-party reduced density matrices in such a way that \(S_k(\psi) = S(\rho_{s_k})\). The last component of this vector is equivalent to a measure of genuine multipartite entanglement that has been introduced in Ref. \[25\] and intensively studied in Ref. \[26\]. Notice that if \(E_k > \sqrt{2(1 - 1/r)}\), this implies that \(r_k \geq r + 1\), i.e. we can lower bound \(r_k \geq \lceil \frac{2}{E_k} \rceil\). Therefore, although the converse is not true, these measures can be used to obtain lower bounds for the Schmidt number vector, thus allowing the possibility of inferring that at least a certain entanglement dimensionality has been achieved. Actually, the measures \(E_k\) are hard to compute in practice \[^{27}\]; however, for simple measures and bipartite systems there exist techniques to estimate certain measures of entanglement using experimentally friendly witness techniques \[^{28, 29}\]. In the following we derive a general framework that allows for the construction of nonlinear witnesses that are experimentally feasible and able to lower bound each \(E_k\) and thus reveal even the non-convex structures of multipartite and multi-dimensional entanglement. In order to do that, let us first consider pure states, which we expand in the computational basis, \(|\psi\rangle = \sum_\eta c_\eta |\eta\rangle\), with \(\eta\) a multi-index of \(N\) entries taking the values 0 and 1. It can be seen that \(S(\rho_{s_k})^2 = \sum_{\eta, \eta'} \langle c_\eta c_{\eta'} - c_{\eta_k} c_{\eta_{k'}} \rangle^2\), where the pair \((c_{\eta_k}, c_{\eta_{k'}})\) is just equal to the pair \((c_a, c_b)\), but with all components of \(\eta\) and \(\eta'\) that are part of the reduction \(s_k\) exchanged. Using that \(|C| \sum_{a_i} |a_i|^2 \geq | \sum_{a_i} a_i |^2 \) \[^{28}\] and that \(|a - b| \geq |a| - |b|\), we have that
\[
S(\rho_{s_k}) \geq \frac{1}{\sqrt{1/|C_k|}} \sum_{\eta, \eta' \in C_k} (|c_\eta c_{\eta'} - c_{\eta_k} c_{\eta_{k'}}|) \quad (5)
\]
for any subset \(C_k\) of multindices of \(N\) entries. Therefore, we can bound our measures \(E_k\) for pure states as
\[
E_k(\psi) \geq \frac{1}{\sqrt{1/|C_k|}} \sum_{\eta, \eta' \in C_k} (|c_\eta c_{\eta'} - \min_{m=1}^k (|c_{\eta_m} c_{\eta'_m}|)\)). \quad (6)
\]

Now we can extend this to mixed states via the observation that \(\inf(A - B) \geq \inf A - \sup B\). First, it is clear that
\[
\inf_{D(\rho)} \sum_i p_i |c_i c_j' \rangle \langle c_i c_j'| \geq | \sum_i p_i c_i c_j' \rangle \langle c_i c_j'| = |\langle \eta | \rho | \eta' \rangle| \quad (7)
\]
For the supremum we can use
\[
\sup_{\mathcal{D}(\rho)} \sum_i p_i \min_{\{s_m\}} \sum_{m=1}^k |c^i_{\eta_{m} \eta'_{m}}|^2 
\leq \min_{\{s_m\}} \sup_{\mathcal{D}(\rho)} \sum_i p_i \sum_{m=1}^k |c^i_{\eta_{m} \eta'_{m}}|^2
\leq \min_{\{s_m\}} \sum_{m=1}^k \sqrt{\sum_i p_i |c^i_{\eta_{m} \eta'_{m}}|^2 (\sum_i p_i |c^i_{\eta_{m} \eta'_{m}}|^2)}
= \min_{\{s_m\}} \sum_{m=1}^k \sqrt{\langle \eta_{m} | \rho | \eta_{m} \rangle \langle \eta'_{m} | \rho | \eta'_{m} \rangle}. \tag{8}
\]

In conclusion, we end up with \( E_k(\rho) \geq W_k(\rho) \), where
\[
W_k(\rho) := \frac{1}{\sqrt{\kappa_k \eta,\eta'}} \sum_{\eta,\eta'} \eta_{m} \eta_{m}' \in C_k \langle \eta | \rho | \eta' \rangle
- \min_{\{s_m\}} \sum_{m=1}^k \sqrt{\langle \eta_{m} | \rho | \eta_{m} \rangle \langle \eta'_{m} | \rho | \eta'_{m} \rangle}. \tag{9}
\]

Thus, we obtain easily computable lower bounds on the Schmidt number vector in terms of the entries of the density matrix. Notice that we are free to play with the subsets \( C_k \) of entries to be considered to obtain the most stringent bounds. Also, the conditions are basis-dependent and one can furthermore optimize over all possible choices of local bases.

It is crucial to investigate how these lower bound nonlinear witness vectors enable a dimensionality classification in the presence of noise. Typically one encounters either white noise or dephasing in experimental situations. So let us consider the following state
\[
\rho_{\text{test}} = \rho_{343} + q \rho_{dp} + \frac{1 - p - q}{64} \mathbb{1}, \tag{10}
\]
where \( \rho_{343} = |\psi_{432}\rangle \langle \psi_{432}| \) is our multidimensionally multipartite entangled target state
\[
|\psi_{432}\rangle = \frac{1}{2} (|000\rangle + |111\rangle + |012\rangle + |123\rangle), \tag{11}
\]
and \( \rho_{dp} \) is the completely dephased state. The crucial step in using the nonlinear witness element as a lower bound on the entropy, and thus the dimensionality is of course the selection of the sets \((\eta, \eta') \in C_k\). We now use a different choice for each entry of the witness vector in order to achieve good noise resistance. For the first component we choose \( C_1 = \{(000, 111), (000, 123), (012, 123)\} \), for the second we choose \( C_2 = \{(000, 111), (000, 123), (012, 123), (000, 012), (111, 123)\} \) and for the maximum entropy we can use the full set \( C_3 = \{(000, 111), (000, 123), (012, 123), (000, 012), (111, 123), (111, 012)\} \). Then using Eq. (9) we arrive at an analytical expression for the entropy lower bounds which we plot in Fig 2.

What is also clearly visible in the example is the fact that using the linear entropy lower bounds to determine the dimensionality of course works best if the distribution of the eigenvalues of the marginals is rather flat. Although this might present itself as a weakness if one aims to characterize fully the dimensionality of mixed states on a theoretical level, we would like to argue that this method actually is advantageous for all practical purposes. First we want to point out that just as in the bipartite case there exist a lot of full rank, indeed even arbitrary dimensionality, states that are \( \epsilon \)-close to the separable states, so even if such a state were to be detected by a more precise criterion, it would immediately introduce problems with experimental precision that would make a meaningful distinction impossible. Secondly the entanglement entropy is at the heart of the advantage of higher dimensional systems, e.g. it directly determines the size of the generated key in a bipartite quantum key distribution scenario (see e.g. Refs. [1, 3]). Using our lower bounds one can achieve two things, first to give a reliable detection method for the dimensionality of multipartite systems and at the same time answer how useful these extra dimensions are in terms of potential applications. In conclusion we have presented for the first time a general classification of multipartite entanglement in terms of multidimensional entanglement. We give necessary and sufficient conditions for the existence of tripartite entanglement classes and necessary...
conditions for any number of parties and with this illustrate the structure of multipartite and multidimensional entanglement and the partial hierarchy of subsets of states it induces. Furthermore we develop a framework of entropy-vector lower bounds that employ nonlinear witness techniques. We explicitly show that these techniques work very well in experimentally feasible and plausible scenarios.

We believe that this not only presents testable conditions about general quantum correlations that are the heart of quantum physics, but also may directly serve as security tests in multidimensional applications of entanglement in quantum key distribution systems. Open challenges include the characterization of entanglement in quantum key distribution systems.

Furthermore, we will employ nonlinear witness techniques. We explicitly show that these techniques work very well in experimentally feasible and plausible scenarios.

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[31] Necessity follows from $r_A = r_{BC} \leq r_{BFC}$. For sufficiency it is enough to consider the state $\sum_{m=1}^{r_A} \sum_{n=0}^{r_B-1} |m(r_A-1)+n\rangle |m\rangle |n\rangle$ which fulfills $r_A = r_{BFC}$. Any state for which $r_A < r_{BFC}$ can be constructed in this way by neglecting some terms in the sum.
[32] A trivial counterexample would be $r_A = r_B = r_C = r = 2$ and $r_{AB} = r_{AC} = r_{BC} = 1$. It obeys the submultiplicativity of ranks, yet it is clearly impossible to realize.
[33] This inequality clearly holds if the tripartite state is pure with equality, for full rank states the left hand side is strictly greater and for all classical distributions it simply follows from the monotonicity of the 0-entropy. It would also rule out the counterexample above.
[34] One can also interpret this definition as the least Schmidt number vector possible if one considers only mixtures of comparable states.