

# An algorithm for characterizing SLOCC classes of multiparticle entanglement

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(Dated: September 11, 2012)

It is well known that the classification of pure multiparticle entangled states according to stochastic local operations leads to a natural classification of mixed states in terms of convex sets. We present a simple algorithmic procedure to prove that a quantum state lies within a given convex set. Our algorithm generalizes a recent algorithm for proving separability of quantum states [J. Barreiro *et al.*, *Nature Phys.* **6**, 943 (2010)]. We give several examples which show the wide applicability of our approach. We also propose a procedure to determine a vicinity of a given quantum state which still belongs to the considered convex set.

PACS numbers: 03.67.-a, 03.67.Mn, 03.65.Aa

## I. INTRODUCTION

The importance of quantum entanglement for quantum computation as well as for many other applications in quantum information processing has raised many fundamental questions regarding its characterization [1]. In mathematical terms, a quantum state is said to be separable, if it can be written as a mixture of projectors onto product states, otherwise it is entangled. Much work has been devoted to the development of criteria (in particular, the well-known tool of entanglement witnesses) which can prove that a quantum state is entangled, which means that it is *outside* of the convex set of separable states [2]. Interestingly, methods which prove that a mixed quantum state is *within* the set of separable states (e.g., by providing an explicit decomposition into product states), are less well known. Nevertheless, for some cases explicit decompositions are known [3–6] and recently even some algorithms for this task have been developed [7–9].

If more than two particles are considered, the problem becomes more complicated, since different classes of multiparticle entanglement exist. One possibility uses the notion of stochastic local operations and classical communication (SLOCC) [10, 11]. For this notion, one can again ask, whether a given state can be decomposed into states of the same SLOCC class, which leads for the case of three spin-1/2 particles to the well known classification into GHZ- and W-states [12]. Distinguishing these classes is a hard task, for partial results see Refs. [12, 13]. Especially if one wishes to prove that a given state is within an entanglement class (such as the W-class), no general methods are known.

In this paper we propose an algorithm which allows

to prove that a given mixed state belongs to a specific SLOCC entanglement class i.e., a decomposition exists where the pure states belong to the specified entanglement class. During the iterative procedure pure states and probabilities of the decomposition are determined as well as the “rest” operator which has an increasing mixedness during the iterations. In case of convergence we determine an explicit decomposition of the initial mixed state in terms of a convex combination of projectors onto pure states with the desired properties as well as a “rest” which is verified to be fully separable. It is not known whether the algorithm converges in all cases, but the method is easy to implement and it turns out to be well working in practice. Our algorithm is a generalization of the algorithm for proving separability from Ref. [9].

Additionally we present a simple method to determine a lower bound on the  $\varepsilon$ -ball of the calculated decomposition [14]. This we achieve by constructing a cross polytope inside the convex set spanned by our decomposition. We find a ball with respect to the Hilbert-Schmidt distance for states in this convex space. This method helps to verify that such properties also hold in case of reasonable small “experimental” errors. In some cases it also helps to get an idea of how far the state is at least away from sets with different properties.

The paper is organized as follows. After an overview about multipartite entanglement and SLOCC entanglement classes in Section II we present in Section III an iterative algorithmic procedure to incrementally determine constituents of a decomposition of a given mixed quantum state. The main ingredient, the maximization of the overlap of a pure state with a given density operator under SLOCC operations, will be presented in Section IV and the properties of the algorithm in terms of convergence as well as scaling is discussed in Sections V-VII. It follows in Section VIII the procedure of determining an  $\varepsilon$ -ball. At the end a series of examples, where decompositions are determined and  $\varepsilon$ -balls are calculated, is presented in Section IX and compared with results already known in the literature. We conclude with possible further improvements and limitations of our procedure.

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## II. DEFINITIONS AND NOTATIONS

Let us first consider pure states. Generally, a pure composite quantum state of  $n$  particles is called entangled if it cannot be written as a tensor product of local states

$$|\psi_E\rangle \neq \bigotimes_{i=1}^k |\phi_i\rangle. \quad (1)$$

where the  $|\phi_i\rangle$  are states on a subset of all  $n$  particles. Depending on the value of  $k$  one can further distinguish the number of parties involved which are not of tensor product form. Consequently, the states are said to be biseparable ( $k = 2$ ), triseparable ( $k = 3$ ), up to  $n$ -separable. If a state does not possess any tensor product structure it is called genuine multipartite entangled.

This classification of pure state entanglement can be refined to the equivalence under stochastic local operations and classical communication (SLOCC) [10, 11]. Physically speaking, SLOCC operations can be implemented with nonzero probability via local operations and classical communication, i.e. a single copy of  $|\psi\rangle$  can be mapped onto  $|\phi\rangle$  using local operations with probability  $p > 0$ , but with probability  $(1 - p)$  some other state may result. If two states can be converted into each other via SLOCC, this implies that both states are in principle useful for the same tasks in information processing, albeit the efficiency might be different. We denote such a class of SLOCC equivalent states by  $\mathcal{C}$ .

Mathematically speaking, a general SLOCC operation can be represented by the action of local operators i.e.,  $A_{\text{SLOCC}} = \bigotimes_i A_i$ , where  $A_i$  are arbitrary operators acting on the  $i$ th party. An SLOCC operation maps the initial state  $|\psi\rangle$  to  $|\phi\rangle$  by

$$|\psi\rangle \mapsto |\phi\rangle = \mathcal{N} A_{\text{SLOCC}} |\psi\rangle, \quad (2)$$

where  $\mathcal{N}$  denotes the normalization.

For mixed quantum states shared between  $n$  parties a state is called entangled if it cannot be written as a convex combination of an  $n$ -fold tensor product of projectors onto pure states [15] i.e.,

$$\varrho_{\text{ent}} \neq \sum_j p_j \bigotimes_{i=1}^n |\psi_i^{(j)}\rangle \langle \psi_i^{(j)}| \quad (3)$$

One can extend this naturally by considering  $k$ -separable states. Finally, a state is genuine multipartite entangled, if it cannot be written as a mixture of biseparable states.

For three qubits and pure genuine entangled states there exist two types of entanglement classes which are not SLOCC equivalent [10]: The two representatives are the GHZ state and the W state

$$\begin{aligned} |GHZ\rangle &= \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle), \\ |W\rangle &= \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle). \end{aligned} \quad (4)$$

Any pure entangled state can either be transformed into  $|GHZ\rangle$  or  $|W\rangle$ , but these two states cannot be converted into each other. The analysis and the hierarchy of the set of mixed W/GHZ states was then developed in Ref. [12]. For more than three qubits already an infinite number of inequivalent SLOCC classes exist [11].

## III. THE MAIN IDEA FOR THE ALGORITHM

### A. Structure of the problem

In this section, we will describe the main idea from Ref. [9] to design an algorithm for proving that a quantum state  $\varrho$  belongs to a given class  $\mathcal{C}$ . In the most general case, the task is to prove that a quantum state  $\varrho$  is a convex combination of some projectors onto pure states  $|\phi_k\rangle$ . This means that we can write

$$\varrho = \sum_k p_k |\phi_k\rangle \langle \phi_k|, \quad (5)$$

where the  $p_k$  form a probability distribution. The  $|\phi_k\rangle \in \mathcal{C}$  are states within a specific class  $\mathcal{C}$ : For instance, if one wishes to prove that  $\varrho$  is fully separable, then  $\mathcal{C}$  is the class of pure fully product states, or if  $\varrho$  should be proven to belong to the W-class for three qubits, then  $\mathcal{C}$  is the class of pure W class states (that is, the SLOCC orbit of  $|W\rangle$ ). In the following, we will denote the set of density matrices that can be decomposed as in Eq. (5) as  $\text{conv}(\mathcal{C})$ , meaning the convex hull of  $\mathcal{C}$ .

In order to design an algorithm to check whether  $\varrho$  can be decomposed as in Eq. (5) we will use the following two facts:

*(a) Convexity:* First, the set of density matrices with a decomposition as in Eq. (5) forms a convex set i.e., if  $\varrho_a$  and  $\varrho_b$  are in  $\text{conv}(\mathcal{C})$ , then  $(1 - p)\varrho_a + p\varrho_b$  is also in  $\text{conv}(\mathcal{C})$ . This is indeed obvious by definition and it will be used as follows: Assume that we have three states  $\varrho_a, \varrho_b$ , and  $\varrho_c$  which obey

$$\varrho_b = \frac{1}{1 - p}(\varrho_a - p\varrho_c) \Leftrightarrow \varrho_a = (1 - p)\varrho_b + p\varrho_c \quad (6)$$

where  $0 \leq p \leq 1$  and  $\varrho_c$  lies in the set  $\text{conv}(\mathcal{C})$ . In this situation, if we can prove that  $\varrho_b \in \text{conv}(\mathcal{C})$ , then  $\varrho_a \in \text{conv}(\mathcal{C})$  must hold, too. We will use this fact in terms of the first part of Eq. (6): starting from  $\varrho_a$  we will subtract a term  $p\varrho_c$  with  $\varrho_c = |\phi_k\rangle \langle \phi_k|$  and  $|\phi_k\rangle \in \mathcal{C}$ . If we can then show that  $\varrho_b \in \text{conv}(\mathcal{C})$ , this implies that  $\varrho_a \in \text{conv}(\mathcal{C})$ .

*(b) Highly mixed states are in  $\text{conv}(\mathcal{C})$ :* As a second fact we need statements which imply that highly mixed states are in  $\text{conv}(\mathcal{C})$ . This, of course, requires a specification of the degree of mixedness and depends on the structure of  $\mathcal{C}$ . For instance, if we consider a bipartite  $N \times M$  system and if  $\mathcal{C}$  denotes the set of pure product states, then it has been shown that if

$$\text{tr}(\varrho^2) \leq \frac{1}{NM - 1} \quad (7)$$

then  $\varrho$  is separable, that is  $\varrho \in \text{conv}(\mathcal{C})$  [16]. Similar results have been obtained for other situations [17–20]. For instance, an  $N$ -qubit state with  $N \geq 3$  for which

$$\text{tr}(\varrho^2) \leq \frac{1}{2^N - \alpha^2} \text{ with } \alpha^2 = \frac{2^N}{\frac{17}{2}3^{N-3} + 1} \quad (8)$$

holds, is fully separable [21]. This condition will be used as a termination condition in the algorithm below.

It should be noted that there are cases, where a condition as Eq. (7) is not directly given. For instance, if  $\mathcal{C}$  is the set of all symmetric product states, then the maximally mixed state is clearly not in  $\text{conv}(\mathcal{C})$ , as  $\text{conv}(\mathcal{C})$  consists of matrices acting on the symmetric space only. Even for the identity operator  $\mathbb{1}_S$  on the symmetric space, a condition like Eq. (7) is not straightforward to derive, since there are non-symmetric states close to  $\mathbb{1}_S$  which are not in  $\text{conv}(\mathcal{C})$ . In our paper, such problems do not play a role, a detailed discussion of symmetric states will be given elsewhere.

## B. The algorithm

Now we can formulate the iterative algorithm to prove that a state  $\varrho$  is in  $\text{conv}(\mathcal{C})$ . The algorithm consists of the following steps:

1. Take the input state  $\varrho$  as  $\varrho_k$  with  $k = 1$ .
2. Consider the optimization problem

$$\max_{|\phi\rangle \in \mathcal{C}} |\langle \phi | \varrho_k | \phi \rangle| \quad (9)$$

and find some state  $|\phi_k\rangle$  within  $\mathcal{C}$  which has a high overlap with  $\varrho_k$ .

The only aim is to find a state with high overlap, one does not need a certified optimal solution of the maximization in Eq. (9). Also one may replace in Eq. (9) the matrix  $\varrho_k$  by  $\sqrt{\varrho_k}$ , which may improve the convergence properties of the algorithm (see Section VII for more discussion).

3. Find an  $\varepsilon_k \geq 0$  such that

$$\varrho_{k+1} := \frac{1}{1 - \varepsilon_k} (\varrho_k - \varepsilon_k |\phi_k\rangle\langle\phi_k|) \quad (10)$$

has no negative eigenvalues and that furthermore  $\text{tr}(\varrho_k^2) \geq \text{tr}(\varrho_{k+1}^2)$  holds. In fact, one can directly calculate the optimal  $\varepsilon_k$ , such that  $\text{tr}(\varrho_{k+1}^2)$  is minimal (see Section VI); this choice is, however, not mandatory. In practical implementations, it can be useful to set an upper bound  $\varepsilon_k \leq \varepsilon_{\max}$ , as this prevents the algorithm from subtracting too much from  $\varrho_k$ .

The main idea is that if  $|\phi_k\rangle$  has a high overlap with  $\varrho_k$ , then it also has a high overlap with the

eigenvector corresponding to the maximal eigenvalue  $\lambda_{\max}(\varrho_k)$  of  $\varrho_k$ . The construction of  $\varrho_{k+1}$  leads typically to  $\lambda_{\max}(\varrho_{k+1}) \leq \lambda_{\max}(\varrho_k)$  and, due to the normalization,  $\lambda_{\min}(\varrho_{k+1}) \geq \lambda_{\min}(\varrho_k)$  holds. Hence,  $\varrho_{k+1}$  will be closer to the maximally mixed state than  $\varrho_k$  and is more likely to obey conditions as in Eq. (7).

4. Check, whether  $\varrho_{k+1}$  fulfills conditions like Eqs. (7, 8). If this is the case, then  $\varrho_{k+1}$  is separable and due to Eq. (6) also  $\varrho_k$  and finally  $\varrho_1$  are in  $\text{conv}(\mathcal{C})$ . Then, the algorithm can terminate.
5. If  $\varrho_{k+1}$  does not fulfill Eqs. (7, 8) return to step 2 and  $k \mapsto k + 1$  and iterate further until Eqs. (7, 8) hold for some  $k$ .

Before discussing and extending this algorithm in detail, two facts must be mentioned: First, it is of course not guaranteed that for a given state in  $\text{conv}(\mathcal{C})$  the algorithm will terminate after a finite number of steps. So we do not claim that the algorithm can in general prove that a state  $\varrho$  is in  $\text{conv}(\mathcal{C})$ , we only claim (and demonstrate in this paper) that the algorithm is a powerful tool which works very well in practice.

Second, a crucial step in the algorithm is the optimization in Eq. (9). As already mentioned, one does not need a certified solution, but still it is important to find a good approximate solution. Clearly, the difficulty of this task depends on the structure of  $\mathcal{C}$ .

For the simple case that  $\mathcal{C}$  are the pure bipartite product states, one can do this as follows: For the optimal  $|\phi\rangle = |a\rangle|b\rangle$  the part  $|a\rangle$  is the eigenvector corresponding to the maximal eigenvalue of  $X_A = \text{tr}_B(\varrho_k \mathbb{1} \otimes |b\rangle\langle b|)$  and  $|b\rangle$  is similarly the vector corresponding to the maximal eigenvalue of  $X_B = \text{tr}_A(\varrho_k |a\rangle\langle a| \otimes \mathbb{1})$ . This can be used to tackle the maximization iteratively: Starting from a random  $|a\rangle$  one computes the optimal  $|b\rangle$  via  $X_B$ , then with this  $|b\rangle$  the optimal  $|a'\rangle$ , then again the optimal  $|b'\rangle$  etc. In practice, this converges quickly against the desired solution. For multiparticle fully separable states, this can be done similarly [22].

If  $\mathcal{C}$  denotes the SLOCC equivalence class of some pure state, however, it is not so clear how to perform the optimization in Eq. (9). For pure three-qubit W class states one may use the explicit parameterization of pure W states from Ref. [12], but for more qubits, such explicit formulae are not available. A central step to extend the algorithm from Ref. [9] to SLOCC classes is therefore a simple algorithm for the maximization in Eq. (9). Such an algorithm will be described in the next section.

Finally, note that the termination conditions Eqs. (7, 8) can also be used for SLOCC classes: From any pure state, one can obtain all pure product states by (non-invertible) SLOCC, hence the fully separable mixed states are a subset of  $\text{conv}(\mathcal{C})$ .

#### IV. MAXIMIZING THE OVERLAP OF $n$ -PARTITE STATES VIA SLOCC

As mentioned in the previous section, a crucial part of the algorithm is to perform the maximization in Eq. (9). If  $\mathcal{C}$  is the SLOCC orbit of a suitably chosen  $n$ -partite pure quantum state  $|\Phi_0\rangle$  in  $\mathcal{H} = \otimes_{i=1}^n \mathcal{H}_i$ , the state after a general SLOCC operation is given by

$$|\Phi'\rangle = \frac{\otimes_{i=1}^n A_i |\Phi_0\rangle}{\sqrt{\langle \Phi_0 | [\otimes_{i=1}^n A_i^\dagger] [\otimes_{i=1}^n A_i] | \Phi_0 \rangle}}, \quad (11)$$

where  $A_i$  is the local filtering (or SLOCC) operator of the  $i$ -th party.

The goal is then to maximize the overlap of  $|\Phi'\rangle$  with a given quantum state  $\varrho$  by applying such an SLOCC operation, so one has to compute

$$\max_{\{A_i\}} \langle \Phi' | \varrho | \Phi' \rangle. \quad (12)$$

The general optimization over the tensor product of SLOCC operators is a hard task. Therefore, one may consider an iterative procedure where in each iteration step ( $\varphi$ ) we optimize the overlap (fidelity) with respect to a single party ( $i$ ) i.e., we calculate a new state by applying a local SLOCC operator of the  $i$ -th party and using the identity for the remaining parties,

$$|\Phi_\varphi\rangle = \frac{\mathbb{1}_{n \setminus i} \otimes A_{i_\varphi} |\Phi_{\varphi-1}\rangle}{\sqrt{\langle \Phi_{\varphi-1} | \mathbb{1}_{n \setminus i_\varphi} \otimes A_{i_\varphi}^\dagger A_{i_\varphi} | \Phi_{\varphi-1} \rangle}}, \quad (13)$$

here  $\mathbb{1}_{n \setminus i_\varphi}$  denotes the identity operator on all parties except the  $i$ -th party. In the following, we will usually omit the symbol  $\mathbb{1}_{n \setminus i_\varphi}$ , when there is no risk of confusion.

In each iteration step the optimizing party is changed, e.g. by going from the first to the second up to the  $n$ -th party and then starting with the first party again. This iterative procedure is continued up to a fixed point, where the state does not change anymore. The calculated SLOCC operator  $A_{i_\varphi}$  is in this case up to some factor proportional to the identity. Note that in general this optimization may converge to a local extremum only, but, as discussed above, global optimality is not required for the separability algorithm.

A possible way to deal with Eq. (13) is to perform a direct numerical optimization over the  $A_{i_\varphi}$ . If  $d_i$  is the dimension of the local Hilbert space  $\mathcal{H}_i$  this requires an optimization over  $2d_i^2 - 1$  real parameters. For multi-qubit states this is directly feasible, however, for larger local dimensions or for a large number of particles  $n$ , it is necessary to have an analytical method to find an  $A_{i_\varphi}$  which increases the overlap. This analytical approach will be explained in the following.

Increasing the overlap in each iteration step is equivalent to (for brevity we use  $i \equiv i_\varphi$ )

$$\langle \Phi_\varphi | \varrho | \Phi_\varphi \rangle = \frac{\langle \Phi_{\varphi-1} | A_i^\dagger \varrho A_i | \Phi_{\varphi-1} \rangle}{\langle \Phi_{\varphi-1} | A_i^\dagger A_i | \Phi_{\varphi-1} \rangle} \geq \langle \Phi_{\varphi-1} | \varrho | \Phi_{\varphi-1} \rangle, \quad (14)$$

or equivalently

$$\begin{aligned} & \langle \Phi_{\varphi-1} | A_i^\dagger \varrho A_i | \Phi_{\varphi-1} \rangle \\ & - \langle \Phi_{\varphi-1} | \varrho | \Phi_{\varphi-1} \rangle \langle \Phi_{\varphi-1} | A_i^\dagger A_i | \Phi_{\varphi-1} \rangle \geq 0. \end{aligned} \quad (15)$$

In this inequality only the operator  $A_i$  is unknown. We denote the overlap (fidelity) of the previous iteration step by  $F_{\varphi-1} = \langle \Phi_{\varphi-1} | \varrho | \Phi_{\varphi-1} \rangle$  and choosing a local orthonormal basis we can rewrite

$$A_i = \sum_{r,s} a_{r,s} |r\rangle \langle s|, \quad (16)$$

$$\varrho = \sum_{r,\xi_1,s,\xi_2} r_{r\xi_1,s\xi_2} |r, \xi_1\rangle \langle s, \xi_2| \quad \text{and} \quad (17)$$

$$|\Phi_{\varphi-1}\rangle = \sum_{r,\xi} c_{r\xi} |r, \xi\rangle, \quad (18)$$

with  $a_{r,s} \in \mathbb{C}$ ,  $r_{r\xi_1,s\xi_2} = r_{s\xi_2,r\xi_1}^* \in \mathbb{C}$ , and  $c_{r\xi} \in \mathbb{C}$ , where we used the multi-indices  $\xi_1, \xi_2$  which denote all index elements of the  $n \setminus i$ -partite system.

With this parametrization the last term of the left hand side in Eq. (15) takes the form

$$\begin{aligned} \langle \Phi_{\varphi-1} | A_i^\dagger A_i | \Phi_{\varphi-1} \rangle &= \text{tr} \left( A_i^\dagger A_i \text{tr}_{n \setminus i} (|\Phi_{\varphi-1}\rangle \langle \Phi_{\varphi-1}|) \right) \\ &= \text{tr} \left( A_i^\dagger A_i C \right) = \sum_{h,j,l} a_{lh}^* a_{lj} (C)_{hj} \\ &= \sum_{h,j,l} a_{lh}^* a_{lj} (\tilde{C})_{lh,lj} = \sum_{\zeta_1, \zeta_2} a_{\zeta_1}^* a_{\zeta_2} (\tilde{C})_{\zeta_1, \zeta_2} \\ &= \langle a | \tilde{C} | a \rangle. \end{aligned} \quad (19)$$

Here,  $C$  is just the matrix representation of  $\text{tr}_{n \setminus i} (|\Phi_{\varphi-1}\rangle \langle \Phi_{\varphi-1}|)$  and we used  $(\tilde{C})_{l_1 h, l_2 j} = \delta_{l_1 l_2} C_{hj}$ , that is

$$\begin{aligned} (\tilde{C})_{\zeta_1=(lh), \zeta_2=(lj)} &= (\text{tr}_{n \setminus i} (|\Phi_{\varphi-1}\rangle \langle \Phi_{\varphi-1}|))_{hj} \\ (\tilde{C})_{\zeta_1=(lh), \zeta_2=(i \neq l j)} &= 0 \end{aligned} \quad (20)$$

and  $\zeta_1, \zeta_2$  is a mapping of a two valued index (the ‘‘matrix element’’ indices of the  $i$ -th party) to a single valued integer index.

The remaining unknown expectation value of the left hand side in Eq. (15) becomes

$$\begin{aligned} \langle \Phi_{\varphi-1} | A_i^\dagger \varrho A_i | \Phi_{\varphi-1} \rangle &= \sum_{\substack{h,\xi_1 \\ j,\xi_2 \\ l,m}} a_{hl}^* c_{l\xi_1}^* r_{h\xi_1,j\xi_2} a_{jm} c_{m\xi_2} \\ &= \sum_{\substack{h,l \\ j,m}} a_{hl}^* a_{jm} \sum_{\xi_1, \xi_2} c_{l\xi_1}^* r_{h\xi_1,j\xi_2} c_{m\xi_2} = \sum_{\substack{h,l \\ j,m}} a_{hl}^* a_{jm} D_{hl,jm} \\ &= \sum_{\zeta_1, \zeta_2} a_{\zeta_1}^* D_{\zeta_1, \zeta_2} a_{\zeta_2} = \langle a | D | a \rangle. \end{aligned} \quad (21)$$

where

$$(D)_{\zeta_1=(hl), \zeta_2=(jm)} = \sum_{\xi_1, \xi_2} c_{l\xi_1}^* r_{h\xi_1,j\xi_2} c_{m\xi_2}. \quad (22)$$

Therefore, we can rewrite Eq. (15) as

$$\langle a | D - F_{\varphi-1} \tilde{C} | a \rangle \geq 0, \quad (23)$$

where  $F_{\varphi-1} = \langle \Phi_{\varphi-1} | \varrho | \Phi_{\varphi-1} \rangle$ . Note that the matrices  $D$  and  $\tilde{C}$  are hermitian and  $F_{\varphi-1}$  is non-negative. The maximum left-hand side corresponds to the maximal eigenvalue ( $\lambda_{\max}$ ) of the matrix  $D - F_{\varphi-1} \tilde{C}$  or likewise the left hand side of Eq. (23) is maximized by using the eigenvector corresponding to the maximal eigenvalue ( $|a_{\max}\rangle$ ). By undoing the mapping we obtain the SLOCC operator,

$$|a_{\max}\rangle \rightarrow \tilde{A}_i. \quad (24)$$

This procedure gives the following insight into the optimization over one local filter as in Eq. (13): If the maximal eigenvalue of  $D - F_{\varphi-1} \tilde{C}$  is positive, one can still increase the overlap with a suitable  $A_i$ . The corresponding eigenvector gives an  $\tilde{A}_i$  which increases the overlap. Note, however, that this  $\tilde{A}_i$  is optimal for Eq. (15), but not necessarily the optimal  $A_i$  for  $\langle \Phi_{\varphi} | \varrho | \Phi_{\varphi} \rangle$  in Eq. 14.

In the practical implementation, especially at the beginning of the optimization procedure it is not helpful to use  $\tilde{A}_i$  directly as the SLOCC operator, because this operator is not necessarily invertible. This could therefore correspond to an irreversible operation which destroys entanglement. It turns out that using

$$A_i = \tilde{A}_i + \lambda_{\max} \mathbb{1}_i \quad (25)$$

avoids this problem. With this SLOCC operator the state for the next iteration step is calculated according to Eq. (13). During the iteration procedure,  $\lambda_{\max}$  will decrease [see Eq. (15)], the SLOCC operators become close to the identity, and the convergence criterion is that  $\lambda_{\max}$  is up to numerical precision zero.

## V. FINDING THE OPTIMAL $\varepsilon_k$

A second optimization occurring in the algorithm is the task to find the best  $\varepsilon_k$  (see Eq. 10). In detail, we want to maximize the decrease in the purity in each iteration, that is

$$\max_{\varepsilon_k} [\text{tr}(\varrho_k^2) - \text{tr}(\varrho_{k+1}^2)] \quad (26)$$

with  $\varrho_{k+1} = (\varrho_k - \varepsilon_k |\phi_k\rangle\langle\phi_k|)/(1 - \varepsilon_k)$ . With the abbreviation  $\langle\phi_k | \varrho_k | \phi_k\rangle = c$  the above maximization leads to

$$\max_{\varepsilon_k} \frac{\varepsilon_k^2 [\text{tr}(\varrho_k^2) - 1] + 2\varepsilon_k [c - \text{tr}(\varrho_k^2)]}{(1 - \varepsilon_k)^2}. \quad (27)$$

Taking the derivative with respect to  $\varepsilon_k$ , we find the maximum as

$$\varepsilon_k^{\max} = \frac{c - \text{tr}(\varrho_k^2)}{1 - c}. \quad (28)$$

In the implementation, in case of  $\varepsilon_k^{\max} > 10^{-2} \lambda_d$ , we define  $\varepsilon_k^{\max} := 10^{-2} \lambda_d$ , where  $\lambda_d$  is the minimal eigenvalue of  $\varrho_k$  (guided by practical experience), to keep the remaining state positive during the iterations. This corresponds to an upper bound on  $\varepsilon_k$ , as mentioned above.

## VI. INCREASING THE MIXEDNESS

A central strategy of the algorithm is to increase the ‘‘mixedness’’ of  $\varrho_k$  in each iteration step i.e., to lower the purity  $\text{tr}(\varrho_k^2)$ . One may wonder, whether this is always possible by subtracting some  $|\phi_k\rangle\langle\phi_k| \in \mathcal{C}$ . Indeed, one can show that this is the case, unless  $\varrho_k$  is outside  $\text{conv}(\mathcal{C})$ , which means that the algorithm has no chance to succeed anyway.

To see this, the condition for an increase of the mixedness can be formulated as

$$\begin{aligned} \text{tr}(\varrho_k^2) &> \text{tr}(\varrho_{k+1}^2) = \text{tr}\left(\left[\frac{\varrho_k - \varepsilon_k |\phi_k\rangle\langle\phi_k|}{1 - \varepsilon_k}\right]^2\right) \\ &= \frac{1}{(1 - \varepsilon_k)^2} [\text{tr}(\varrho_k^2) - 2\varepsilon_k \text{tr}(\varrho_k |\phi_k\rangle\langle\phi_k|) + \varepsilon_k^2] \\ &\approx \frac{1}{1 - 2\varepsilon_k} [\text{tr}(\varrho_k^2) - 2\varepsilon_k \langle\phi_k | \varrho_k | \phi_k\rangle] \end{aligned}$$

for small  $\varepsilon_k$ . It follows that iff

$$\langle\phi_k | \varrho_k | \phi_k\rangle > \text{tr}(\varrho_k^2). \quad (29)$$

the state  $|\phi_k\rangle\langle\phi_k|$  can be subtracted with a small weight, and the mixedness increases.

If condition Eq. (29) is not fulfilled for any  $|\phi_k\rangle$  the mixedness cannot increase. But this implies that

$$\sup_{|\phi\rangle \in \mathcal{C}} \langle\phi | \varrho_k | \phi\rangle \leq \text{tr}(\varrho_k^2). \quad (30)$$

Consequently,  $\text{tr}(\varrho_k \mathcal{W}) \leq 0$  for the observable

$$\mathcal{W} = \alpha \mathbb{1} - \varrho_k \quad (31)$$

with  $\alpha = \sup_{|\phi\rangle \in \mathcal{C}} \langle\phi | \varrho_k | \phi\rangle$ . This  $\mathcal{W}$  is nothing but a witness [2] which discriminates between  $\text{conv}(\mathcal{C})$  and the remaining states, and  $\text{tr}(\varrho \mathcal{W}) < 0$  implies that a state is not in  $\text{conv}(\mathcal{C})$ . Therefore, states which cannot fulfill the condition in Eq. (29) are either not in  $\text{conv}(\mathcal{C})$  or (in case that  $\text{tr}(\varrho_k \mathcal{W}) = 0$ ) they may lie at the border of  $\text{conv}(\mathcal{C})$ . This, however, is a set of measure zero and not of practical relevance.

## VII. CONVERGENCE BEHAVIOR OF THE ALGORITHM

Let us now discuss some practical issues. The question, whether or not the algorithm converges depends first on the type of state and decomposition to be determined and second on the distance of the state from the boundary of

the considered convex set. The closer the state is to a boundary the slower is the convergence. The algorithm does e.g. not work with rank deficit states, because overlap of the optimized pure states with the kernel of the density operator cannot be avoided i.e., it is not possible to ensure  $\rho_{k+1} \geq 0$ . In the three- and four-qubit case the decompositions consists of the order of  $10^3$  states (meaning that the algorithm requires this number of iterations, until the conditions in Eqs. (7, 8) apply) i.e., usually such decompositions contain many more states than the Caratheodory-bound of  $d^2$ .

In practice, the overlap optimization in Eq. (9) with the square root  $\sqrt{\varrho}$  instead of  $\varrho$  has a better convergence behavior. Also other fractional powers of  $\varrho$  show a similar advantage. Note that replacing  $\varrho$  by  $\sqrt{\varrho}$  does not affect the proof that the iterated state is separable, if Eqs. (7, 8) apply.

### VIII. LOWER BOUND ON THE $\varepsilon$ -BALL VIA CROSS POLYTOPE

The presented algorithmic procedure allows to determine a decomposition of the state  $\varrho$  with the specified SLOCC properties. After  $n$  iterations we have a decomposition i.e., the set  $\mathcal{S} = \{ \{ |\phi_i\rangle\langle\phi_i|, \varrho_n \}$ , of our initial state of the form

$$\varrho = \sum_{i=1}^n p_i |\phi_i\rangle\langle\phi_i| + q_n \varrho_n, \quad (32)$$

where the probabilities  $p_i$  are given by  $p_i = \varepsilon_i q_{i-1}$  and  $q_i = \prod_{j=1}^i (1 - p_j)$  with  $q_0 := 1$  and  $\varrho_0 := \varrho$ .

By construction, our convex set  $\mathcal{S}$  has specific ‘‘entanglement’’ properties which are valid for all states in its convex hull. However, if we obtained the state  $\varrho$  from experimental data, we have to deal with errors and imperfections, and so the starting state  $\varrho$  is affected by uncertainties. Therefore it is of great importance to give some statements about the ‘‘stability’’ of the determined decomposition, or an estimate of the probability that an experimental states lies inside this convex set.

A first possibility to deal with this problem was used in Ref. [9]: There, starting from the experimentally obtained state  $\varrho_{exp}$  the measurements were simulated via a Monte-Carlo simulation, and 200 sampled states were reconstructed via a maximum likelihood approximation. Then, separability of the state  $\varrho_{exp}$  was only claimed, when the algorithm could prove that  $\varrho_{exp}$  as well as all samples were separable. Note that the generation of states via Monte-Carlo simulation of the measurements is a standard technique to estimate errors in ion-trap experiments.

A different possibility can be obtained by answering the question, how much can an experimental state deviate from  $\varrho$  such that the state still belongs to the set  $\mathcal{S}$ . Although this question is in general not easy to answer

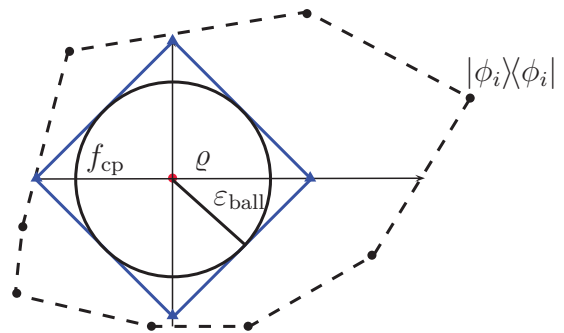


FIG. 1: (Color online) Schematic two-dimensional example for a decomposition of  $\varrho$  (red dot). The convex hull of the states of the decomposition i.e., the set  $\mathcal{S}$ , is denoted by the dashed line. The cross polytope is shown in blue, the vertex states of the cross polytope are marked by blue triangles and the  $\varepsilon_{\text{ball}}$  corresponds to the circle.

[23], we can determine a lower bound on the minimal Hilbert-Schmidt-distance of the state  $\varrho$  with respect to the convex hull of  $\mathcal{S}$ .

The idea is to show that if the state deviates from  $\varrho$  in different directions, then it remains in the convex set. More precisely, we construct a symmetric cross polytope [14] with the state  $\varrho$  in the center (see Fig. 1 for a 2-dimensional example). For a quantum state  $\varrho$  with Hilbert space dimension  $d$  the set needs at least  $d^2$  constituents s.t. a nonzero volume object in this space is possible. The cross polytope is a symmetric polytope with  $2(d^2 - 1)$  vertex states. The vertex states of the cross polytope are defined by  $\varrho_{\pm i}^{\text{cp}} = \bar{\varrho} \pm f_{\text{cp}} \bar{e}_i$ , where we used a vector representation of the density operator in  $(d^2 - 1)$ -dimensional Euclidian space by mapping

$$A = \begin{pmatrix} a_1 & a_d + ia_{d+1} & \cdots & a_{3d-3} + ia_{3d-2} \\ \vdots & \vdots & \vdots & \vdots \\ \cdots & \cdots & a_{d-1} & \cdots \\ \cdots & \cdots & a_{d^2-2} - ia_{d^2-1} & 1 - \sum_{i=1}^{d-1} a_i \end{pmatrix} \longrightarrow \vec{A} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{d^2-1} \end{pmatrix}.$$

The elements of the basisvectors in this notation are given by  $(\bar{e}_i)_j = \delta_{ij}$ .

The Euclidian distance of the vertex states of the cross polytope with respect to the state  $\varrho$ , which is given by  $f_{\text{cp}}$ , is maximized under the constraint that the vertex states are contained in the convex hull of our set  $\mathcal{S}$  (see Fig. 1).

First, using a divide and conquer algorithm we calculate the maximal parameter  $f$  of each state  $\varrho_{\pm i} = \bar{\varrho} \pm f \bar{e}_i$  such that it is contained in the convex hull of our set  $\mathcal{S}$ . Whether a state is contained in the convex set can be decided by using a linear program, e.g. via the Matlab

routine `linprog`. The vertex state with the smallest parameter  $f_{cp}$  is used for defining the vertex states of the cross polytope inside our convex hull. The parameter  $f_{cp}$  also depends on the relative orientation of the chosen orthogonal basis  $\{\vec{e}_i\}$ , here an additional optimization is possible.

Then, the smallest Hilbert-Schmidt distance of  $\varrho$  with respect to any point in the convex hull of the cross polytope is given by  $\varepsilon_{\text{ball}} = \frac{f_{cp}}{\sqrt{d^2-1}}$ , where  $d$  is the dimension of the Hilbert space and  $f_{cp}$  is the maximal parameter such that the cross polytope is contained inside the set  $S$  [14]. We will present an example below.

## IX. EXAMPLES

In this section, we present several examples for the application of our algorithm outlined above.

### A. GHZ states affected by white noise

First, we consider the GHZ state of  $n$  qubits affected by white noise

$$\varrho_{\text{GHZ}_n}(p) = p|\text{GHZ}_n\rangle\langle\text{GHZ}_n| + \frac{1-p}{2^n}\mathbb{1}, \quad (33)$$

where  $|\text{GHZ}_n\rangle = \frac{1}{\sqrt{2}}(|0\dots 0\rangle + |1\dots 1\rangle)$ . For three qubits, these states have the following properties:

- $\varrho_{\text{GHZ}_3}$  is fully separable iff  $p \leq 1/5 = 0.2$  [24],
- $\varrho_{\text{GHZ}_3}$  is genuine multipartite (tripartite) entangled iff  $p > 3/7 \approx 0.4286$  [25],
- $\varrho_{\text{GHZ}_3}$  belongs to the GHZ class iff  $p \gtrsim 0.6955$ . For a detailed discussion see Ref. [13].

With our algorithm we can determine separable and biseparable decompositions up to the threshold values of  $p$ . A bound with a threshold value of  $p = \frac{559}{805} \approx 0.6944$  for existing W-class decomposition was obtained with our algorithm, which is close to the optimal threshold value of  $p \approx 0.6955$ .

#### 1. The $\varepsilon$ -ball and the robustness depending on $p$

With our algorithm it is possible to obtain W-decompositions of the state  $\rho_{\text{GHZ}_3}$  up to  $p = 0.6944$ . Due to the ‘‘small’’ number of vertex states forming the convex set the size of an  $\varepsilon$ -ball generated via the procedure of Sec. VIII will be small in comparison to the maximum possible ball which fulfills the considered properties. However the lower bound on the size of this ball will also depend on the distance of the considered state to the border where the properties are not fulfilled anymore. In Fig. 2 the lower bound on the size of the  $\varepsilon$ -ball

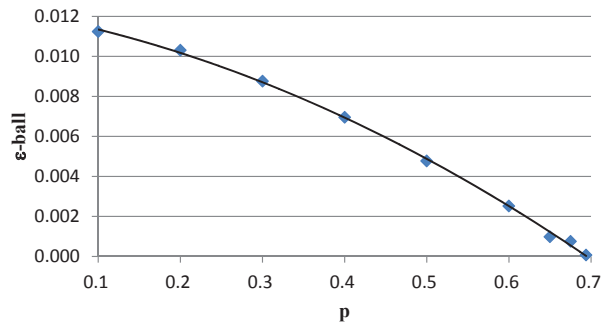


FIG. 2: (Color online) The lower bound on the size of the  $\varepsilon$ -ball of the state given in Eq. (33) as a function of  $p$ . The decompositions are obtained with the procedure of Sec. VIII. The line is a polynomial fit of the points for guiding the eye. The ball-size strongly depends on the number of constituents in the decomposition, especially if states far away from the border are considered. Therefore here decompositions are compared which all consists of about 4000 pure states.

is plotted versus the parameter  $p$ . As expected for the almost maximally mixed state (small  $p$ ) the ball is quite large, but it decreases by several orders of magnitude as  $p$  approaches the threshold value of the considered convex set.

From our  $\varepsilon$ -ball we can also deduce that any state  $\varrho'$  which has an Euclidean distance from  $\varrho$  which is smaller equal the radius of the  $\varepsilon$ -ball is contained in our convex set i.e., using the Hilbert-Schmidt-distance between two operators  $A$  and  $B$  given by  $d = \sqrt{\text{tr}((A-B)^2)}$ , we can calculate the distance between two GHZ-Werner states, see Eq. (33), with purity  $p$  and  $p' = p + \delta$  to be given by

$$\begin{aligned} d^2 &= \text{tr}([\varrho_{\text{GHZ}}(p) - \varrho_{\text{GHZ}}(p')]^2) \\ &= \frac{7}{8}\delta^2. \end{aligned} \quad (34)$$

If we have an  $\varepsilon$ -ball in the surrounding of  $\varrho_{\text{GHZ}}(p)$  with radius  $\varepsilon_{\text{ball}}$  then we can deduce that also the state  $\varrho_{\text{GHZ}}(p')$  with

$$\delta \leq \sqrt{\frac{8}{7}}\varepsilon_{\text{ball}} \quad (35)$$

belongs to the same convex set, allowing to increase the threshold parameter accordingly.

#### 2. Entanglement properties of $\rho_{\text{GHZ}_4}(p)$

The maximal parameter  $p_{\text{opt}} \approx 0.467$  for biseparability of the four-qubit GHZ-state mixed with white noise was derived in Ref. [25]. Our algorithm is able to determine decompositions for values of  $p$  up to  $p \approx 0.466$ .

For four qubits there is already a continuous set of inequivalent SLOCC entanglement classes, and it can happen that a state can be decomposed into biseparable states, but not into SLOCC equivalents of some genuine multipartite entangled states. To investigate this,

we considered the state  $\rho_{\text{GHZ}_4}(p)$  and asked when it can be decomposed into SLOCC equivalents of the four-qubit W-state,  $|W_4\rangle = \frac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle)$ . This seems to be only possible for  $p \leq 0.32$ , but for the larger parameter regime  $p \leq 0.467$  the state is biseparable.

An intuitive argument for such a behavior is that the four qubit W-state can be transformed via SLOCC into a three-qubit GHZ state as well as to a two-qubit Bell state tensored with a product state, but it is *not* possible to reach  $|\phi_4\rangle = |\phi^+\rangle \otimes |\phi^+\rangle$ , we even have  $\max_{W \in \text{SLOCC}(W_4)} |\langle W | \phi_4 \rangle|^2 = 0.5$ [34]. States like  $|\phi_4\rangle$ , however, are essential in the biseparable decomposition of  $\rho_{\text{GHZ}_4}(p)$  [25]. Many lower entangled pure states are SLOCC inequivalent to specific genuine multipartite entangled pure states.

### B. W-states with white noise

In order to give an example where the algorithm is not capable of computing the threshold of separability, we consider states of the form

$$\varrho_{W_n}(p) = p|W_n\rangle\langle W_n| + \frac{1-p}{2^n}\mathbb{1}, \quad (36)$$

where the three-qubits W state  $|W_3\rangle$  is given in Eq. (4) and for four qubits we have  $|W_4\rangle = \frac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle)$ . The border to the class of biseparable states can only be roughly approached by the algorithm. In the three-qubit case we have a gap of about  $\Delta p = 0.03$ , the exact value  $p = 0.4790$  is known from Ref. [26]. For the four-qubit W-state with white noise the gap with respect to the upper bound obtained by an semidefinite-programming-witness (SDP-witness) [26] is approximately  $\Delta p_4 = 0.04$  i.e., we determined a decomposition for  $p = 1 - 0.526 - 0.04 = 0.434$ .

### C. Bound entangled state from an unextendible product basis

As a second example, we consider the bound entangled states arising from an unextendible product basis [27]. These states are defined via using the product vectors  $|\psi_0\rangle = |0\rangle(|0\rangle - |1\rangle)/\sqrt{2}$ ,  $|\psi_1\rangle = (|0\rangle - |1\rangle)|2\rangle/\sqrt{2}$ ,  $|\psi_2\rangle = |2\rangle(|1\rangle - |2\rangle)/\sqrt{2}$ ,  $|\psi_3\rangle = (|1\rangle - |2\rangle)|0\rangle/\sqrt{2}$ ,  $|\psi_4\rangle = (|0\rangle + |1\rangle + |2\rangle)(|0\rangle + |1\rangle + |2\rangle)/3$ . Then the state

$$\varrho_{\text{BE}} = \frac{1}{4} \left( \mathbb{1} - \sum_{i=0}^4 |\psi_i\rangle\langle\psi_i| \right) \quad (37)$$

is an entangled state on a  $3 \times 3$  system, which is not detected by the PPT criterion. We considered the family of states

$$\varrho_{\text{UPB}}(p) = p\varrho_{\text{BE}} + (1-p)\mathbb{1}/9. \quad (38)$$

They have often been used as a test-bed for separability criteria. To our knowledge, the best criterion for these

states is the first step of the algorithm of Doherty et al. [28] which detects them to be entangled for  $p > 0.8691$ . Our algorithm proves that these states are separable for  $p \leq 0.83$ .

### D. Thermal states with the Heisenberg interaction

Let us consider the thermal state

$$\varrho_{\text{H}}(T) \sim \exp\{-H_{\text{H}}/T\} \quad (39)$$

of three spin-1/2 particles interacting with the Heisenberg interaction,

$$H_{\text{H}} = \sum_{i < j} h_{ij} \quad \text{with} \quad h_{ij} = \sum_{k=x,y,z} \sigma_k^{(i)} \otimes \sigma_k^{(j)}, \quad (40)$$

where  $i, j \in \{1, 2, 3\}$ . In Ref. [29] the entanglement properties of this system were investigated, and it was shown that the spin-squeezing inequality  $(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 \geq N/2$  with  $J_k = 1/2 \sum_i \sigma_k^{(i)}$  detects these states as entangled for  $T \leq 5.461$ . Remarkably, the spin-squeezing inequality shows that for  $4.329 \leq T \leq 5.461$  the thermal state is biseparable with respect to any bipartition, but not fully separable. Direct application of our algorithm gives that for  $T \geq 5.462$  the thermal state is fully separable, giving strong evidence that the spin-squeezing inequality is a necessary and sufficient criterion for the thermal state. For more than three spins, however, this does not seem to be the case.

### E. Experimental pseudo bound entangled state

In Ref. [12] a class of three-qubit bound entangled states with rank seven were introduced. We consider the specific state where the entanglement is maximally robust with respect to white noise [30]:

$$\begin{aligned} \rho_{\text{BE}3} = \frac{1}{N} & \left( 2|\text{GHZ}\rangle\langle\text{GHZ}| + \right. \\ & a|001\rangle\langle 001| + a|010\rangle\langle 010| + \frac{1}{a}|011\rangle\langle 011| + \\ & \left. a|100\rangle\langle 100| + \frac{1}{a}|101\rangle\langle 101| + \frac{1}{a}|110\rangle\langle 110| \right), \end{aligned} \quad (41)$$

where  $|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ ,  $a = 0.3460$ , and the normalization is  $N = (2 + 3(a + \frac{1}{a}))$ . The state has the curious property that it is biseparable with respect to any bipartite splitting, but it is nevertheless entangled. A pseudo bound entangled state of this form was experimentally generated and characterized in Ref. [31], see Fig. 3. It was shown via a witness operator that the state is entangled and PPT with respect to any bipartite splitting. Now with our algorithm we are able to prove that this state is biseparable with respect to the split B-AC with an  $\varepsilon$ -ball of  $\varepsilon_{\text{ball}} = 4 \cdot 10^{-4}$ .



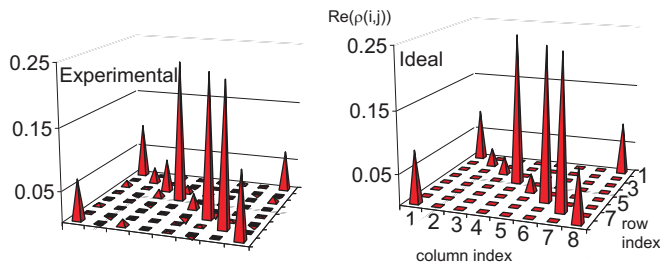


FIG. 3: (Color online) Experimental pseudo bound entangled state [31]. All imaginary elements of the experimental state are small and therefore not shown.

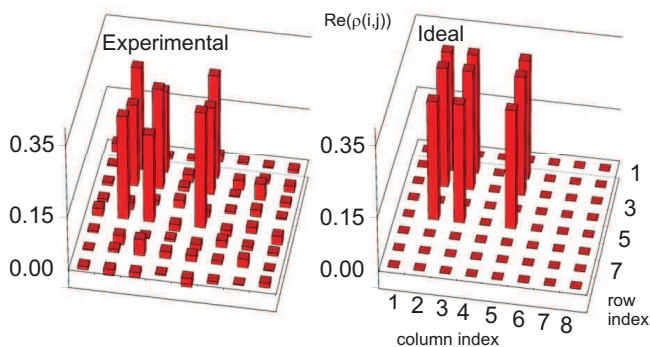


FIG. 4: (Color online) Real part of the experimental W-state from Roos *et al.* [32] (left) in comparison to the ideal W-state (right). All imaginary elements of the experimental state are small and therefore not shown.

### F. Experimental three-qubit W-state

Nowadays it is possible in several experimental setups to generate quantum states which are e.g. close to the three-qubit W-state. The generated states are characterized by quantum state tomography. Here we use data from an experiment by Roos *et al.* [32]. This “typical” experiment (see Fig. 4) led to a fidelity of  $F = \sqrt{\langle W | \varrho_{\text{exp}} | W \rangle} = 0.9$ , where we can prove via an entanglement witness that this state is genuine multipartite entangled. Now the question arises whether this state really belongs to the W-class of entanglement. With our algorithm it is not possible to find a W-class decomposition of  $\varrho_{\text{exp}}$ , so probably the state belongs to the class of GHZ-entangled-states. On the other hand we can find for the slightly depolarized version of this state, e.g.  $\varrho' = 0.96\varrho_{\text{exp}} + \frac{0.04}{8}\mathbb{1}$ , a W-decomposition and we can prove that it is genuine multipartite entangled.

### G. Summary of the algorithmic performance

In this section we summarize the obtained threshold parameters for the various examples considered. Our standard approach was to consider different types of quantum states mixed with white noise of the form:

$$\varrho_i(p) = p\varrho_i + (1-p)\mathbb{1}/d. \quad (42)$$

Then we determined the threshold parameters  $p$  for various types of entanglement which we can achieve via our algorithm, and to compared them with bounds from the literature or with exact values if they are known. The only exceptional parameterization was the case of the thermal equilibrium Heisenberg spin chain state (Sec. IX D) which depends on the temperature. In Table I we summarize the threshold parameters reached via our algorithm and show the best known bounds from the literature. For several cases we also calculated lower bounds on the  $\varepsilon$ -ball for our determined decompositions (see Sec. VIII). For all cases where the exact bounds are known we can reproduce the threshold parameters quite well by our procedure, apart from the three-qubit W state, where there is a small gap. It is remarkable that our algorithm seems to work independently of the type of decomposition to be determined. For the given examples the calculation needs less than 5 min on a standard personal computer. The number of terms calculated in the decomposition strongly depends on the distance to the border of the convex set. I.e. already a very small change on the  $p$ -threshold values has a huge influence on the number of terms in the decomposition. For threshold values with the given precision in Table I it is possible to find decomposition within the order of  $\sim 5000$  terms.

### X. CONCLUSIONS

We presented an easy to implement, fast and straightforward method for finding decompositions of quantum states with specific SLOCC entanglement properties. For a large variety of examples decompositions were determined for those parameters, where they are known to exist. For instance, is it possible to find separable decompositions of Werner states with minimal amount of white noise. Also the threshold values for biseparability can be reproduced in most cases for three- and four-qubit states. Especially interesting are the cases where the exact parameter range for the existing decompositions is not known. It was e.g. possible to investigate bound entangled states with our algorithm. This method of determining specific decompositions of a quantum state is a complementary tool to entanglement criteria such as entanglement witnesses. Together these tools allow to extensively specify the entanglement properties of a given quantum state. In the future we would like to understand better the convergence behavior of the algorithm, especially why optimally decreasing the purity of the quan-

State	Ent.	Bound	Decomp.	$\varepsilon$ -ball
$\varrho_{\text{GHZ3}}$	S	$1/5^*$ (a)	0.199	$8.1 \cdot 10^{-5}$
	BS	$0.429^*$ [26]	0.4285	$9.2 \cdot 10^{-6}$
	W	$0.6955^*$ [13]	0.694	$7.1 \cdot 10^{-5}$
$\varrho_{\text{GHZ4}}$	S	$1/9^*$ (a)	0.111	
	BS	$0.467^*$ [26]	0.466	
	W		0.316	
$\varrho_{\text{W3}}$	S	$3/11$ (a)	0.1727	$7.6 \cdot 10^{-4}$
	BS	$0.479^*$ [26]	0.45	$1.1 \cdot 10^{-3}$
$\varrho_{\text{W4}}$	S	$1/5$ (a)	0.09	
	BS	$0.474$ [26]	0.434	
$\varrho_{\text{UPB}}$	S	0.87 [28]	0.83	$1.2 \cdot 10^{-4}$
$\varrho_{\text{BE3}}$	S	$0.786^*$ [33]	0.726	$2.0 \cdot 10^{-4}$
	BS (AB-C)	$1^*$ [12]	0.9	$1.1 \cdot 10^{-3}$
$\varrho_{\text{H}}(T)$	S	5.61 [29]	5.62	$2.1 \cdot 10^{-5}$
	BS (AB-C)	4.329 [29]	4.33	$7.2 \cdot 10^{-6}$

TABLE I: Threshold values for  $p$ , see Eq. (42). With an asterisk we denote exact values from the literature and with (a) we denote bounds obtained via the PPT criterion. The column Decomp. contains the parameter threshold up to which we are able to determine S (separable), BS (biseparable), W (W-type) decompositions. The specific methods used to obtain bounds on the threshold values are discussed in the corresponding paragraph of the examples.

tum state in each iteration is at the end not necessarily a good strategy.

We would like to thank J. Barreiro, M. Kleinmann, M. Mertz, M. Piani, C. Roos, and A. Streltsov for valuable discussions. This project was financially supported by the Austrian Science Fund (FWF): Y376-N16 (START prize), the EU (Marie Curie CIG 293993/ENFOQI), the BMBF (Chist-Era Project QUASAR) and the Deutsche Forschungsgemeinschaft (DFG).

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- [1] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, *Rev. Mod. Phys.* **81**, 865 (2009).
- [2] O. Gühne and G. Tóth, *Phys. Rep.* **474**, 1 (2009).
- [3] W. K. Wootters, *Phys. Rev. Lett.* **80**, 2245 (1998).
- [4] A. Sanpera, R. Tarrach, and G. Vidal, *Phys. Rev. A* **58**, 826 (1998).
- [5] R. Unanyan, H. Kampermann, and D. Bruß, *J. Phys. A* **40**, F483 (2007).
- [6] A. Kay, *Phys. Rev. A* **83**, 020303(R) (2011).
- [7] F. M. Spedalieri, *Phys. Rev. A* **76**, 032318 (2007).
- [8] M. Navascues, M. Owari, and M. B. Plenio, *Phys. Rev. Lett.* **103**, 160404 (2009).
- [9] J. Barreiro, P. Schindler, O. Gühne, T. Monz, M. Chwalla, C. Roos, M. Hennrich, and R. Blatt, *Nat. Phys.* **6**, 943 (2010).
- [10] W. Dür, G. Vidal, and J. I. Cirac, *Phys. Rev. A* **62**, 062314 (2000).
- [11] F. Verstraete, J. Dehaene, B. DeMoor, and H. Verschelde, *Phys. Rev. A* **65**, 052112 (2002).
- [12] A. Acin, D. Bruß, M. Lewenstein, and A. Sanpera, *Phys. Rev. Lett.* **87**, 040401 (2001).
- [13] C. Eltschka and J. Siewert, *Phys. Rev. Lett.* **108**, 020502 (2012).
- [14] C. Wilmott, H. Kampermann, and D. Bruß, *J. Phys. A* **43**, 505306 (2010).
- [15] R. F. Werner, *Phys. Rev. A* **40**, 4277 (1989).
- [16] L. Gurvits and H. Barnum, *Phys. Rev. A* **66**, 062311 (2002).
- [17] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, *Phys. Rev. A* **58**, 883 (1998).
- [18] S. L. Braunstein, C. M. Caves, R. Jozsa, N. Linden, S. Popescu, and R. Schack, *Phys. Rev. Lett.* **83**, 1054 (1999).
- [19] V. M. Kendon, K. Nemoto, and W. J. Munro, *J. Mod. Optics* **49**, 1709 (2002).
- [20] J. I. de Vicente, *Quantum Inf. Comput.* **7**, 624 (2007).
- [21] R. Hildebrand, *Separable balls around the maximally mixed state for a 3-qubit system* (2006), quant-ph/0601201.
- [22] O. Gühne, M. Reimpell, and R. F. Werner, *Phys. Rev. Lett.* **98**, 110502 (2007).
- [23] B. Grünbaum, *Convex Polytopes* (Springer, 2003), 2nd ed.
- [24] W. Dür and J. I. Cirac, *Phys. Rev. A* **61**, 042314 (2000).
- [25] O. Gühne and M. Seevinck, *New J. Phys.* **12**, 053002 (2010).
- [26] B. Jungnitsch, T. Moroder, and O. Gühne, *Phys. Rev. Lett.* **106**, 190502 (2011).
- [27] C. H. Bennett, D. P. DiVincenzo, T. Mor, P. W. Shor, J. A. Smolin, and B. M. Terhal, *Phys. Rev. Lett.* **82**, 5385 (1999).
- [28] A. C. Doherty, P. A. Parrilo, and F. M. Spedalieri, *Phys. Rev. Lett.* **88**, 187904 (2002).
- [29] G. Tóth, C. Knapp, O. Gühne, and H. J. Briegel, *Phys. Rev. Lett.* **99**, 250405 (2007).
- [30] P. Hyllus, C. M. Alves, D. Bruß, and C. Macchiavello,

Phys. Rev. A **70**, 032316 (2004).

- [31] H. Kampermann, D. Bruß, X. Peng, and D. Suter, Phys. Rev. A **81**, 040304(R) (2010).
- [32] C. Roos, *private communication*.
- [33] P. Hyllus, Ph.D. thesis, Universität Hannover (2005).
- [34] This property can e.g. be supported by considering the

Schmidt-rank of  $|W_4\rangle$  with respect to the split 1,3 vs 2,4 which is 2, whereas the corresponding Schmidt rank of  $|\phi^+\rangle\otimes|\phi^+\rangle$  is 4. It is not possible to increase the Schmidt-rank of a state via SLOCC operations.