Estimating multipartite entanglement measures

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We investigate the lower bound obtained from experimental data of a quantum state $\rho$, as proposed independently by Gühne et al. and Eisert et al. and apply it to mixed states of three qubits. The measure we consider is the convex-roof extended three-tangle. Our findings highlight an intimate relation to lower bounds obtained recently from so-called characteristic curves of a given entanglement measure. We apply the bounds to estimate the three-tangle present in recently performed experiments aimed at producing a three-qubit GHZ state. A non-vanishing lower bound is obtained if the GHZ-fidelity of the produced states is larger than $3/4$.

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I. INTRODUCTION

Since entanglement has been recognized as a possible valuable resource for quantum information processing $^1$, its analysis, detection and quantification are major goals $^2-5$. Except for simple measures that are polynomial invariants of degree 2, as e.g. the concurrence, already the calculation of that measure for a known mixed state poses a hard problem. In the laboratory, however, the states to work with are mixed states with major weight on a desired entangled state and additional uncontrolled admixture of different states due to systematic or non-systematic errors in the preparation process. Even though in principle full state tomography can be performed, it is experimentally increasingly expensive with the number of qubits.

It is for this reason that entanglement witnesses $^6$ play an important role for experimental detection of entanglement. Witness operators are constructed such to have negative expectation values only on states that carry a specific class of entanglement; all states that do not belong to this class have positive expectation value of the witness. Then, a negative expectation value implies that the mixed state $\rho$ carries the specific entanglement class detected by the witness. Recently, also quantitative estimates have been obtained for a variety of entanglement measures from (e.g. experimental) values for one or more witness operators $^7,8$, and for non-linear combinations of expectation values $^9-13$, by using methods of convex optimization $^14$. Further lower bounds have been obtained using a different approaches in a similar context $^15-20$. A connection of the problem of entanglement estimation from uncomplete information to Jaynes principle has been discussed already in $^21$.

Here, we investigate the tight lower bound for convex-roof extended measures as introduced in Refs. $^7,8$ for measures quantifying true multipartite entanglement in order to compare them with lower bounds obtained from different premises $^{22}$. The computation of the lower bound involves a supremum over some parameters and an infimum over pure states. One of our central observations is that the bound can be alternatively computed in a way which involves an infimum over pure states only, followed by the convexification of the resulting function. This observation establishes a connection between the methods from Refs. $^7,8$ and Ref. $^{22}$.

To this end we focus on the three-tangle, where a specific analytic solution of the convex roof can be used as a benchmark.

The work is laid out as follows. In the next section we briefly sketch the estimation method from witness operators as proposed in Ref. $^7,8$ and introduce the three-tangle and general multipartite entanglement witnesses. We then turn to the application of the method in Section III using expectation values of entanglement witnesses designed to detect true three-partite entanglement. We first consider a specific class of rank two mixed three qubit states for two different witness operators. The estimation using the data of the first witness is directly related to the results of Ref. $^{22}$. Then, we compute a lower bound for an important witness, which can directly be used to estimate the three-tangle produced in recent experiments. Finally, we report on further interesting observations as the effect of common symmetries of the Witness operators and the entanglement measure in Section IV where we also sketch a proof for the possible reduction to the related problem for pure states. Section V contains our conclusions.

II. BASIC CONCEPTS

A. Lower bound on entanglement

We consider the following situation: assume that a source can be described by the (unknown) density matrix $\rho$ and that $K$ expectation values $w_k = \text{tr} [\rho W_k]$ are measured and then collected in a vector $w$. The operators $W_k$ are further assumed to be witness operators. The lowest value of the entanglement of the state $\rho$ consistent with the measurement results is formally given by the solution of the problem

$$\inf_{\rho} E(\rho) \big|_{\text{tr} [W_k \rho] = w_k} .$$

In Refs $^7,8$ it has been shown that the solution of this optimization problem can be approximated from below with affine functions by $e(w) = \sup_{r} \left( r \cdot w - E(\sum_k r_k W_k) \right)$, where $E(W) = \sup_{\rho} (\text{tr} [\rho W] - E(\rho))$ is the Legendre transform.
of $E$. It was further shown that for pure state entanglement measures extended via the convex roof construction as

$$E(\rho) := \inf_{\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|} \sum_i p_i E(|\psi_i\rangle),$$

(2)

where $\sum_i p_i = 1$ and $p_i \geq 0$, the Legendre transform can be computed by optimizing over pure states only, leading to

$$\epsilon(w) = \sup_r \inf_{|\psi\rangle} \left( \sum_{k=1}^K r_k (w_k - \langle \psi | W_k |\psi\rangle) + E(|\psi\rangle) \right).$$

(3)

This bound is tight due to the convexity of the problem [7, 8].

A key observation is that Eq. (3) is the dual problem to the minimization of $E(\psi)$ on pure states subject to the witness conditions. It is therefore solved by an approximation of the pure state problem

$$\inf_{\psi} E(\psi) \big|_{|\psi\rangle W_k |\psi\rangle = w_k}$$

(4)

from below with affine functions. Hence the result coincides with the function convex hull of the pure state problem [37]. In other words, in order to solve the problem (1) for convex-roof extended entanglement measures, we could alternatively solve the problem (4) and convexify the resulting function. In cases where $K$ is small, this could reduce the computational cost. This point is illustrated in Section III A, where we explicitly solve (5) and (4) for a restricted situation, and the equivalence of both problems is highlighted explicitly. The origin of this equivalence is further investigated in Section IV A for arbitrary $K$.

The entanglement measure we consider is the three-tangle and its square; it distinguishes the two classes of global entanglement for three qubits: W and GHZ.

B. Three-tangle

The three-tangle of a general pure three qubit state expanded in a product basis $|\psi\rangle = \sum_{i,j,k=0}^1 \psi_{ijk} |i,j,k\rangle$ is given by [23]

$$\tau_3 = 4 |d_1 - 2d_2 + 4d_3|,$$

(5)

$$d_1 = \psi_{000}^2 \psi_{111}^2 + \psi_{001}^2 \psi_{110}^2 + \psi_{010}^2 \psi_{101}^2 + \psi_{100}^2 \psi_{011}^2,$$

$$d_2 = \psi_{000} \psi_{111} \psi_{011} \psi_{100} + \psi_{000} \psi_{111} \psi_{101} \psi_{010} + \psi_{001} \psi_{110} \psi_{011} \psi_{100} + \psi_{010} \psi_{101} \psi_{010} \psi_{101} + \psi_{100} \psi_{011} \psi_{100} \psi_{011} + \psi_{101} \psi_{010} \psi_{101} \psi_{010} + \psi_{110} \psi_{011} \psi_{100} \psi_{011} + \psi_{111} \psi_{010} \psi_{100} \psi_{010},$$

$$d_3 = \psi_{000} \psi_{111} \psi_{011} \psi_{100} + \psi_{001} \psi_{110} \psi_{011} \psi_{100} + \psi_{010} \psi_{101} \psi_{010} \psi_{101} + \psi_{100} \psi_{011} \psi_{100} \psi_{011} + \psi_{101} \psi_{010} \psi_{101} \psi_{010} + \psi_{110} \psi_{011} \psi_{100} \psi_{011} + \psi_{111} \psi_{010} \psi_{100} \psi_{010}.$$

It can be extended to mixed states via the convex roof construction [4].

The three-tangle is non-vanishing on true 3-partite entangled states only and vanishes on any bi-separable state such as $|\psi_{AB}\rangle \otimes |\phi_C\rangle$ for the parties $A$, $B$, and $C$, but also for W states introduced below. Also the convex-roof extended measure has this property for mixtures of bi-separable states, possibly for different partitions of the parties. Summarizing, it distinguishes the two classes of three-partite entanglement that are inequivalent under stochastic local operations and classical communications (SLOCC) [24]. The representative of one class is the W-state

$$|W\rangle = \frac{1}{\sqrt{3}} (|001\rangle + |010\rangle + |100\rangle)$$

(6)

and the representative of the other class is the GHZ state [23]

$$|\text{GHZ}\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle).$$

(7)

The three-tangle vanishes on all states of the W-class while it is non-vanishing for states of the GHZ-class. This classification can be extrapolated to mixed states in the sense that a mixed state belongs to the W-class if it has a decomposition into pure states exclusively out of the W-class [26]. In analogy, a mixed state belongs to the GHZ-class if it has a decomposition into pure states of the GHZ-class.

C. Multipartite entanglement witnesses

Multipartite entanglement witnesses can be constructed as [27]

$$W = \alpha \mathbb{I} - |\phi\rangle \langle\phi|,$$

(8)

where $\alpha = \max_{|\phi\rangle} |\langle\phi|\phi\rangle|^2$ is the maximal overlap of $|\phi\rangle$ with any state for which a given entanglement measure $E(|\phi\rangle) = 0$. In the case that global entanglement is concerned, $|\phi\rangle$ would be all biseparable states, whereas only W-states were included if only states with a GHZ component are of interest [23, 24]. We will highlight the latter situation and use the three-tangle, $E := \tau_3$, since it is non-zero only for states of the GHZ class.

For such witnesses, Eq. (3) becomes

$$\sup_r \left\{ -\sum_{k=1}^K r_k \langle \phi_k | \rho |\phi_k\rangle + \inf_{|\psi\rangle} \left( E(|\psi\rangle) + \sum_{k=1}^K r_k |\langle \phi_k |\psi\rangle|^2 \right) \right\}.$$  

(9)

This tells us that the trivial part $\alpha \mathbb{I}$ of the witness is irrelevant for the estimation. Hence, it does not seem to be essential that the expectation values are measured with respect to witnesses; an operator which projects onto a suitable subspaces seems to be sufficient [28].

For a single witness of this form it is straightforward to check that $r \geq 0$ leads to $\epsilon(w) = 0$; indeed, in this case the infimum over all states $|\psi\rangle$ would be those states perpendicular to $|\phi\rangle$ for which $E(|\psi\rangle) = 0$. This is always possible for a single witness. Another peculiar case is when $\langle \phi | \rho |\phi\rangle = 0$. In this case the estimate is independent of the density matrix under consideration and hence can only be zero. This corresponds to a bad choice for the witness operator. For the three-tangle, choosing $|\phi\rangle$ outside the GHZ class also leads to $\epsilon(w) = 0$ since then the infimum in (9) is reached by choosing $|\psi\rangle = |\phi\rangle$ for $r < 0$.

The above reasoning has interesting implications. First, $r$ can be taken to be negative for a single witness operator detecting the class of entanglement measured by $E$. Second, it
will admit to relax the restriction for $\mathcal{W}$ to being a witness, and a wider class of observables might lead to a reasonable estimation of $E$. In these cases, $r$ can possibly also be positive [38]. For more than one witness, the situation is more complicated and then even observables that are not useful at all for detecting entanglement could possibly be useful for improving the lower bound.

III. APPLICATION

We illustrate the results of the previous Section by explicitly solving the optimization problem (3) for special cases where knowledge about the state is assumed to be given and by showing explicitly that the result coincides with the one obtained by solving problem (4) and convexifying the solution. Then, we numerically solve the general problem for a general witness which allows to estimate the three-tangle from experiments where the GHZ state was produced and the fidelity $\langle \text{GHZ}, \rho_{\text{exp}} \rangle |\text{GHZ}|$ was estimated for the produced state $\rho_{\text{exp}}$.

A. Restricted optimization

We will demonstrate the Legendre transform at work on a simple example, where the Hilbert space for minimization with respect to $\psi$ is restricted to the range of the actual density matrix. This amounts to an idealized situation where the experimenter knows precisely which states are possibly produced in the laboratory to be part of the resulting mixed state. The specific example is about the three-tangle of the three qubit mixed states

$$\rho(p) = p \pi_{\text{GHZ}} + (1 - p) \pi_{\text{W}},$$

for which the analytic convex roof is known [28]. Here, $\pi_{\text{GHZ}}$, $\pi_{\text{W}}$ are the projectors onto the $\ket{\text{GHZ}}$ and $\ket{\text{W}}$ state, respectively. The vectors in the range of $\rho(p)$ are given by

$$\ket{Z(q, \phi)} = \sqrt{q} \ket{\text{GHZ}} - e^{i \phi} \sqrt{1 - q} \ket{\text{W}},$$

with its three-tangle given by

$$\tau_3(q, \phi) := \tau_3(Z(q, \phi)) = \left| q^2 - \frac{8 \sqrt{6}}{9} \sqrt{q(1 - q)} \right| e^{3i \phi}.$$

In the following, we want to apply the method of Refs [7,8] in order to get lower bounds for the three-tangle of general states $\rho$ in the GHZ-W subspace, using two qualitatively different single witnesses by performing the optimization of Eq. (3). We compare the result with that obtained by solving the problem (4) and by convexifying the solution.

1. GHZ witness

The first witness we would like to consider is

$$\mathcal{W}_{\text{GHZ}} = \alpha \mathbb{I} - \pi_{\text{GHZ}}.$$

For $\alpha = \frac{1}{3}$, this is a witness for multiparticle entanglement, while for $\alpha = \frac{3}{4}$, it detects states of the GHZ class only [26]. For this witness, $w = \text{tr} [\mathcal{W} \rho] = \frac{1}{3} p$, where we defined $p \equiv \langle \phi | q \rangle$. We perform the infimum with respect to $|\psi\rangle$ only over the restricted set of states $|Z(q, \phi)\rangle$ in the range of $\rho$. This is useful for obtaining a bound on the tangle of the rank 2 state $q$ and relies on the assumption that we know the subspace that $q$ lives in. As we will show below, knowing the expectation value of the witness (13) corresponds to knowing $q$ in Eq. (11). Hence the only free parameter in the pure state problem (4) is the phase $\phi$, which is minimized for $\phi = 0$ [28]. By the argument of Section 11 the lower bound to the problem is then given by the function convex hull $\tau_3(q, 0)$ (see Eq. (12) and Fig. 1), corresponding to the convexified solution of problem (4). It has emerged as so-called characteristic curve from a different approach to obtain lower bounds on entanglement measures pursued in Ref. [22].

Let us compare this result to the problem problem (3) which can be solved explicitly in this simple case. We have to determine

$$\epsilon(w) = \sup_{r \in q, \phi} \left( r(q - p) + \tau_3(q, \phi) \right)$$

and we show in what follows that $\epsilon(w) = \tau_3(p)$ is obtained also in this case. As mentioned above, the infimum over $\phi$ is always obtained for $\phi = 0$ so that we have to optimize over $q$ only. $\tau_3(q, 0)$ is plotted in Fig. 1. Graphically, optimization in Eq. (14) means to tilt the $x$-axis about the fixpoint $(x, y) = (p, 0)$, resulting in a curve with local minima for each tilting slope $r$. The largest of these minima is the estimated lower bound for the entanglement measure, here $\tau_3$. This seesaw argument is shown for two cases in Fig. 3.

As already discussed earlier, assuming $r > 0$ leads to an infimum at $q = 0$ for all $p \in [0, 1]$ and we are left with the trivial bound $\epsilon(w) = \sup_{r} (-rp) = 0$. So we take $r < 0$ and focus at the infimum $\inf_{q} ( -|r q + \tau_3(q, 0))$, formally looking for
local extrema in intervals where \( \tau_3(q) \) is twice differentiable. The differential minimum condition is then

\[
|r| = \tau_3(q, 0) = 0
\]

The second condition simply demands that \( \tau_2(q, 0) \) be convex (see the discussion in Section IV A for the general case). Where \( \tau_3(q, 0) \) is concave, the infimum is found at the border of some interval, which has to be determined. We have to find the global infimum and three cases have to be treated separately.

Unregarded the value of \( p \) there are three separate regions for the variable \( r \): (i) \( 0 < r > r_0 \), (ii) \( r_0 > r > r_1 \), and (iii) \( r_1 > r \) with \( r_0, r_1 \) to be specified below. The three cases can be understood graphically from Fig. 1. In region (i), the infimum is taken at \( q_0 = \frac{-1 + \sqrt{2}}{4 + \sqrt{2}} \approx 0.627 \) until the slope of the function \( -|r|q + \tau_3(q, 0) \) (for \( q > q_0 \)) at \( q = q_0 \) vanishes. This happens for \( r_0 = -\tau_3(q_0, 0) \approx -2.52 \). In region (ii), the function \( -|r|q + \tau_3(q, 0) \) has a unique local minimum at some position \( q_1 \in [q_0, q_1] \) given by Eq. (15), where \( q_1 \) is determined below. This local minimum is also the global minimum. We see that \( -|r|q + \tau_3(q, 0) \) is convex in this region, when zooming into the plot, as shown in the right panel of Fig. 1. Finally, \( r_1 \) is the value for \( r \) below which the infimum is located at \( q = 1 \). The values of \( r_1 \) and \( q_1 \) can be computed as follows: at \( r = r_1 \) the infimum is reached both at \( q_1 \) and at \( q = 1 \). We therefore have \( r_1 q_1 + \tau_3(q_1, 0) = r_1 + \tau_3(1, 0) \), and hence \( r_1 = -\tau_3(q_1) \). Also at this point, the slope of \( \tau_3(q, 0) \) equals that of the straight line connecting the points \((q_1, \tau_3(q_1, 0))\) and \((1, 1)\), hence \( r_1 = -\tau_3(q_1) \). Both conditions determine \( q_1 = \frac{1}{2} + \frac{1}{10} \sqrt{465} \approx 0.70868 \). Reinserting \( p \), we are left with the following optimization problems in the three regions: (i) \( \sup_r r(q_0 - p) \), (ii) \( \sup_r r(q_r - p) + \tau_3(q_r, 0) \), \( (q_r \in [q_0, q_1]) \), while in region (iii), the infimum is given by \( -|r| + 1 \), and \( \epsilon(w) = \sup_p (-|r|(1 - p) + 1) = 1 - |r|(1 - p) \). This curve is the straight line connecting the points \((q_1, \tau_3(q_1))\) and \((1, 1)\), as already mentioned before.

The question we address now is, which of the above depicted three regions corresponds to a given \( p \). For \( p \leq q_0 \), choosing \( r \) from region (i) yields \( \epsilon(p) = 0 \) since \( r < 0 \) and \( q_0 - p > 0 \). In regions (ii) and (iii) the infimum is at negative values (see Fig. 3). For \( q_0 < p \leq q_1 \), we find \( \epsilon(i) = \tau_0(p - q_0) \) in region (i), and \( q_r = p \) in region (ii), hence \( \epsilon(ii) = \tau_3(p, 0) \).

In region (iii) the infimum is at negative values again. Due to the convexity of \( \tau_3(p, 0) \) in \( p \in [q_0, q_1] \), \( \tau_3(p, 0) > r_0(p - q_0) \), and hence \( \epsilon(w) = \tau_3(p, 0) \). Finally, for \( q_1 < p \leq 1 \) the supremum of the infima is located in region (iii), and \( \epsilon(w) = 1 - |r|(1 - p) \). Altogether, this yields \( \epsilon(w) = \tau_3(q) \) as claimed above.

This is further illustrated by numerically applying both methods to \( \tau_3^2 \) [39], as shown in Fig. 2. The region, where the
function convex hull must be applied is clearly distinguished from the numerical uncertainty.

Quite generally, lower bounds can be obtained from the characteristic curve of a given entanglement measure [22]. Here this lower bound coincides with that bound obtained from the approach in Refs [7, 8], and even gives the analytic convex roof. In this sense, the bound is tight.

2. Off-diagonal witness

Clearly, the previous discussion marks an ideal situation in that the infimum over the admissible states $\psi$ was easy to handle. As already mentioned in Section II, it is essential for the operator $\mathcal{W}$ to have a nontrivial overlap with the set of density matrices of interest. With nontrivial we mean that $tr \rho \mathcal{W} \neq const$. For GHZ-W mixtures it implies that $W$ must be able to distinguish both states. Consequently, $\mathcal{W} = -\alpha [W] \langle W \rangle - \beta \langle \text{GHZ} \rangle \text{ (GHZ)}$ can be employed (unless $\alpha = \beta$), but also $\mathcal{W}' = -|111\rangle \langle 111|$, both without changing the resulting lower bound as obtained above for the particular GHZ witness $\mathcal{W}_{\text{GHZ}} = \frac{1}{2} \mathbb{1} - \pi_{\text{GHZ}}$. We emphasize however that this is due to the restricted Hilbert space we consider here. To point it differently: more ab initio information about the state admits more freedom to the observables in order to get sensible lower bounds.

A more generic situation occurs when we admit for off-diagonal operators like

$$\mathcal{W}_{\text{skew}} = -\pi_{\text{GHZ}} - \omega |\text{GHZ}\rangle \langle W | - \omega^* |W\rangle \langle \text{GHZ}| . \quad (17)$$

We obtain

$$\epsilon(p) = \sup_r \inf_{q,\phi} \left(r(q-p+2\sqrt{q(1-q)}\text{Re} \omega e^{i\phi}) + \tau_3(q,\phi)\right). \quad (18)$$

In this case, the infimum cannot be taken separately for $q$ and $\phi$. It is clear from the specific situation that the off-diagonal part would result in a decrease of the lower estimate of the three-tangle (see Fig. 4). The fact that $r$ is a prefactor of $\sqrt{q(1-q)}$ in the function to be optimized leads to the feature that even the estimate at $p = 1$ is below the exact value 1. We analyze this case in detail because it exhibits relevant features an improper choice for the witness might have. This type of experimental “error” might be due to e.g. incomplete knowledge about relative phases in the state under consideration or a not perfectly symmetric setup for the production of e.g. a GHZ state. The restriction to a two-dimensional Hilbert space admits to depict both possible effects and their origin.

Also in this case we determine the bound $\epsilon(w)$ with the two methods. We first solve problem (3), consisting in numerically reaching the supremum of the infimum. Then, we apply the witness restrictions directly to the pure states (see Eq. (4)). Here, this leads to

$$q_{\text{min}}(p, \phi) = \frac{p + 2\omega^2 \cos^2 \phi \pm 2|\omega \cos \phi| \sqrt{\omega^2 \cos^2 \phi + p - p^2}}{1 + 4\omega^2 \cos^2 \phi} \quad (19)$$

where $\omega \cos \phi < 0$ must be imposed, and the infimum is then obtained for the minus sign in (19).

In the second case, the lower bound of the three-tangle is then obtained as the function convex hull of $\min_{\phi} \tau_3(q_{\text{min}}(p, \phi), \phi)$. For $\tau_3^2$, this curve is indicated with circles in the left panel of Fig. 5 together with the result from the numerical approach; their agreement is perfect [39].

B. Unrestricted optimization

Now let us consider the situation relevant for most experiments. A state $\rho$ is created and $w = tr [\rho \mathcal{W}_{\text{GHZ}}]$ is measured [40]. From this value we would like to obtain an estimate of the tangle. This corresponds to obtaining a bound on the three-tangle given the fidelity of the state with respect to the GHZ-state, $p = tr[\rho |\text{GHZ}\rangle \langle \text{GHZ}|]$, since $w = \alpha - p$. We have solved the problem (3) for this case numerically. The results are plotted in Fig. 5. In Table I, the corresponding bound on the three-tangle are listed for experiments where $p$ has been measured. It is a curious fact that the results agree with those obtained by solving (4), where the optimization was performed only over states which are symmetric under the exchange of particles. We add some more comments on this curious fact in Section IV B.

The problem restricted on pure states amounts to finding the steepest descent of the three-tangle when the GHZ state is superposed with some other state out of the orthogonal complement, which is numerically found to be reached using only the states $W$ and its bit-flipped form, $\bar{W}$. The value zero is assumed for the weight $p = 3/4$ of the GHZ-state. For GHZ-

![Fig. 4: (Color online) For visualizing how the estimated lower bound is decreased by the off-diagonal part of the witness [17], we assume the term $\sqrt{q(1-q)} \cos \phi$ to appear without $r$ as a prefactor for a moment. It then simply modifies the characteristic curve as shown here for $\omega = 1$. The function convex hull of the lowest enveloping curve (thick full red line) would then constitute the lower bound estimate from the off-diagonal witness. However, this estimate would still lead to the correct value at $p = 1$. Even this is spoiled when the contribution from the off-diagonal part of the witness is actually $r$-dependent, as is the case here.](image)
states mixed with white noise

\[ \gamma \pi_{\text{GHZ}} + (1 - \gamma) \mathbb{I}/8, \quad \gamma \in [0, 1], \]  

which we will refer to as noisy GHZ states, this leads to zero three-tangle at \( \gamma = 5/7 \). This coincides of course with the known bound for GHZ-entanglement in these states: by construction, if \( p > 3/4 \) they are detected by the optimal GHZ witness \( W_{\text{opt}}^{\text{GHZ}} = \frac{1}{2} \mathbb{I} - \pi_{\text{GHZ}} \) (see Ref. \[26\]). Since this is a lower bound, and we do not know whether this bound is tight for the noisy GHZ states, we give an upper bound for its three-tangle at \( p = 3/4 \).

To this end, a decomposition of the noisy GHZ state must be constructed, and we use our result that the minimum value for the three-tangle is assumed for symmetric states containing \( W \) and \( \bar{W} \) alone and with equal weight. Imprinting local phases, we can induce relative phases for the \( W \) and the \( \bar{W} \) state, that are mutually inverse. When keeping the phase of the GHZ state fixed and averaging over these relative phases, this leads almost to a state of the form \[20\], but with the orthogonal GHZ state with relative minus sign, \( \text{GHZ}_{-} \), missing. Convexity of the convex-roof applied to the resulting decomposition leads to an upper bound of 1/9 for the three-tangle of the noisy GHZ state \[20\] with GHZ weight \( p = 3/4 \).

An interesting question to ask here is for the full convex set of states with zero three-tangle and GHZ weight \( 3/4 \). If the interior of this polytope contained a state of the form \[20\], this would mean that the lower bound was even tight for these states. Otherwise the bound is not tight and the threshold weight for GHZ-entanglement (as measured by the three-tangle) would definitely be smaller than \( 3/4 \).

A lower bound \( p_{\text{sub}} = 1/3 \) and \( \gamma_{\text{sub}} = 5/21 \) for the weight of GHZ in a state \[20\] without three-tangle can be obtained

\[
\Delta \tau^2 := \tau^2 - \tau_{\text{opt}}^2, \quad \tau_{\text{opt}} = \inf_\rho \frac{2}{\sqrt{3}} \text{Tr} (\rho \sigma_{\text{GHZ}}),
\]

where the estimated \( \tau^2_{\text{opt}} \) is shown for a given GHZ fidelity \( p \). This captures also the GHZ-identity mixture. Two different methods are compared: full scale numerical optimization and the optimization restricted to symmetric states satisfying the constraint given by the GHZ witness \( \frac{1}{2} \mathbb{I} - \pi_{\text{GHZ}} \), which fixes the value of \( p \). Both methods lead to the same result (modulo taking the function convex hull in the latter method), as it should be. Inset: close to \( p = 1 \) the curve obtained by imposing the witness constraint directly on the pure states is seen to lie above the curve resulting from numerical optimization; in this region, the pure state curve is not convex. The function convex hull agrees with the curve from the full scale optimization.

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### Table I: (Color online) Lower bounds on \( \tau_3 \) for recent experiments where the estimated \( p \) exceeded 3/4. The used data is the same as that used for Fig. 5

| Experiment     | GHZ-fidelity | \( p(p) \)       |
|----------------|--------------|-------------------|
| ion trap [29]  | 0.86 ± 0.03  | 0.42 ± 0.12       |
| diamond centers [30] | 0.87 ± 0.06 | 0.46 ± 0.24       |
| ion trap [31]  | 0.979 ± 0.002 | 0.914 ± 0.009    |

FIG. 5: (Color online) The estimate for \( \tau_3^2 \) from an off-diagonal witness for various relative weights \( \omega := \alpha/\gamma \) of the off-diagonal part. The insets show the deviation \( \Delta \tau_3^2 \) to the exact convex roof for \( \tau_3^2 \). Increasing \( \omega \) the estimate quickly decreases and finally becomes the trivial bound, which is reached well before \( \omega = \infty \), which means a purely off-diagonal witness. This is only due to the special choice of basis we did: the off-diagonal part does not detect neither GHZ nor \( W \) state. The lower panel shows that negative \( \omega \) is more destructive. The circles and squares indicate the solution obtained from setting the part proportional to \( \tau \) of the functional to zero; they lie on top of the numerical curves.

FIG. 6: (Color online) The unrestricted optimized lower bound for the three-tangle \( \tau_3 \) is shown for a given GHZ fidelity \( p \). This captures also the GHZ-identity mixture. Two different methods are compared: full scale numerical optimization and the optimization restricted to symmetric states satisfying the constraint given by the GHZ witness \( \frac{1}{2} \mathbb{I} - \pi_{\text{GHZ}} \), which fixes the value of \( p \). Both methods lead to the same result (modulo taking the function convex hull in the latter method), as it should be. Inset: close to \( p = 1 \) the curve obtained by imposing the witness constraint directly on the pure states is seen to lie above the curve resulting from numerical optimization; in this region, the pure state curve is not convex. The function convex hull agrees with the curve from the full scale optimization.
from a phase average of states of the form
\[ \gamma(p_0 \pi_{\text{GHZ}} + (1 - p_0)\pi_{W_\alpha}) + \frac{1 - \gamma}{2}(\pi_{\text{GHZ}_-} + \pi_{W_\alpha}) \]
which are known to have zero three-tangle \([32]\). The index \(\alpha\) indicates that relative phases have been introduced into the state by means of local phases.

C. The effect of more witness constraints

If the expectation values of more than one witness operator has been measured, then the class of states over which the optimization is performed is restricted. For instance, the problem discussed in Section [III.A] is recovered if \(p = (\pi_{\text{GHZ}})\) and \(\tilde{p} = (\pi_{\text{GHZ}_-})\) are known and in addition \(p + \tilde{p} = 1\) holds. In Ref. [27], \(p\) and \(\tilde{p}\) have been measured with a setup intended to produce a W-state. As expected, the lower bound on \(\tau_3\) obtained from the data is equal to zero.

Note that if the pure state problem [4] returns zero as an estimate, the final lower bound is also zero, since the function convex hull is smaller or equal to the original function.

IV. FURTHER OBSERVATIONS

A. Restriction to pure states

The problem [3] can be written as
\[ \sup_{\vec{r}} \inf_{\vec{x}} \left\{ \vec{r}(\bar{w} - \vec{W}(\vec{x})) + E(\vec{x}) \right\} , \]
(21)
where \(\bar{x}\) is assumed to be a minimal set of parameters that uniquely describes the pure states of the system. It is worth mentioning that due to \(\nabla_{\vec{r}} \nabla_{\vec{r}} \{\ldots\} = 0\), the order of the extrema is relevant. Therefore, we consider at first \(\nabla_{\vec{r}} \{\ldots\} = 0\), which leads to \(\vec{r} = \vec{W}(\bar{x}) - E(\bar{x})\). If \(\vec{W}\) is invertible in a neighborhood of the optimal point this is formally equivalent to
\[ \vec{r} = \nabla_{\vec{W}} E , \]
(22)
that is, the vector of Lagrange multipliers equals the gradient of the entanglement measure with respect to the witness values. The consecutive supremum in \(\vec{r}\), inserting this condition, leads to
\[ \vec{W}(\bar{x}) = \bar{w} , \]
(23)
i.e., the pure states themselves already satisfy the experimental witness constraint.

A remark is in order: the number of witness constraints will typically be significantly smaller than the number of parameters describing the states. Then, for each set \(\bar{w}\) of witness constraints, there will be a corresponding submanifold in the parameter space \(\bar{x}\). In order that \(\vec{W}\) can be invertible, we have to take the infimum of \(E\) in that manifold and call it \(E_c(\bar{w})\), which is the characteristic value of \(E\) as introduced in [22], and we can henceforth use \(\bar{w}\) as the parameters describing those states with minimal value for the entanglement measure subject to the constraint \(\langle \psi | \hat{W} | \psi \rangle = \bar{w}\).

For positive semidefinite second derivative we have an infimum; after straightforward algebra, this leads to the condition that the matrix with entries
\[ \frac{\partial^2 E_c}{\partial w_i \partial w_m} - \frac{\partial E_c}{\partial w_k} \frac{\partial^2 w_k}{\partial w_i \partial w_m} = \frac{\partial^2 E_c}{\partial w_i \partial w_m} \]
(24)
be positive definite. This requires convexity of \(E_c\). The equality holds where \(\vec{W}\) is invertible and the witness constraints are independent, i.e. we assumed \(\delta_{j\tilde{j}} \omega_k = \delta_{k\tilde{k}}\). Wherever \(E_c(\bar{w})\) is not convex, the infimum will be assumed at the boundary of some interval, and the function convex hull will have to be taken at the end.

Interestingly, invertibility of \(\vec{W}\) and \(\frac{\partial^2 E_c}{\partial w_i \partial w_m}\), when inserted into the second derivative w.r.t. \(\vec{r}\) leads to
\[ \nabla_{\vec{r}} \nabla_{\vec{r}} \{\ldots\} \text{extrema conditions} = -\left(\nabla_{\vec{w}} E_c(\bar{w})\right)^{-1} , \]
which should be positive semidefinite, since we maximize with respect to \(\vec{r}\). This is consistent with our above result that \(\nabla_{\vec{w}} E_c(\bar{w})\) had to be positive definite.

This analysis generalizes the explicit calculation for a single witness performed in Section [III.A.1] it underpins the deep connection to the concept of characteristic curves as proposed in Ref. [22]. In the presence of non-convex regions in \(E_c(\bar{w})\) the extrema are assumed at the boundary \(\partial I_{\bar{w}}\) of some interval \(I_{\bar{w}}\); in complete analogy to the discussions on optimal decompositions in Refs. [22, 28, 32] this means that no pure state satisfying the witness conditions leads to the lower bound for this case. The lower bound is then achieved by mixed states made of some pure states in \(\partial I_{\bar{w}}\), and the lower bound is affine within the whole interval \(I_{\bar{w}}\). For a single witness, this boundary consists of precisely two states and then prescribes a mixed state solution of the problem.

B. Simplification due to symmetry

The problem also simplifies, when both the entanglement measure to be estimated and the observables measured in the experiment have a common symmetry [41]. Let us assume that both \(E(\rho)\) and \(\rho \mathcal{W}_k\) are invariant under \(\rho \rightarrow \hat{Q}_j(\rho) \equiv Q_j(\rho)Q_j^\dagger\), where the operators \(Q_j\) form a group \(G\) with \(J\) elements. The symmetry group encountered later on is the symmetric group \(S_n\) of n qubit permutations; therefore we assume that \(J\) is finite in what follows. The result is more general and also applies to compact continuous groups. Let us define \(\tilde{\rho} = \frac{1}{J} \sum_{j=1}^J \hat{Q}_j(\rho)\) given a state \(\rho\). Clearly, \(\hat{Q}_j(\tilde{\rho}) = \tilde{\rho}\) holds, and then convexity and invariance of \(E\) with respect to \(\mathcal{J}\) imply \(E(\rho) \leq E(\tilde{\rho})\). Note that also \(\tilde{\rho}\) fulfills the experimental constraints \(w_k = \text{tr} \mathcal{W}_k \tilde{\rho}\) since also the witnesses \(\mathcal{W}_k\) are assumed to be \(\mathcal{G}\) invariant. Hence we can restrict ourselves to optimize over density matrices which are invariant under the action of the symmetry group.
However, this does not imply that we can restrict the optimization over pure states \(\psi\) to pure states with this symmetry, since the optimum of the convex roof for a symmetric states \(\bar{\rho}\) is not necessarily taken for symmetric pure states. To see this, assume that the problem \(\rho\) gives the correct minimum of the problem \(\psi\) for a state \(\psi_{\text{min}}\). Then the symmetric mixed state \(\bar{\rho}_{\text{min}} := \frac{1}{d} \sum_{j=1}^d Q_j |\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|\) also satisfies the constraints \(\bar{\rho}_{\text{min}} W_k = w_k \) and fulfills \(E(\bar{\rho}_{\text{min}}) = E(|\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|)\). In general, for every \(\psi_{\text{min}}\) that minimizes the problem \(\rho\) we find \(E(\bar{\rho}) \leq E(|\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|)\) for (without loss of generality) \(G\) symmetric states \(\bar{\rho}\). Equality holds if all states in the optimal decomposition of \(\bar{\rho}\) minimize \(\rho\) separately. If we now assume that a \(Q_{j_0} \in G\) exists such that \(Q_{j_0} |\psi_{\text{min}}\rangle \neq |\psi_{\text{min}}\rangle\), i.e. that \(|\psi_{\text{min}}\rangle\) is not \(G\) symmetric, then the \(G\)-orbit of all minimal pure states constitutes a set of optimal decomposition vectors of a flat roof \(\mathcal{G}\).

The main problem we encounter in trying to extend the above proof for symmetric mixed states to symmetric pure states is that the coherent symmetrization \(\sum_j \sqrt{Q_j} |\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|\) will typically not satisfy the constraint, unless the witnesses have no off-diagonal matrix elements for the \(Q_j |\psi_{\text{min}}\rangle\), i.e. unless \(|\psi_{\text{min}}\rangle Q_j |\psi_{\text{min}}\rangle \propto \delta_{ji}\). If this condition would be satisfied, then - since all decomposition states of \(\bar{\rho}_{\text{min}}\) are superpositions of the \(Q_j |\psi_{\text{min}}\rangle\) - two cases would occur:

\[ a) \ E(\sum_j \sqrt{Q_j} |\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|) \equiv E(|\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|) \text{ for all } q_j; \sum_j q_j = 1. \]

\[ b) \text{ A state } |\tilde{\psi}\rangle \text{ exists in the range of } G |\psi_{\text{min}}\rangle \text{ such that } E(\tilde{\psi}) < E(|\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|). \]

From a) we conclude that also the \(G\) symmetric state \(\psi_{\text{symm}} := \frac{1}{d^2} \sum_{i=1}^d Q_i |\psi_{\text{min}}\rangle\langle \psi_{\text{min}}|\) is a solution of the problem \(\rho\) by virtue of the orthogonality condition \(|\psi_{\text{min}}\rangle Q_i^\dagger W_k Q_i |\psi_{\text{min}}\rangle \propto \delta_{ji}\). The alternative b) is a contradiction to the initial assumption that \(|\psi_{\text{min}}\rangle\) solves \(\rho\). This would complete the proof that we can restrict ourselves to optimize over \(G\)-invariant pure states. However, the orthogonality condition we used in the proof seems a rather stringent at first sight; furthermore, in order to test it one would need to find the \(|\psi_{\text{min}}\rangle\) first, which amounts to solving the problem without imposing the symmetry argument. We leave this discussion for future research. Curiously, in the cases considered in this work, the minizing pure states turned out to be symmetric.

V. CONCLUSIONS

We have analyzed the method proposed in Refs. \([7, 8]\) for obtaining a lower bound for entanglement measures from expectation values of witness operators. To this end, we have applied the latter method to the convex-roof extended three-tangle of mixed three qubit states. As a first general result we show that a solution to the problem is obtained, when the constraints from the experimental knowledge about the quantum state are imposed on pure states instead of mixed states. The function convex hull of the thus constructed curve gives the solution to the full problem. This elegant simplification can be seen as a corollary to the results in Refs. \([7, 8]\), that has not been noticed before. Furthermore, this result highlights a close relation to lower bounds obtained from so-called characteristic curves \([22]\).

We applied both the full and pure state approach to a simplified situation, where the state is assumed to be of the form \(\exp(\frac{1}{2} J)\), in order to explicitly demonstrate the Legendre transformation at work, using three different witnesses. This situation corresponds to an experiment with dominating systematic errors: in our example, the only occurring error consists in the admixture of a W state. This analysis is useful, because it also clearly points out the need for a convexification after the related pure-state problem \(\rho\) has been solved. Interestingly, the thus obtained bound coincides with the exact value of the three-tangle as obtained in Ref. \([28]\). Note that this restricted approach can be generally applied if a bound on the entanglement of a family of states is desired. In addition, we have analyzed off-diagonal elements in the witness for the same setting, in order to mimic the effect of not properly chosen witness operators. The main effect is to reduce the estimated lower bound as compared to a perfect witness, even for a pure state at hand.

We then considered the experimentally relevant case where the fidelity of the produced state with respect to the GHZ state has been measured, and no prior information about the state is assumed to be available. The result is plotted in Fig. \(6\) and has been used to estimate the three-tangle produced in recent experiments, summarized in Table I. We only considered experiments where the fidelity \(|\text{GHZ}| \rho_{\text{exp}} |\text{GHZ}\rangle\) exceeds \(3/4\), since a lower fidelity is compatible with a state with no three-tangle. As to be expected, the witness bound \(\gamma = 5/7\) for having three-tangle in a GHZ-identity mixture, is reproduced.

It is a curious observation that the lower bound seems to be obtained using permutation symmetric pure states only. Although the effect of common symmetries of witness and entanglement measure - as we have here - is directly reflected in mixed state solutions of the optimization problem, the same conclusion does not seem to be straightforward for pure state solutions.

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For convex-roof extended measures, we obtain taking the convex roof commute in this case [22].

For similar arguments see Refs [8, 33–35] and exercise 4.4 from [14].

A trivial example is the "anti-witness" \( \bar{\mathcal{W}} \).

Such a singular situation is a general feature of the bound in the language of the Lagrange dual problem [14].

The Lagrange dual function to problem (1) is defined as \( g(\tau) = \inf_{\rho} E(\rho) + \sum_{k} r_k (\nu_k - \text{tr} [\mathcal{W}_k \rho]) \), where the Lagrange multipliers \( r_k \) are real numbers. This is a lower bound to the optimal solution of the first problem since if \( \tilde{\rho} \) is a state fulfilling all the constraints then the terms proportional to \( r_k \) vanish. For convex-roof extended measures, we obtain \( \inf_{\rho} \{ E(\rho) + \sum_{k} r_k (\nu_k - \text{tr} [\mathcal{W}_k \rho]) \} = \inf_{(\nu_i, |\psi_i\rangle)} \sum_{i} p_i \left( E(|\psi_i\rangle) + \sum_{k} r_k (\nu_k - \langle \psi | \mathcal{W}_k | \psi \rangle) \right) \geq \inf_{|\psi\rangle} \{ E(|\psi\rangle) + \sum_{k} r_k (\nu_k - \langle \psi | \mathcal{W}_k | \psi \rangle) \} \), where \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i | \) is the projector on the state \( |\psi\rangle \). The fact that \( E(\rho) \) is defined via the convex-roof extensions from its value on pure states enters in the first inequality. The optimal lower bound is then obtained by taking the supremum over all Lagrange multipliers \( \tau \), leading to Eq. (3). The claim follows from the fact that the final expression above is the Lagrange dual function of the pure state problem [4].

A trivial example is the “anti-witness” \( \bar{\mathcal{W}} = -\mathcal{W} \) of a witness \( \mathcal{W} \).

Whereas the discussion in the text is done for the three-tangle itself, the numerical analysis has been performed for the square of the three-tangle. The motivation is two-fold: first, it avoids square roots and hence leads to a continuous derivative, which simplifies the numerical optimization routine; second, it reduces the interval in which the characteristic curve is concave (this can be seen by considering the second derivative of a positive semi-definite function \( f(x) \) exponentiated with \( n > 1 \): \( d^n f/dx^n = n f^{n-1} f'' + n(n-1) f^{n-2} (f')^2 \), where \( f' = df/dx \). Since \( f \geq 0 \) holds, \( d^2 f^2/dx^2 \geq 0 \) wherever \( f'' \geq 0 \). It must be kept in mind though that \( \tau_0^2 < \tau_1^2 \), and that \( \sqrt{\tau_1^2} \) is not convex.

We consider the GHZ-witness because the GHZ-state is most frequently aimed at in experiments [29, 30]. Generally, any witness based on a projector of a state of the GHZ-class as defined in [24] can lead to a bound \( \epsilon > 0 \).

For similar arguments see Refs [8, 33, 35] and exercise 4.4 from [14] by P. Parrilo.

It is a very peculiar optimal decomposition; namely, where all decomposition states have the same value for the entanglement measure \( E \). Such a singular situation is a general feature of sufficiently simple entanglement measures, as the concurrence [36], and has interesting consequences. Particularly interesting among them is that taking a function of the measure and taking the convex roof commute in this case [22].

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