# Complete hierarchies of efficient approximations to problems in entanglement theory

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We investigate several problems in entanglement theory from the perspective of convex optimization. This list of problems comprises (A) the decision whether a state is multiparty entangled, (B) the minimization of expectation values of entanglement witnesses with respect to pure product states, (C) the closely related evaluation of the geometric measure of entanglement to quantify pure multiparty entanglement, (D) the test whether states are multiparty entangled on the basis of witnesses based on second moments and on the basis of linear entropic criteria, and (E) the evaluation of instances of maximal output purities of quantum channels. We show that these problems can be formulated as certain optimization problems: as polynomially constrained problems employing polynomials of degree 3 or less. We then apply very recently established known methods from the theory of semidefinite relaxations to the formulated optimization problems. By this construction we arrive at a hierarchy of efficiently solvable approximations to the solution, approximating the exact solution as closely as desired, in a way that is asymptotically complete. For example, this results in a hierarchy of efficiently decidable sufficient criteria for multiparticle entanglement, such that every entangled state will necessarily be detected in some step of the hierarchy. Finally, we present numerical examples to demonstrate the practical accessibility of this approach.

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## I. INTRODUCTION

One of the reasons for the superior performance of quantum devices for computation and communication compared to their classical counterparts is simply due to the fact that in quantum mechanics, one has a very large space at hand to work with: the dimension of the state space of a number of quantum bits is exponentially larger than the corresponding configuration space of classical bits. This renders the simulation of a quantum computer on a classical device a difficult task. But it is not only the sheer size of state space that makes the assessment of quantum states a difficult problem. In fact, even to decide whether quantum states have certain properties that are of central interest in quantum-information science often amounts to solving computationally hard problems on a classical computer. Most prominently, to decide whether a known state $\rho$ of a finite-dimensional bipartite system is separable or entangled, i.e., whether or not it can be written as a convex combination of product states

$$\rho = \sum_{i=1}^{n} p_i \rho_1^{(i)} \otimes \rho_2^{(i)}, \tag{1}$$

is already an *NP* hard problem in the system size [1]. A state is separable if there is a preparation of the state that involves only local quantum operations and shared classical randomness. Such states are correlated, but classically correlated, as the source for the correlations can be thought of as resulting entirely from the shared source of randomness [2]. Due to the central status of the concept of entanglement in quantum information, a very significant amount of research has been dedicated to the problem of finding good criteria for separability that are suitable for specific contexts [3].

To state whether a state is separable or not is equivalent to stating whether a state is in the convex hull of product states. Also, the evaluation of many measures of entanglement essentially require the solution of a convex problem. So in recent years, it has increasingly been realized that a good deal of insight into several problems in quantum information and in particular in entanglement theory could in fact come from the field of research that is primarily concerned with questions of this type [1,4–10]: this is the theory of convex optimization. Many problems are already of the required form, and powerful tools such as the concept of Lagrange duality readily deliver bounds for the problems at hand. Examples include the evaluation of measures of entanglement that reasonably quantify the degree of entanglement of a given state, such as the distillable entanglement or the asymptotic relative entropy of entanglement [4,5]. Also, it has been realized that while the complete solution of the question of separability is *NP* hard, one can nevertheless find hierarchies of sufficient criteria for entanglement in the bipartite setting. In each step, by solving an efficiently solvable convex optimization problem, one finds an answer to the problem in the form (i) one can assert that the state is entangled, or (ii) one cannot assert it, and has to go one (computationally more expensive) step further [8]. The problem of testing for multipartite entanglement has been related to robust semidefinite programming and a hierarchy of relaxations in Ref. [9].

This paper is concerned with a link of the theory of entanglement to the theory of convex optimization in a similar

 

spirit. The central observation of this paper is very simple yet potentially very useful: many problems related to entanglement can be cast into the form of optimization problems with polynomial constraints of degree 3. This includes (A) the question whether a state is entangled or not, notably not only in the bipartite, but also for the several separability classes of the multipartite setting. Then, (B) the construction of nondecomposable witnesses involves a problem of this kind, as well as (C) the evaluation of the geometric measure of entanglement to quantify multipartite entanglement. (D) Also, when considering entanglement witnesses based on second moments rather than on first moments one has to solve a problem of this form. We will also discuss criteria based on linear entropies (i.e., $p$-norms for $p=2$). (E) Finally, we will briefly mention the evaluation of maximal output purities of quantum channels with respect to $p$-norms for $p=2$. This structure is due to the fact that in all these instances one essentially minimizes over product state vectors of a multipartite quantum system.

This polynomial part of the optimization problems is still nonconvex and computationally expensive to solve. Yet, applying results from relaxation theory of nonconvex problems [11–15], notably the method of Lasserre [13], we find hierarchies of solutions to our original problems, and each step is a better approximation than the previous one. Each step itself amounts to solving an efficiently implementable semidefinite program [16]. Moreover, the hierarchy is asymptotically complete, in the sense that the exact solution is asympotically attained. The increase of the size of the vector of objective variables of these semidefinite problems grows notably polynomially in the label of the hierarchy.

We will first clearly state how one can introduce auxiliary variables to cast the considered problems from entanglement theory into the desired form. Then, we will investigate the hierarchies of relaxations in detail, and study numerical examples. Finally, we will summarize what has been achieved.

## II. PROBLEMS IN ENTANGLEMENT THEORY AS OPTIMIZATION PROBLEMS

The problems that we will encounter are of the following type or similar. At the core are typically minimizations over product vectors, originating from the very definition of the concept of entanglement. Given a $W=W^\dagger$, we seek the minimum of

$$\mathrm{tr}[|\psi_1\rangle\langle\psi_1| \otimes \cdots \otimes |\psi_N\rangle\langle\psi_N| W], \tag{2}$$

where the minimum is taken with respect to product state vectors of a composite quantum systems with parts labeled $1,\ldots,N$, with Hilbert space $\mathcal{H}=\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_N$. Throughout the paper, the respective Hilbert spaces are assumed to have finite dimensions, $\mathcal{H}_j=\mathbb{C}^{d_j}$, $j=1,\ldots,N$.

One way of solving this problem is to choose a specific basis for the Hilbert space and to explicitly parametrize the state vectors. This yields a complex polynomial in these parameters, in general of very high order. This is obviously not a convex problem in these variables: a solution can be found, albeit not in an efficient manner. For small systems, algorithms such as simulated annealing may be employed, delivering upper bounds to the optimal solution, as no control is possible as to what extent one is far away from the global optimum.

The general strategy of this paper is in instances of the above type to introduce additional variables, giving rise to one vector $x\in\mathbb{R}^t$, $x=(x_1,\ldots,x_t)^T$, which is the objective variable, parametrizing the product states. The problem is then cast into the form of a linear objective function, simply as

$$\text{minimize } c^T x \tag{3}$$

with a (fixed) $c\in\mathbb{R}^t$, subject to constraints which are polynomials in the objective variables. These constraints will then be relaxed to semidefinite problems. So two types of constraints will be encountered in the present paper.

*Semidefinite constraints*. These are constraints of the form

$$F_0+\sum_{s=1}^{t} x_s F_s \geqslant 0, \tag{4}$$

where $F_0,\ldots,F_t$ are Hermitian matrices of arbitrary dimensions. The resulting matrix has to be positive semidefinite; therefore it is referred to as a semidefinite constraint. Optimization problems of this type, exhibiting a linear objective function and semidefinite constraints, are called semidefinite programs [16]. Such instances of convex optimization problems can be efficiently solved, for example by means of the interior-point methods [16]. Moreover, the idea of Lagrange duality [17] readily delivers lower bounds for the problem. Typically, the dual optimization problem yields an optimal value which is identical to the optimal value for the primal problem (unless there is a duality gap). Many problems in quantum information theory have already the form of a semidefinite program [6,8]. In fact, it may be convincingly argued that to specify the solution of a problem in form of a semidefinite program has the same status as stating a result in terms of the spectrum of a matrix, as this again merely means that efficient methods are available to find the eigenvalues of a given matrix.

*Polynomial constraints*. This means that we can write the constraints as

$$g_l(x)\leqslant 0, \tag{5}$$

$l=1,\ldots,L$, where $g_l:\mathbb{R}^t\to\mathbb{R}$ are real polynomials of some degree. Quadratic constraints are of the form

$$x^T A_l x + b_l^T x + c_l \leqslant 0, \tag{6}$$

$l=1,\ldots,L$. The matrices $A_l$ are, however, not necessarily positive semidefinite. This is by no means a minor detail: if all matrices $A_1,\ldots,A_L$ were positive matrices, $A_l\geqslant 0$, this would yield a convex quadratic program, which can be efficiently solved (they are in fact also instances of semidefinite programs and of second-order cone programs). In stark contrast, if the matrices are not all positive semidefinite, one obtains a very hard, nonconvex optimization problem. This structure is yet dictated by the problems from quantum information theory at hand.

The central point is to employ known methods from the theory of relaxations of nonconvex optimization problems, to

obtain complete hierarchies of cheaply computable approximations, approximating the solution as closely as desired. The idea of a relaxation is to introduce new variables and to formulate the problem as a convex problem in a larger space. This idea can be exemplified in the simplest form of a relaxation, the Shor relaxation [11]. For example, let $A_1$ in (6) be a matrix which is not positive semidefinite, and let us assume that $b_1=0$ and $c_1=0$ for simplicity. Then, one can still write the constraint equivalently as

$$\mathrm{tr}[XA_1] \geqslant 0, \quad X = xx^T, \tag{7}$$

using a $t\times t$ symmetric matrix $X$. The equality $X=xx^T$ is equivalent with the convex constraint

$$X \geqslant xx^T, \tag{8}$$

together with the nonconvex one $X\leqslant xx^T$. Shor's relaxation amounts to taking only the convex part into account, thereby delivering an efficiently solvable convex problem which yields a lower bound to the original problem [11]. Such relaxations in terms of semidefinite constraints will be employed, yet instead of one many such relaxations, forming a complete hierarchy.

As pointed out before, we will show that the encountered optimization problems can be written as polynomially constrained problems of degree 3. That this is possible is based on the observation that any Hermitian $m\times m$ matrix $O$ for which

$$\mathrm{tr}[O^2] = 1, \quad \mathrm{tr}[O^3] = 1 \tag{9}$$

is one that satisfies

$$\mathrm{tr}[O] = 1, \quad O = O^2, \quad O \geqslant 0, \tag{10}$$

i.e., it corresponds to a pure state (compare also Ref. [18]). This follows from the fact that, denoting the decreasingly ordered list of eigenvalues of $O$ by $\lambda^{\downarrow}(O)$, the only vector consistent with

$$\sum_{i=1}^{m} \lambda_i^{\downarrow}(O)^2 = 1, \quad \sum_{i=1}^{m} \lambda_i^{\downarrow}(O)^3 = 1 \tag{11}$$

is the vector $\lambda^{\downarrow}(O)=(1,0,\ldots,0)$. The quantities $\lambda_i^{\downarrow}(O)^2$ and $\lambda_i^{\downarrow}(O)^3$ are unitarily invariant, and hence the above statements can be shown to be valid on the level of probability distributions. Essentially, $\Sigma_{i=1}^{m}\lambda_i^{\downarrow}(O)^2=1$ already requires all absolute values of eigenvalues to be smaller than or equal to 1, such that the only ordered vector of real numbers consistent with $\Sigma_{i=1}^{m}\lambda_i^{\downarrow}(O)^3=1$ becomes (1,0,…,0).

For systems where the individual constituents are qubit systems, $d_j=2$ for all $j=1,\ldots,N$, the constraints can further be simplified by merely requiring as constraints $\mathrm{tr}[O]=1$, $\mathrm{tr}[O^2]=1$, as for Hermitian $2\times 2$ matrices these conditions alone imply that

$$O \geqslant 0, \quad O = O^2. \tag{12}$$

When applied to our specific problems at hand, these constraints will appear in the following form. We will require that Hermitian matrices $P$ are, except from normalization, products of pure states with respect to all constituents. This will be incorporated as follows. Denoting by $I=\{1,\ldots,N\}$ the index set labeling the subsystems and by $\mathrm{tr}_{I\backslash j}$ the partial trace with respect to all systems except the one with label $j$, the lines

$$\mathrm{tr}\big[\mathrm{tr}_{I\backslash j}[P]^2\big] = (\mathrm{tr}[P])^2, \tag{13}$$

$$\mathrm{tr}\big[\mathrm{tr}_{I\backslash j}[P]^3\big] = (\mathrm{tr}[P])^3 \tag{14}$$

for all $j\in I$ indeed enforce that the matrices are products. If reductions are pure, the global state must be a pure product state. This can be seen as follows. For states $\rho$, the only possibility for

$$\mathrm{tr}\big[\mathrm{tr}_{I\backslash j}[\rho]^2\big] = 1, \quad \mathrm{tr}\big[\mathrm{tr}_{I\backslash j}[\rho]^3\big] = 1 \tag{15}$$

to hold for all $j\in I$ is that $\rho$ is of the form of the 9 product pure state,

$$\rho = |\phi_1\rangle\langle\phi_1| \otimes \cdots \otimes |\phi_N\rangle\langle\phi_N|. \tag{16}$$

If an additional constant $\alpha>0$ is included, these conditions read $\mathrm{tr}\big[\mathrm{tr}_{I\backslash j}[\alpha\rho]^2\big]=(\mathrm{tr}[\alpha\rho])^2=\alpha^2$ and $\mathrm{tr}\big[\mathrm{tr}_{I\backslash j}[\alpha\rho]^3\big]=(\mathrm{tr}[\alpha\rho])^3=\alpha^3$, which explains the above constraint [19]. Having stated the general strategy, let us now look at the specific instances of problems in quantum information we will be considering in this paper.

### A. Tests for bipartite and multipartite entanglement

The approach is here to consider for a given state $\rho\in\mathcal{S}(\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_N)$ the minimal Hilbert-Schmidt norm with respect to the set of separable states. For simplicity of notation, we explicitly formulate the optimization problem for the instance of full separability, without loss of generality. That is, we test whether $\rho$ can be written as

$$\rho = \sum_{i=1}^{n} p_i \rho_1^{(i)} \otimes \cdots \otimes \rho_N^{(i)}, \tag{17}$$

with $\{p_i\}_i$ forming a probability distribution. The question whether a state is fully separable is hence equivalent to asking whether a state is an element of the convex hull of product vectors with respect to all subsystems. According to Caratheodory's theorem [20], for any $k$-dimensional subset $S\subset\mathbb{R}^m$, any point of the convex hull of $S$ can be written as a convex combination of at most $k+1$ points from $S$. Hence, the number of elements in the convex combination given by Eq. (17) can be restricted to $n=\Pi_{j=1}^{N}d_j^2$, again without loss of generality. To decide whether a state $\rho$ is fully separable or not, we may solve the following optimization problem:

$$\text{minimize } \|\rho - P\|_2^2 = \mathrm{tr}(\rho - P)^2, \tag{18}$$

$$\text{subject to } P \text{ is fully separable}.$$

We make use of the Hilbert-Schmidt norm as it is quadratic in the matrix entries.

The task is to write this problem in terms of a polynomially constrained problem. Each relaxation (see Sec. III), labeled with $h=h_{\min},h_{\min}+1,\ldots$, then delivers a lower bound of the Hilbert-Schmidt distance to the set of fully separable

states. Hence, asserting that the state is not fully separable whenever we obtain a value larger than the one that we accept as accuracy of the computation [21], each step delivers a sufficient criterion for multipartite entanglement in its own right, and the hierarchy is complete in the sense that each entangled state is detected by some step. The associated optimization problem can now be written as

$$\text{minimize } x, \tag{19}$$

$$\text{subject to } x \geqslant \mathrm{tr}(\rho - P)^2,$$

$$P - \sum_{i=1}^{n} P^{(i)} = 0,$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^2] = (\mathrm{tr}[P^{(i)}])^2$$

$$\text{for all } i = 1, \ldots, n, \quad j \in I,$$

$$\sum_{i=1}^{n} \mathrm{tr}[P^{(i)}] = 1,$$

$$P^{(i)} \geqslant 0 \quad \text{for all } i = 1, \ldots, n.$$

The line $\Sigma_{i=1}^{n}\mathrm{tr}[P^{(i)}]=1$ takes the normalization of the whole state into account. This is a quadratic program, combined with a semidefinite constraint for the positivity of the matrices $P^{(i)}$. As pointed out above, the problem can also be formulated as a polynomial problem without a semidefinite constraint, but now with constraints that are of degree 3:

$$\text{minimize } x, \tag{20}$$

$$\text{subject to } x \geqslant \mathrm{tr}(\rho - P)^2,$$

$$P - \sum_{i=1}^{n} P^{(i)} = 0,$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^2] = (\mathrm{tr}[P^{(i)}])^2$$

$$\text{for all } i = 1, \ldots, n, \quad j \in I,$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^3] = (\mathrm{tr}[P^{(i)}])^3$$

$$\text{for all } i = 1, \ldots, n, \quad j \in I,$$

$$\sum_{i=1}^{n} \mathrm{tr}[P^{(i)}] = 1.$$

This is a global optimization problem with polynomial constraints of degree 3, but no semidefinite constraint.

Here one tests the hypothesis that the state is fully separable against the alternative that the state is entangled in some sense. To assert that the state is multiparticle entangled and not separable with respect to any separability class, several tests are hence required. In this way, the various classes of genuine multiparticle entanglement can be detected. Note that when even applied to the bipartite case, the resulting hierarchy of semidefinite relaxations is inequivalent to the one in Ref. [8], and also inequivalent to the robust semidefinite programming approach in Refs. [9]. The above formulation in the optimization problem in terms of full separability still does not constitute a restriction of generality, as this includes all separability classes with respect to all possible splits.

Alternatively to the above approach, one may write each test in the form of a feasibility problem, a problem with a vanishing objective function,

$$\text{minimize } 0, \tag{21}$$

$$\text{subject to } \rho \text{ satisfies the test of step}$$

$$h = h_{\min}, h_{\min+1}, \ldots \text{ in the hierarchy}.$$

Either one finds no solution (which is to say, the problem is not primal feasible), and one can assert that the state is not fully separable, or one has to go on one step in the hierarchy. In each step of the hierarchy forming a semidefinite problem, the dual problem can then be employed to prove the infeasibility of the above primal problem serving as a certificate [16] (see also Ref. [8]).

In general the total problem can in each step be written as a semidefinite problem of the form

$$\text{minimize } 0, \tag{22}$$

$$\text{subject to } H_0 + \sum_{s=1}^{T} z_s H_s \geqslant 0,$$

with appropriate matrices $H_s$, $s=1,\ldots,T$. The associated Lagrange dual problem [17] is again a semidefinite program,

$$\text{maximize } -\mathrm{tr}[ZH_0], \tag{23}$$

$$\text{subject to } \mathrm{tr}[ZH_s] = 0, \quad s = 1, \ldots, T,$$

$$Z \geqslant 0$$

In the context of our feasibility problem above, any feasible solution of the dual problem with $\mathrm{tr}[ZH_0]<0$ proves the infeasibility of the primal (original) problem. That is, we can use the dual problem to prove properties of our original problem at hand.

Finally, it is important to point out that in problem (19), one may keep the semidefinite constraint provided by the last line, and look for the intersection of the feasible sets of the semidefinite part and the constraint set of the relaxations. Then, in each step we can assert either whether the state is entangled, or that one cannot say whether it is entangled or not. In this way, it may happen, yet, that the state is entangled, although this entanglement is not detected in any step of the hierarchy. One hence obtains a hierarchy of sufficient criteria, albeit one which is not necessarily asymptotically complete. This will be discussed in more detail in the section on the hierarchy of relaxations.

In an implementation of this optimization problem, one has to choose a basis of Hermitian matrices for each Hilbert space,

$$\{\sigma_1, \ldots, \sigma_{d_j^2}\}, \tag{24}$$

for $j=1,\ldots,N$, suppressing an additional index labeling the subsystems. These Hermitian matrices satisfy $\mathrm{tr}[\sigma_1]=1$ and

$$\mathrm{tr}[\sigma_k]=0, \quad k=2,\ldots,d_j^2, \tag{25}$$

and have a Hilbert-Schmidt scalar product

$$\mathrm{tr}[\sigma_k\sigma_l]=\xi_{d_j}\delta_{kl} \tag{26}$$

with a dimension-dependent constant $\xi_{d_j}$ (and similarly for terms of third order). For the case of qubit subsystems, the appropriately normalized familiar Pauli matrices can be taken. In terms of this basis of Hermitian matrices, the matrices $P^{(i)}$ and $P$ can be written as

$$P^{(i)}=\sum_{\kappa=(k_1,\ldots,k_N)} p_\kappa^{(i)}\Sigma_\kappa, \tag{27}$$

$$P=\sum_{\kappa=(k_1,\ldots,k_N)} p_\kappa\Sigma_\kappa, \tag{28}$$

where $\kappa=(k_1,\ldots,k_N)$, is a multi-index, with $k_j=1,\ldots,d_j^2$ for $j\in I$, and

$$\Sigma_\kappa=\sigma_{k_1}\otimes\sigma_{k_2}\otimes\cdots\otimes\sigma_{k_N}. \tag{29}$$

This parametrization will be used in the section presenting numerical examples. Before we present the hierarchy of relaxations explicitly, we discuss the other applications which are similar in structure from the point of view taken in this paper.

### B. Nondecomposable witnesses

Optimization problems of the type of the one in Eq. (2) often appear in the construction of entanglement witnesses [23]. An entanglement witness is a Hermitian observable $W=W^\dagger$ with the property that $\mathrm{tr}[W\rho]\geqslant 0$ holds for all separable $\rho$; thus a negative expectation value signals the presence of entanglement. So entanglement witnesses can be used for an experimental verification that a given state is entangled, and, in fact, they have already been implemented [24].

The detection of entanglement is not only of interest for fundamental reasons, it can also be of practical interest. This is the case in quantum crytography, since it has been shown that the provable presence of quantum correlations in such protocols is a necessary precondition for secure key distillation [25]. Entanglement witnesses are particularly suited to deliver this entanglement proof, even when the quantum state shared by the users cannot be completely reconstructed. In turn, by measuring *all* accessible witnesses, one can decide whether the measurable correlations of the state origin from an entangled state or may be compatible with a separable state.

There are many strategies to construct entanglement witnesses [26,27]. As an example in which such optimization problems occur we choose the construction of nondecomposable witnesses for PPT entangled states [27]. These are entangled states which have a positive partial transpose [28]. We discuss our example in the bipartite setting for simplicity. In the theory of PPT entangled states the extreme points of the set are of central interest, and often referred to as edge states. A state $\rho$ is a PPT entangled edge state if it has a positive partial transpose, while for all product vectors $|a,b\rangle$ in the range of $\rho$ the vector $|a,b^*\rangle$ is not in the range of the partially transposed $\rho^{T_B}$ [23,27]. Here the asterisk refers to complex conjugation.

To construct witnesses for these states, one proceeds as follows. Let $R=K(\rho)$ and $Q=K(\rho^{T_B})$ be the projectors onto the kernels of $\rho$ and of $\rho^{T_B}$, respectively. Then a witness allowing the detection of the state $\rho$ is given by [27]

$$W'=R+Q^{T_B}-\varepsilon\mathbb{1}, \tag{30}$$

where

$$\varepsilon=\min_{|a,b\rangle}\mathrm{tr}[|a,b\rangle\langle a,b|(R+Q^{T_B})]. \tag{31}$$

Since $\rho$ is an edge state, we have $\varepsilon>0$. This implies that $\mathrm{tr}[W'\rho]<0$; thus, $\rho$ is detected. Also, it is clear that the difficult part of this construction is the minimization procedure in Eq. (31)—which is just of the type of Eq. (2).

This method can also be used to obtain a finer witness from a given one $\tilde{W}$, i.e., a witness that detects the same states as $\tilde{W}$ and more. If $\tilde{\varepsilon}=\min_{|a,b\rangle}\mathrm{tr}[|a,b\rangle\langle a,b|\tilde{W}]>0$ then $\tilde{W}-\tilde{\varepsilon}\mathbb{1}$ is a finer witness than $\tilde{W}$. This can also be applied in the scenario where only a restricted set of observables is available, since the observable $\mathbb{1}$ is always accessible. In practical situations, given a particular implementation of a quantum-key-distribution (QKD) scheme, it is sufficient to obtain one relevant entanglement witness as a first step toward the demonstration of the feasibility of the scheme. Here is where the method presented in this section can be used. Although this method requires one, as a starting point, to have already a valid entanglement witness for the given QKD protocol, note that this operator does not need to be an entanglement witness in the strict sense, but can be a positive operator from the restricted set which is more easy to characterize than an entanglement witnesses [31]. Moreover, during several steps of the method, better entanglement witnesses can be obtained from it, belonging to the same restricted set.

The construction of the witness above can also be used for multipartite PPT witnesses [32]. The other approaches for the construction of entanglement witnesses also need similar optimization processes [26]. For the sake of generality, we formulate the optimization strategies directly in the multipartite setting as in Eq. (2). For a given entanglement witness $W=W^\dagger$, the optimization problem looks as follows. The aim is to solve the problem

$$\text{minimize } x \tag{32}$$

$$\text{subject to } x\geqslant\mathrm{tr}[WP],$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P]^2]=1 \text{ for all } j\in I,$$

$$\mathrm{tr}[\mathrm{tr}_{\Lambda j}[P]^3] = 1 \text{ for all } j \in I.$$

Again, for multiparty qubit systems this can be written as a polynomially constrained problem with polynomials of degree 2.

### C. Estimating the geometric entanglement to quantify multiparticle entanglement

The same tools can be used in order to quantify multiparticle entanglement for pure quantum states. Needless to say, the question of quantifying multiparticle entanglement is much more involved that the analogous question in the bipartite setting: in the bipartite setting, the degree of entanglement of pure states can be uniquely quantified in terms of the entropy of entanglement. Any pure state can be asymptotically reversibly transformed into any other, the achievable rates being given by just this measure of entanglement. In this sense, any bipartite entanglement of pure states is essentially equivalent to that of the maximally entangled pair of qubits, which forms the so-called minimal reversible entanglement-generating set (MREGS) [33]. The situation is very different in the multipartite case, where the MREGS's have not even been identified for three-qubit systems, let alone for more general settings [34]. In view of this fact, several more pragmatic (and inequivalent) measures of entanglement have been proposed, reasonably grasping the degree of multiparticle entanglement [35–37]. To evaluate these quantities typically amounts to solving a computationally hard problem.

One of the reasonable quantities to quantify multiparticle entanglement is the geometric measure of entanglement [35,36,38]: for a given state vector $|\psi\rangle \in \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$, essentially, entanglement is then quantified in terms of the solution of the maximization problem

$$\Lambda^2 = \max |\langle \psi | \phi \rangle|^2, \tag{33}$$

such that the geometric measure of entanglement becomes

$$E(|\psi\rangle\langle\psi|) = 1 - \Lambda^2. \tag{34}$$

The maximization is performed over all state vectors $|\phi\rangle$ which are products with respect to all subsystems. Setting $\rho = |\psi\rangle\langle\psi|$ and

$$P = |\phi\rangle\langle\phi| = |\phi_1\rangle\langle\phi_1| \otimes \cdots \otimes |\phi_N\rangle\langle\phi_N|, \tag{35}$$

we arrive at

$$\text{minimize } t, \tag{36}$$

$$\text{subject to } \mathrm{tr}[P\rho] + t \geqslant 1,$$

$$\mathrm{tr}[\mathrm{tr}_{\Lambda j}[P]^2] = 1 \text{ for all } j \in I,$$

$$\mathrm{tr}[\mathrm{tr}_{\Lambda j}[P]^3] = 1 \text{ for all } j \in I,$$

which is the same optimization as in the previous subsection, except for one line in the list of constraints.

### D. Entanglement witnesses based on second moments and entropic criteria

In this subsection we will consider again entanglement witnesses, but not in the original sense, which involve only expectation values of Hermitian operators. It is also possible to introduce nonlinear functionals with similar properties: these are entanglement witnesses based on second moments, on variances of observables. Such entanglement criteria based on second moments are very popular in the study of infinite-dimensional quantum systems having canonical coordinates [39]. There, to measure arbitrary observables is often by far unfeasible, whereas the estimation of second moments of canonical coordinates is very accessible. In optical systems, the appropriate measurements are available in homodyne detection. Similarly, one may also for finite-dimensional systems look at variances rather than at first moments themselves [40]. In Ref. [41], second-order witnesses related to variances of operators were constructed, and the relation to entanglement criteria for continuous variable systems based on second moments was shown. The advantage in a practical context is that one specifies some observables which are the most accessible, and tests whether the obtained second moments are consistent with a separable state. The application of such a test always requires the solution of an optimization problem as pointed out below.

Let us specify a set of observables $M_1, \ldots, M_K$. Then we can define the real symmetric $K \times K$ covariance matrix $\gamma_\rho$ of a state $\rho$ associated with these observables as

$$(\gamma_\rho)_{k,l} = (\mathrm{tr}[M_k M_l \rho] + \mathrm{tr}[M_l M_k \rho])/2 - \mathrm{tr}[M_k \rho]\mathrm{tr}[M_l \rho], \tag{37}$$

with $k, l = 1, \ldots, K$. This is completely analogous to the familiar covariance matrix of systems with canonical coordinates. Then, it turns out that—in the previous notation—any fully separable state $\rho$ has the property that there exist states

$$\rho_1^{(i)}, \ldots, \rho_N^{(i)}, \quad i = 1, \ldots, n, \tag{38}$$

$n = \Pi_{j=1}^N d_j^2$, and probability distributions $\{p_i\}_i$ such that

$$\gamma_\rho \geqslant \sum_i p_i \gamma_{\rho_1^{(i)} \otimes \cdots \otimes \rho_N^{(i)}}. \tag{39}$$

So one would fix those observables that are the most accessible, and estimate the appropriate second moments. This would yield an estimate of the elements of the covariance matrix to some accuracy. Then, the question that arises is: do states and probability distributions exist that satisfy (39)? If not, we can conclude that the state must have been entangled. It is important to note that this judgement is not based on the knowledge of the entire state, but only on the knowledge of the covariance matrix with respect to a previously selected set of observables. This is a problem that can be cast into a feasibility problem, again in the form that we envision. As it is a feasibility problem, the objective function can be set to zero. This can be written as follows:

$$\text{minimize } 0, \tag{40}$$

$$\text{subject to } Q - \sum_{i=1}^{n} p_i Q^{(i)} = 0,$$

$$Q_{k,l}^{(i)} = (\mathrm{tr}[M_k M_l P^{(i)}] + \mathrm{tr}[M_l M_k P^{(i)}])/2 - \mathrm{tr}[M_k P^{(i)}]\mathrm{tr}[M_l P^{(i)}],$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^2] = (\mathrm{tr}[P^{(i)}])^2 \quad \text{for all } i = 1, \ldots, n, \quad j \in I,$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^3] = (\mathrm{tr}[P^{(i)}])^3 \quad \text{for all } i = 1, \ldots, n, \quad j \in I,$$

$$\sum_{i=1}^{n} \mathrm{tr}[P^{(i)}] = 1,$$

$$\gamma_\rho - Q \geqslant 0.$$

In each step of the hierarchies of relaxations, we can assess whether there is a feasible solution or not. If there is no feasible solution in some step, we can conclude that the state is entangled, and multiparticle entanglement is hence detected. This is now a problem which is still a combination of a polynomially constrained problem, together with a semidefinite constraint. Here, two strategies may be applied.

On the one hand, one can keep the semidefinite constraint, and can proceed as pointed out in Sec. II A. This means that one can in each step assert that the state was entangled, or one has to go one step further. This is computationally cheaper, but comes at the price of losing asymptotic completeness. For practical purposes, however, this method is expected to be the method of choice; in particular in the light of the fact that for a given set of observables, typically not every entangled state is anyway detected by the entanglement witness based on second moments.

The other strategy, on the other hand, is to formulate $\gamma_\rho - Q \geqslant 0$ as a set of polynomial constraints. A Hermitian matrix is positive if and only if the determinants of all its submatrices are positive (see also Ref. [31]). This gives rise to a set of polynomial constraints, for which the relaxations can be applied, leading to an asymptotically complete hierarchy of tests. This comes at the price of being computationally more expensive.

In view of Refs. [40,41], it is useful to employ arguments along the following line. If we can show that no fully separable state can have the image that we estimate in an experiment, we can assert that the state must have been entangled. This observation can, while being fairly obvious, still be practically very relevant. For example, we may for any observable $M = M^\dagger$ look at the minimum of second moments that are consistent with a separable state, i.e., the solution of

$$\text{minimize } \mathrm{tr}[M^2 P] - \mathrm{tr}[MP]^2, \tag{41}$$

$$\text{subject to } P \text{ is fully separable}, \tag{42}$$

and use this as a criterion for detecting entangled states. This gives rise to the optimization problem

$$\text{minimize } x, \tag{43}$$

$$\text{subject to } x \geqslant \mathrm{tr}[M^2 P] - \mathrm{tr}[MP]^2,$$

$$P - \sum_{i=1}^{n} P^{(i)} = 0,$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^2] = (\mathrm{tr}[P^{(i)}])^2 \text{ for all } i = 1, \ldots, n, \quad j \in I,$$

$$\mathrm{tr}[\mathrm{tr}_{I\setminus j}[P^{(i)}]^3] = (\mathrm{tr}[P^{(i)}])^3 \text{ for all } i = 1, \ldots, n, \quad j \in I,$$

$$\sum_{i=1}^{n} \mathrm{tr}[P^{(i)}] = 1.$$

It should be clear at this point that the same method can be used for entanglement criteria based on linear entropies, that is, $p$-norms for $p=2$ (see, in the rich literature on the subject, e.g., Refs. [42]). For any expression that is linear in the linear entropies of the whole state $\rho$

$$\|\rho\|_2 = \mathrm{tr}[\rho^2] \tag{44}$$

of a multipartite system and in the linear entropies of the reductions

$$\|\mathrm{tr}_{j\setminus I}[\rho]\|_2 = \mathrm{tr}[(\mathrm{tr}_{j\setminus I}[\rho])^2], \quad j = 1, \ldots, n, \tag{45}$$

one can in the same manner find the largest value consistent with a separable state. Any state that delivers a larger value is then clearly entangled. In practical considerations, these linear entropies can be estimated in a fairly feasible manner [42], for example, when assessing entanglement in Bose-Hubbard-type models.

### E. Maximal output purities of quantum channels

Similar arguments, it will finally be briefly discussed, can immediately be applied to assess minimal output purities of channels

$$\rho \mapsto \mathcal{E}(\rho) = \sum_{i=1}^{k} R_i \rho R_i^\dagger, \tag{46}$$

where $\Sigma_{i=1}^{k} R_i^\dagger R_i = \mathbb{1}$, with respect to $p$-norms for $p=2$ (and other integer $p$); see, e.g., Refs. [43]. One may then investigate the maximal output purity

$$\nu_2(\mathcal{E}) = \max_\rho \|\mathcal{E}(\rho)\|_2, \tag{47}$$

where it does not constitute a restriction of generality to maximize not over all states $\rho$, but merely over all pure states (compare also Ref. [7]). The central question here is to see whether this quantity is multiplicative in general. That is whether generally

$$\nu_2(\mathcal{E}_1 \otimes \mathcal{E}_2) = \nu_2(\mathcal{E}_1)\nu_2(\mathcal{E}_2) \tag{48}$$

holds, which means that it is never an advantage to allow for entangled inputs when maximizing the output purity. In the previously used language, this optimization problem can be written as follows:

$$\text{maximize } x \tag{49}$$

$$\text{subject to } x \leqslant \mathrm{tr}\left[\left(\sum_{i=1}^{k} R_i P R_i^\dagger\right)\left(\sum_{j=1}^{k} R_j P R_j^\dagger\right)\right],$$

$$\mathrm{tr}[P^2] = 1,$$

$$\mathrm{tr}[P^3] = 1,$$

as a polynomially constrained problem with polynomials of degree 3.

## III. COMPLETE HIERARCHIES OF RELAXATIONS TO APPROXIMATE THE SOLUTIONS

We will now state how the theory of relaxations can be applied to the described problems in entanglement theory. In all of the above cases (except in Sec. II D), we obtained an optimization problem of the following structure: for $x \in \mathbb{R}^t$,

$$\text{minimize } c^T x, \tag{50}$$

$$\text{subject to } g_l(x) \geqslant 0,$$

for $l=1,\ldots,L$, the global optimum value being denoted as $p^*$, where $g_l$ is a polynomial of at most degree 3. The constraint set given by

$$\mathcal{M} = \{x \in \mathbb{R}^t : g_l(x) \geqslant 0,\ l = 1,\ldots,L\} \tag{51}$$

is not a convex set. We may however apply Lasserre's method of semidefinite relaxations to treat this part (see the Appendix). This will yield a sequence of semidefinite programs, labeled with an index $h=h_{\min}, h_{\min}+1,\ldots$, such that each of the efficiently solvable steps yields an approximation of the original problem. The minimal step $h_{\min}$ is 1 if the highest degree of the constraint polynomials is 2 and $h_{\min}=2$ if constraints of degree 3 are required. The case $h=h_{\min}$ is the first semidefinite relaxation leading to the first approximation, $h=h_{\min}+1$ is the second, and so on. Often, in practice the global optimum is already achieved after a small number of steps in the hierarchy.

### A. Semidefinite relaxations

Instead of considering an optimization problem in $x \in \mathbb{R}^t$, this is turned into an optimization problem in a larger real vector $y \in \mathbb{R}^{D_{2h}}$, $D_{2h}$ being a natural number defined in the Appendix. This larger dimension is due to the uplifting procedure used in Lasserre's method [13,14] for approximating the quadratic part of our problems, and goes back to work in Ref. [44]. For each instance of the hierarchy of semidefinite programs, the objective function will be the same, but uplifted, namely,

$$y \mapsto d^T y, \tag{52}$$

where

$$d^T = (0, c_1, \ldots, c_t, 0, \ldots, 0), \tag{53}$$

with $c \in \mathbb{R}^t$ being defined as above. Lasserre's method now gives rise to a sequence of semidefinite programs approximating the solutions of

$$\text{minimize } c^T x, \tag{54}$$

$$\text{subject to } g_l(x) \geqslant 0,$$

for $l=1,\ldots,L$ in the following form: For $h=h_{\min}$, $h_{\min}+1,\ldots$, each instance is of the form

$$\text{minimize } d^T y, \tag{55}$$

$$\text{subject to } F^{[h]}(y) \geqslant 0,$$

$$G_l^{[h]}(y) \geqslant 0, \quad l = 1,\ldots,L$$

with matrices $F^{[h]}(y)$ and $G_l^{[h]}(y)$ that are linear in the elements of $y$ that increase in dimension with increasing $h$ (see the Appendix). This method is based on recent results in real algebraic geometry; see also Ref. [15].

In Ref. [13] convergence to the solution of (54) is guaranteed if certain conditions are satisfied. Convergence in the limit $h \to \infty$ is guaranteed if there exist polynomials $u_0, u_1, \ldots, u_L$, all sums of squares, such that the set

$$\left\{ x \in \mathbb{R}^t : u_0(x) + \sum_{l=1}^{L} u_l(x) g_l(x) \geqslant 0 \right\} \tag{56}$$

is compact. This is, however, the case in all of the specific situations from entanglement theory considered above. The set in Eq. (56) is compact if there exists an $l \in \{1,\ldots,L\}$ such that the set

$$\{x \in \mathbb{R}^t : g_l(x) \geqslant 0\} \tag{57}$$

is compact. In each of the discussed cases, we find that due to the linear constraints incorporating the trace requirement and the quadratic constraints coming from the purity of the reduced states, there exists an $a>0$ such that $a^2 - \|x\|^2 \geqslant 0$ for all $x \in \mathcal{M}$. This follows from the fact that for each of the involved matrices, the trace is bounded from above, and positivity of the matrices enforces boundedness of all elements. Hence, to ensure asymptotic completeness, we may add the constraint $g_{L+1}(x) = a^2 - \|x\|^2 \geqslant 0$ to the list of quadratic constraints, such that the condition in Eq. (57) is certainly satisfied. Hence, one can conclude that

$$\min_{y \in \mathcal{M}^{[h]}} d^T y \to \min_{x \in \mathcal{M}} c^T x \tag{58}$$

for $h \to \infty$, and for

$$\mathcal{M}^{[h]} = \{y \in \mathbb{R}^{D_{2h}} : F^{[h]}(y) \geqslant 0,\ G_l^{[h]}(y) \geqslant 0,\ l = 1,\ldots,L+1\}. \tag{59}$$

This is not only meant as a numerical procedure: instead, as each step is an analytically accessible semidefinite program, in each step one may assess the approximations with analytical means. Moreover, symmetries of the involved states under certain groups can be carried over to symmetries in the Hermitian matrices in the semidefinite programs, similarly to the strategy employed in Ref. [5] for semidefinite programs, and in Ref. [4] for convex but not semidefinite programs.

In Sec. II D, we encountered an additional semidefinite constraint. Then, Lasserre's method may be applied using

polynomials of higher order, as described above. Or, one may combine the semidefinite relaxations with the semidefinite constraint itself. This gives rise to a hierarchy of sufficient tests, without the property of asymptotic completeness. To see how they can be combined, let us consider an additional semidefinite constraint such as $\gamma_\rho - Q \geqslant 0$. In terms of the $y \in \mathbb{R}^{D_{2h}}$, we have the feasible set of the additional semidefinite constraint

$$\mathcal{F} = \left\{ y \in \mathbb{R}^{D_{2h}} : F_0 + \sum_{s=1}^{t} y_{s+1} F_s \geqslant 0 \right\}, \tag{60}$$

with appropriate matrices $F_0, \ldots, F_t$. Therefore, we can write the full hierarchy of semidefinite programs as

$$\text{minimize } d^T y \tag{61}$$

$$\text{subject to } F^{[h]}(y) \geqslant 0,$$

$$G_l^{[h]}(y) \geqslant 0, \quad l = 1, \ldots, L,$$

$$F_0 + \sum_{s=1}^{t} y_{s+1} F_s \geqslant 0,$$

$h = h_{\min}, h_{\min+1}, \ldots$ being the label of the element of the hierarchy. The projection of the feasible sets $\mathcal{M}^{[h]}$ onto the plane of first-order moments, i.e., onto the plane

$$\{ y \in \mathbb{R}^{D_{2h}} : y = (0, y_2, \ldots, y_{t+1}, 0, \ldots, 0) \}, \tag{62}$$

conceived as a subset of $\mathbb{R}^t$, converges (pointwise) to the convex hull of $\mathcal{M}$ [12–14]. Therefore, we have that

$$\min_{y \in \mathcal{M}^{[h]} \cap \mathcal{F}} d^T y \leqslant p^* \tag{63}$$

for all $h \to \infty$. Moreover, $\min_{y \in \mathcal{M}^{[h]} \cap \mathcal{F}} d^T y$ is a monotone increasing sequence in $h$, such that the sufficient criteria become more powerful with an increasing order of the hierarchy.

### B. Size of the relaxations

A relevant issue is how large the semidefinite relaxations are in each step of the hierarchy. In the worst-case scenario, where the polynomial constraints is a polynomial involving all basis elements of the basis of polynomials of the respective degree, one obtains the subsequent sizes of the relaxation matrices. The matrix $F^{[h]}$ is of dimension $D_h \times D_h$ (for a definition of $D_h$, see the Appendix). As a formula for $D_h$ we arrive at

$$D_h = \sum_{k=0}^{h} \binom{t+k-1}{k}. \tag{64}$$

For example,

$$D_2 = 1 + t + \frac{t(t+1)}{2}. \tag{65}$$

In the number of variables $t$, this is a manifestly polynomial expression. In step $h$ the vector $y$ is of the length $D_{2h}$. Notably, in each of the steps, the effort of a numerical solution of the associated semidefinite program is polynomial in the dimension of the matrices [16]. Hence, each problem can be solved in an efficient manner.

In terms of the step $h$ in the hierarchy, it turns out that the scaling is also polynomial. Approximating the above sum by an integral expression, we arrive at

$$D_h = O(h^t). \tag{66}$$

That is, for a fixed number of variables (which is the setting considered here), the size of the vector of the objective variables increases also only polynomially in the step $h$ in the hierarchy. Moreover, in many small- and medium-size problems, the program detects optimal solutions in the first iteration steps at relatively low computational cost [45]. Also, the sparsity of the moment matrices may be exploited. The issue of computational effort will be discussed in more detail elsewhere. Another point of interest is that it is possible in some cases to trade in a lower number of variables $t$ for a higher lowest relaxation step $h_{\min}$, as in the examples in the subsequent section. In some cases, this might simplify the problem, as in our example in the next section.

## IV. NUMERICAL EXAMPLES

In this section we present some numerical examples, in order to show that the approach is also feasible in practice. We will provide three examples, two for the geometric measure of entanglement and one for the construction of entanglement witnesses for bound entangled three-qubit states.

### A. Geometric measure for three-qubit states

Let us start with the calculation of the geometric measure of entanglement for three-qubit states. As we have shown in Sec. II the computation of the geometric measure of entanglement for a given pure three-qubit state vector $|\psi\rangle$ requires essentially the calculation of

$$\Lambda^2 = \max_{|a,b,c\rangle} |\langle a,b,c|\psi\rangle|^2. \tag{67}$$

As already mentioned above, we use here a different parametrization from the general one described in Sec. II. In terms of the Pauli matrices forming a basis of Hermitan matrices, we can write

$$|\psi\rangle\langle\psi| = \frac{1}{8} \sum_{i,j,k=0}^{3} \lambda_{ijk} (\sigma_i \otimes \sigma_j \otimes \sigma_k), \tag{68}$$

$$|a,b,c\rangle\langle a,b,c| = \frac{1}{8} \sum_{i,j,k=0}^{3} a_i b_j c_k (\sigma_i \otimes \sigma_j \otimes \sigma_k), \tag{69}$$

where $\lambda_{000} = a_0 = b_0 = c_0 = 1$. The coefficients $\lambda_{ijk}$, $i,j,k = 0, \ldots, 3$, are determined from the known state vector $|\psi\rangle$. We have to impose constraints that guarantee that $\rho_A$ is a pure state on the coefficients $(a_1, a_2, a_3)$ describing the state $\rho_A = \sum_{i=0}^{3} a_i \sigma_i / 2$ [and similarly $(b_1, b_2, b_3)$ and $(c_1, c_2, c_3)$]. We have seen before that for qubit systems, instead of requiring $\mathrm{tr}[\rho_A^2] = 1$ and $\mathrm{tr}[\rho_A^3] = 1$, we may alternatively merely require

that $\mathrm{tr}[\rho_A]=1$ and $\mathrm{tr}[\rho_A^2]=1$ (where $\mathrm{tr}[\rho_A]=1$ is already a consequence of the parametrization). So we arrive at the optimization problem

$$\text{minimize}_{a_i,b_j,c_k} \frac{1}{8}\sum_{i,j,k=0}^{3}\lambda_{ijk}a_i b_j c_k, \tag{70}$$

$$\text{subject to } a_1^2+a_2^2+a_3^2=1,$$

$$b_1^2+b_2^2+b_3^2=1,$$

$$c_1^2+c_2^2+c_3^2=1.$$

This polynomial optimization problem can be solved with the help of Lasserre's method (see the Appendix). For these calculations the package GLOPTIPOLY [45] based on SEDUMI [46] is freely available, and we have used it for our calculations. The package GLOPTIPOLY has a number of desirable features, in particular, it provides a certificate for global optimality.

Note that with this parametrization, the number of objective variables is $4N$, $N$ being the number of qubits, in contrast to $4^N$ parameters which are necessary to parametrize a general $N$ qubit state as decribed in Sec. II A. From Eq. (70) it is clear that the objective function will be a polynomial of degree $N$ which increases $h_{\min}$ (see the Appendix).

First, we present a nontrivial example for the calculation of the geometric measure of entanglement, in a case where its value is already known. In this way we can test our methods. We aim at computing the geometric measure of entanglement for state vectors of the form

$$|\psi(s)\rangle=\sqrt{s}|W\rangle+\sqrt{1-s}|\tilde{W}\rangle, \tag{71}$$

$s\in[0,1]$, where $|W\rangle$ and $|\tilde{W}\rangle$ are state vectors of three-qubit W states [47] in different bases,

$$|W\rangle=(|001\rangle+|010\rangle+|100\rangle)/\sqrt{3}, \tag{72}$$

$$|\tilde{W}\rangle=(|011\rangle+|101\rangle+|110\rangle)/\sqrt{3}. \tag{73}$$

For the geometric measure of entanglement of $|\psi(s)\rangle$ a formula has been developed in Ref. [36], exploiting the permutation symmetry of the states. The comparison between the theoretical value and the numerical calculation using Lasserre's method for $h=2$ is shown in Fig. 1. Details of the performance are summarized in Table I. The results indicate clearly the usefulness of the presented approach. As a matter of fact, this is a case where already a very small number of steps in the hierarchy detects the global optimum, as is typical for this relaxation, as has been pointed out in Ref. [45], based on numerical experiments.

### B. Geometric measure for four-qubit states

We calculate the geometric measure of entanglement also for the following one-parameter family of state vectors:

$$|\psi_4(p)\rangle=\sqrt{p}|\mathrm{GHZ}'\rangle-\sqrt{1-p}|\psi^+\rangle\otimes|\psi^+\rangle, \tag{74}$$

where

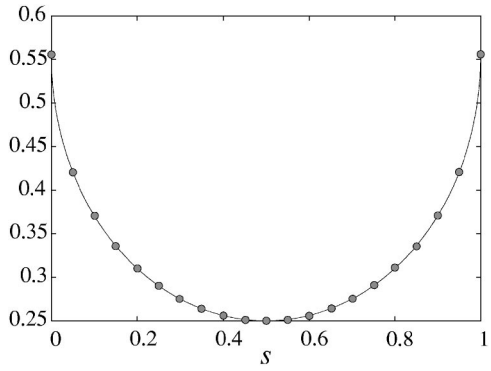


FIG. 1. The numerical values of the geometric measure of entanglement $E$ of the family of states of Eq. (71), plotted on top of the analytical values of Ref. [36].

$$|\mathrm{GHZ}'\rangle=(|0011\rangle+|1100\rangle)/\sqrt{2}, \tag{75}$$

$|\psi^+\rangle=(|01\rangle+|10\rangle)/\sqrt{2}$, and $p\in[0,1]$. The state vector $|\psi_4(2/3)\rangle$ corresponds to the four-qubit singlet state, i.e., the state vector satisfying

$$U^{\otimes 4}|\psi\rangle=|\psi\rangle \tag{76}$$

for all unitary $U$ [48]. For the two individual states in the above superpositions in Eq. (74), the geometric measure can be directly evaluated [36]: For $p=1$ we find $\Lambda^2=1/2$, and for $p=0$ we obtain $\Lambda^2=1/4$ from $\Lambda^2_{\psi^+}=1/2$. The numerical results for the geometric measure of entanglement for other values of $p$ are plotted in Fig. 2.

It is interesting to note that at the singlet value $p=2/3$, the behavior of the geometric measure changes. From there up to $p=1$ the optimum is attained for the choices $|0011\rangle$ or $|1100\rangle$ of the product state which gives rise to the linear behavior.

The family of states specified in Eq. (74) is invariant under the exchange $(AB)\leftrightarrow(CD)$. Because of this symmetry, one may without loss of generality assume that the product state vector leading to the maximal value of $\Lambda^2$ is given by $|\phi_1,\phi_2,\phi_1,\phi_2\rangle$, where $|\phi_{1,2}\rangle=e^{i\chi_{1,2}}\cos\theta_{1,2}|0\rangle+e^{i\eta_{1,2}}\sin\theta_{1,2}|1\rangle$, where the optimal phases can be shown to be $\chi_1=\chi_2=\eta_1=\eta_2=0$. This gives rises to an optimization problem with polynomial constraints with only four variables which can be solved exactly by GLOPTIPOLY. The results coincide with the results above.

TABLE I. Details of the relaxations in the three numerical examples discussed above for one point of each example. The provided CPU time refers to a machine with an Intel Xeon Processor, 2.2 GHz, 1 Gbyte RAM, using GLOPTIPOLY 2.2E [45], SEDUMI 1.05 [47], and MATLAB 6.5.1.199709 (release 13). In all cases $h=h_{\min}=2$, so that the result was obtained after the first relaxation step.

| Subsection | Relaxation $h$ | Number of variables | dim($y$) | CPU time |
|---|---|---|---|---|
| A | 2 | 9 | 714 | 10.92 *s* |
| B | 2 | 12 | 1819 | 103.97 *s* |
| C | 2 | 9 | 714 | 6.14 *s* |

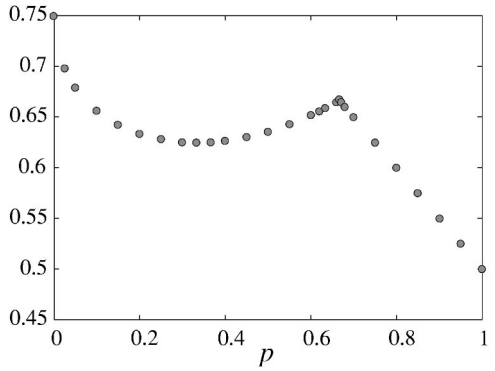


FIG. 2. The numerical values of the geometric measure of entanglement $E$ of the family of states of Eq. (74).

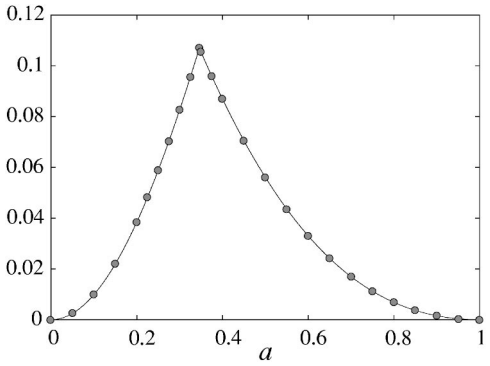


FIG. 3. The numerical values of $\varepsilon$ for $\overline{W}$ of Eq. (79) plotted on top of the results of Ref. [32].

### C. Witness for three-qubit PPT entangled states

Employing the same strategy, we would like to calculate the value of $\varepsilon$ as defined in Sec. II for the family of witnesses constructed for the PPT (bound) entangled states

$$\rho = \left( a|001\rangle\langle 001| + b|010\rangle\langle 010| + c|011\rangle\langle 011| + \frac{1}{c}|100\rangle\langle 100| + \frac{1}{b}|101\rangle\langle 101| + \frac{1}{a}|110\rangle\langle 110| + 2|\mathrm{GHZ}\rangle\langle \mathrm{GHZ}| \right) \Big/ C, \tag{77}$$

where $C=2+a+b+c+1/a+1/b+1/c$, and $a,b,c>0$, $ab \neq c$, and

$$|\mathrm{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}. \tag{78}$$

In Ref. [32], upper bounds for the values of $\varepsilon$ were obtained by using a multivariable minimization routine for the parameter range $a=b=1/c \in (0,1)$. The minimization over the product states has to be performed with respect to [32]

$$\begin{aligned}\overline{W} = {} & \frac{1}{2}(|000\rangle\langle 000| + |111\rangle\langle 111|) + \frac{1}{1+c^2}(c^2|100\rangle\langle 100| \\ & + |011\rangle\langle 011|) + \frac{1}{1+b^2}(|010\rangle\langle 010| + b^2|101\rangle\langle 101|) \\ & + \frac{1}{1+a^2}(|001\rangle\langle 001| + a^2|110\rangle\langle 110|) - \left(\frac{1}{2} + \frac{c}{1+c^2} \right. \\ & \left. + \frac{b}{1+b^2} + \frac{a}{1+a^2}\right)(|000\rangle\langle 111| + |111\rangle\langle 000|). \end{aligned} \tag{79}$$

The numerical results are plotted in Fig. 3. Again, the global optimum is achieved, and the found values agree with the values found in Ref. [32]. For details concerning the relaxations, see Table I.

## V. SUMMARY AND OUTLOOK

In this paper, we have reconsidered several problems in entanglement theory with the tools and language of convex optimization. The central point of the paper was that many problems where a minimization over pure product vectors is required can be written as instances of certain optimization problems involving polynomial constraints of degree 2 or 3, or with additional semidefinite constraints. For such polynomially constrained problems, which are generally instances of nonconvex optimization problems, hierarchies of semidefinite relaxations can be found. In this sense, one additional intention of this paper is to communicate these recently achieved results in the theory of relaxations and to show that they can be fruitfully applied in the quantum-information context. One arrives at hierarchies of more and more refined tests detecting entangled or separable states, or better and better lower bounds to optimization problems. In all instances, recently achieved known results from semialgebraic geometry guarantee that asymptotically, the achieved minimum is indeed approaching the globally optimal one. In this sense, the statements are similar in spirit with yet more versatile than the ones presented in Refs. [8]. Moreover, we have seen that the size of the optimization problems to be solved in each test grows polynomially with the steps in the hierarchy, and that for small problems, often already a small number of steps is required to find the exact solution.

The presented method is on the one hand meant as a numerical method to achieve good bounds to problems that are of relevance in the study of multiparticle entanglement, in the construction of entanglement witnesses in the bipartite and multipartite case, in the context of quantum-key distribution, and to assess maximal output purities. On the other hand, each instance of the hierarchy delivers a semidefinite program which is readily accessible with analytical methods, and where properties of the Lagrange dual can be exploited. It is hoped that these techniques shed light on the structure of optimization problems underlying the questions of entanglement and separability of several constituents.

Finally—and shifting perspective to some extent—it seems worth noticing that very similar techniques may be expected to be useful tools to assess ground-state properties of many-body Hamiltonians. Often variational approaches deliver already a good approximation to properties of the true ground state. For example, in the Gutzwiller ansatz for the ground state of the Bose-Hubbard model in a lattice one optimizes the energy functional over product states with respect to the sites. Similar techniques can be used for spin systems and matrix product states. Then, relaxations in the way discussed above could potentially be applied for a rea-

sonable size of the system. Such studies could complement numerical techniques yielding upper bounds, such as simulated annealing techniques, delivering provable lower bounds for the ground state energy.


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## APPENDIX: LASSERRE'S METHOD

For completeness, in this appendix we briefly sketch the method to construct sequences of semi-definite relaxations of global optimization problems with multivariate real-valued polynomial objective function and constraints due to Lasserre [13]. The class of problems is of the following form:

$$\text{minimize } c^T x, \quad x \in \mathbb{R}^t \tag{A1}$$

$$\text{subject to } g_l(x) \geqslant 0, \quad l = 1, \ldots, L, \tag{A2}$$

where $g_1, \ldots, g_L : \mathbb{R}^t \to \mathbb{R}$ are real-valued polynomials of degree 2 or 3. Although we consider only polynomials of degree of at most 3, it will be convenient to formulate the subsequent sequence of semidefinite programs in terms that formally involve higher-order polynomials. For any $r \in \mathbb{N}$, we consider the basis of polynomials of degree $r$ in the variables $x_1, \ldots, x_t$ as

$$(1; x_1, \ldots, x_t; x_1^2, x_1 x_2, \ldots, x_1 x_t; x_2^2, x_2 x_3, \ldots, x_t^r) \tag{A3}$$

in this ordering. The dimension of this basis will be denoted as $D_r$. For clarity of notation, we will not specify $t$ as an index, as this will stay the same throughout the procedure. Any polynomial of degree of at most $r$ can then be identified with a vector $p \in \mathbb{R}^{D_r}$. It is convenient to introduce two labelings, connected with each other by a function

$$f_r : \{1, \ldots, D_r\} \to \left\{ \alpha = (\alpha_1, \ldots, \alpha_t) : \sum_{s=1}^{t} \alpha_s \leqslant r \right\}, \tag{A4}$$

such that the $i$th element $z$, $i = 1, \ldots, D_r$, of the basis given by Eq. (A3) is written as

$$z = \prod_{i=1}^{t} x_i^{\alpha_i}, \tag{A5}$$

characterized by $\alpha = (\alpha_1, \ldots, \alpha_t) \in \mathbb{N}_0^t$. Note that for a given $k \in \mathbb{N}$ there are $\binom{t+k-1}{k}$ possible vectors $\alpha$ such that $\Sigma_{s=1}^t \alpha_s = k$. It follows that the dimensions $D_h$ are given by Eq. (64).

In the following we give the required matrices from Lasserre's method for general polynomials [13] and discuss the cases occuring in the paper explicitly afterward. Let $\delta_l$ be the degree of the polynomial constraint $l \in \{1, \ldots, L\}$ and $\lceil \delta_l / 2 \rceil$ be the smallest integer greater than or equal to $\delta_l / 2$. We assume that the objective function is linear, which is no restriction of generality, as other polynomials can always be incorporated in the constraints as in Sec. II. Then the first possible relaxation step of Lasserre's method is $h_{\min} = \max_l \lceil \delta_l / 2 \rceil$. For $h \geqslant h_{\min}$ the matrix $F^{[h]}(y)$ is of dimension $D_h \times D_h$ and linear in a vector $y \in \mathbb{R}^{D_{2h}}$,

$$[F^{[h]}(y)]_{i,j} = y_{f_{2h}^{-1}[f_h(i) + f_h(j)]}. \tag{A6}$$

In turn, the matrices $G_l^{[h]}(y)$, one for each of the constraint polynomials, $l = 1, \ldots, L$, are of dimension $D_{\tilde{h}_l} \times D_{\tilde{h}_l}$, where $\tilde{h}_l = h - \lceil \delta_l / 2 \rceil$. Each polynomial $g_l$ is characterized according to the above procedure by a vector $v_l$. The matrices $G_l^{[h]}(y)$ are then defined as

$$[G_l^{[h]}(y)]_{i,j} = \sum_{\alpha} v_{f_{\delta_l}^{-1}(\alpha)} y_{\{f^{-1}_{\delta_l + 2\tilde{h}_l}[f_{\tilde{h}_l}(i) + f_{\tilde{h}_l}(j)] + \alpha\}}. \tag{A7}$$

For qubits, $h_{\min} = 1$, because the maximal degree of the constraint polynomials is 2. For higher-dimensional systems, the highest occurring order is 3 due to the positivity constraints. In this case, $h_{\min} = 2$.


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$$\text{minimize} \quad c^T x,$$

$$\text{subject to } F_0 + \sum_{s=1}^{t} x_s F_s \geqslant 0,$$

one can formulate the Lagrange-dual problem, which is again a semidefinite problem. It is given by

$$\text{maximize} \quad -\text{tr}[F_0 Z],$$

$$\text{subject to } \text{tr}[F_s Z] = c_s, s = 1, \ldots, t,$$

$$Z \geqslant 0.$$

The key point of Lagrange duality is that any solution of the dual problem is a lower bound to the optimal solution of the primal problem. This is what is referred to as weak duality. Under certain conditions (in particular, if there is a solution $x$ satisfying $F_0+\Sigma_{s=1}^{t} x_s F_s > 0$, the optimal values of the dual and the primal problem are identical. In this case, which is rather the typical one, one refers to strong duality. The idea of Lagrange duality is a powerful tool to formulate rigorous lower bounds to solutions of optimization problems.

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$$\|x - y\|_2 \leqslant \delta,$$

and with $B(S, -\delta)$ the set of all $x \in S$ for which $y \in S$ for all $y \in \mathbb{Q}^m$ with $\|x-y\|_2 \leqslant \delta$. So clearly, $S$ is a strict subset of $B(S, \delta)$, and $B(S, -\delta)$ is a strict subset of $S$. The weak membership problem allows for two alternatives: given a rational element $x \in \mathbb{Q}^m$ and a rational number $\delta > 0$ either (i) assert that $x \in B(S, \delta)$, or (ii) assert that $x \neq B(S, -\delta)$.

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