Estimating Entanglement Measures in Experiments

O. Gühne,1 M. Reimpell,2 and R. F. Werner2

1Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, A-6020 Innsbruck, Austria
2Institut für Mathematische Physik, Technische Universität Braunschweig, Mendelssohnstraße 3, D-38106 Braunschweig, Germany
(Received 2 August 2006; published 16 March 2007)

We present a method to estimate entanglement measures in experiments. We show how a lower bound on a generic entanglement measure can be derived from the measured expectation values of any finite collection of entanglement witnesses. Hence, witness measurements are given a quantitative meaning without the need of further experimental data. We apply our results to a recent multiphoton experiment [M. Bourennane et al., Phys. Rev. Lett. 92, 087902 (2004)], giving bounds on the entanglement of formation and the geometric measure of entanglement in this experiment.

Introduction.—Deciding whether or not a given state is entangled is one of the basic tasks of quantum information theory. In principle, one can determine the full quantum state via state tomography, and apply some separability criteria afterwards. However, the tomography requires an effort which is growing exponentially with the number of parties. For practical implementations, it is therefore highly desirable to verify entanglement on the basis of only a few, maybe only one measurement. Entanglement witnesses [1] are just the observables for this purpose: by definition they have positive expectation on every separable state, so when a negative expectation is found in some state, it must be entangled. Consequently, entanglement witnesses have been used in many experiments [2–4], and their theory is far developed [5–7].

Besides the mere detection, the quantification of entanglement is an even more challenging problem in the field. Here one aims at characterizing the amount of entanglement by so-called entanglement measures. Many entanglement measures have been introduced for this purpose [8]. But even if a quantum state is fully known, the computation of given entanglement measure is often not straightforward. Needless to say that the efficient determination of an entanglement measure in experiments is even more complicated.

In this Letter we present a method to estimate entanglement measures in experiments. We show that entanglement witnesses can not only be used for the detection of entanglement, but also for its quantification: any measured negative expectation value of a witness can be turned into a nontrivial lower bound on a generic entanglement measure. Hence, if witnesses are already used for entanglement detection, the estimation of an entanglement measure requires no extra experimental effort. We describe the procedures for computing such bounds in detail for entanglement of formation [9] and the geometric measure of entanglement [10]. Our method can not only be applied to the measurement of a single witness, but extends to incomplete tomography in general: for any finite set of measured expectation values we characterize the best possible lower bound on any convex entanglement measure (or, more generally, any convex figure of merit) consistent with these expectations. Finally, we apply our results to a recent multiphoton experiment [3].

The theoretical context of our method is the theory of Legendre transforms (also called Fenchel transforms or conjugate functions) [11]. This method has already been used to characterize additivity properties of entanglement measures [12]. The question how to estimate the entanglement when only partial knowledge is given was, to our knowledge, first addressed in Ref. [13]. Bounds on some entanglement measures from special Bell inequalities or entanglement witnesses have been obtained in Refs. [6,14], and methods to estimate measures in experiments by making measurements on several copies of a state have been discussed in Ref. [15].

Main idea of the estimation.—Let us consider $n$ witness operators (or indeed any Hermitian operators [17]), $W_1, \ldots, W_n$ on the same Hilbert space, and some entanglement measure $E$, assigning to every density operator $\rho$ a numerical value $E(\rho)$ characterizing its entanglement. We assume for the moment only that $\rho \mapsto E(\rho)$ is convex and continuous. Suppose now that, for some state $\rho$, we have measured the expectations of the $W_k$, i.e., that we are given the real numbers $w_k = \text{Tr}(\rho W_k)$ for $k = 1, \ldots, n$. On the basis of these numbers we would like to calculate a lower bound on $E(\rho)$ or, more precisely, the best lower bound

$$\epsilon(w_1, \ldots, w_n) = \inf_{\rho} \{E(\rho) | \text{Tr}(\rho W_k) = w_k\},$$

(1)

where the infimum is understood as the infimum over all states compatible with the data $w_k = \text{Tr}(\rho W_k)$.

The idea of our estimate is to characterize a convex function such as $\epsilon: \mathbb{R}^n \to \mathbb{R}$ or the entanglement measure $E$ itself as the supremum of all affine (i.e., linear + constant)
functions below it. So let \( r = (r_1, \ldots, r_n) \) and \( w = (w_1, \ldots, w_n) \) be vectors, which we use to define the linear function \( w \mapsto r \cdot w = \sum_k r_k w_k \), and consider bounds of the type

\[
\varepsilon(w) \geq r \cdot w - c
\]

for arbitrary \( r \) and \( c \). Note that by definition of \( \varepsilon \) this is the same as saying that \( E(\rho) \geq r \cdot w - c \) for every \( \rho \) giving the expectation values \( w_k \) as in (1). The constant \( c \), which we try to choose as small as possible, hence needs to satisfy, for any \( \rho \), the inequality

\[
c \geq \sum_k r_k \text{Tr}(\rho \ W_k) - E(\rho),
\]

where we already inserted the condition \( w_k = \text{Tr}(\rho \ W_k) \). Obviously, the best choice of \( c \) is the supremum of the right hand side, which only depends on the operator \( W = \sum_k r_k W_k \). Hence we can write

\[
c = \hat{E}\left( \sum_k r_k W_k \right)
\]

with

\[
\hat{E}(W) = \sup_{\rho} [\text{Tr}(\rho \ W) - E(\rho)].
\]

Here (5) is just the definition of \( \hat{E} \) as the Legendre transform of the entanglement measure \( E \). We now use the formula (4) of the optimal constant \( c \) in (2) to compute \( \varepsilon \). As a convex function it is the supremum over all affine functions below it, which are now parametrized by the “slopes” \( r \) (see also Fig. 1). Hence we arrive at the main formula of this Letter, characterizing the lower bound on \( E \), obtainable from the measured expectations \( w_k \):

\[
\varepsilon(w) = \sup_r \left\{ r \cdot w - \hat{E}\left( \sum_k r_k W_k \right) \right\}.
\]

Once again this is a Legendre transform formula, saying that \( \varepsilon \) is the Legendre transform of \( \hat{E}(r) = \hat{E}(\sum r_k W_k) \).

Of course, we want to apply formula (6) mainly when \( n = 1 \), or at least when \( n \) is very small compared to the dimension of the full space of Hermitian operators. It does involve the computation of two Legendre transforms: on the one hand, we have to compute \( \hat{E} \) from (5). For any choice of coefficients \( (r_1, \ldots, r_n) \) the computation of \( c = \hat{E}(\sum r_k W_k) \) already gives a partial solution to our problem of giving a lower bound on \( E(\rho) \) in terms of the measured expectations, namely, a best linear lower bound of the form (2). Optimizing over \( r \) then gives the best overall lower bound (6) for which the Legendre transform has to be taken over a low (i.e., \( n \)-) dimensional space only (see Fig. 1). In any case the success of the method depends on the possibility of efficiently computing \( \hat{E} \). Clearly this will depend on the entanglement measure \( E \) and the witness \( W \) chosen. We will demonstrate now for important examples how the computation can be done.

**Convex roof constructions.**—Many entanglement measures are defined by a standard extension process, which extends a function \( |\psi\rangle \mapsto E(|\psi\rangle) \) defined only on pure entangled states to all mixed states, namely, as

\[
E(\rho) = \inf_{p_i,|\psi_i\rangle} \sum_i p_i E(|\psi_i\rangle),
\]

where the \( p_i \) are convex weights, and \( \sum_i p_i |\psi_i\rangle \langle \psi_i| = \rho \). The convex roof (or “convex hull”) is just the largest convex function smaller than \( E \) on pure states, and can therefore be computed as the supremum of its affine lower bounds, i.e., once again as a Legendre transform. \( \hat{E} \) can then be simplified to a variational problem over pure states only:

\[
\hat{E}(W) = \sup_{\rho} \left[ \text{Tr}(\rho \ W) - \inf_{p_i,|\psi_i\rangle} \sum_i p_i E(|\psi_i\rangle) \right]
\]

\[
= \sup_{|\psi\rangle} \sup_{|\phi\rangle} \left\{ \sum_i p_i (|\psi_i\rangle \langle \psi_i| W |\psi\rangle - E(|\psi\rangle)) \right\}
\]

\[
= \sup_{|\psi\rangle} \left( \langle \psi| W |\psi\rangle - E(|\psi\rangle) \right). \tag{8}
\]

Here, at the second equality, we converted the “\(-\inf\)” into a “\(-\sup\)” and substituted \( \rho \) from the constraint \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \). The constraint then becomes redundant, because the sup is taken over all values \( \rho \), too. The sup over the \( p_i \) can furthermore be dropped, because convex combinations of expressions of the form (8) cannot be larger than the largest of these values. So in the end we can use the Legendre formula (5) for \( \hat{E} \), with the simplification that we need only vary over pure states.

In many cases the variation can be simplified by varying first over orbits of the local unitary group, i.e., to consider vectors \( |\psi\rangle = (U_1 \otimes U_2)|\phi\rangle \) with \( U_1, U_2 \) unitary matrices.
and $|\phi\rangle$ fixed. Since, by definition, entanglement measures are invariant under such transformations, the second term in (8) is independent of the $U_i$, so we can maximize the first term separately.

Consider, for example, witness operators of the form $\hat{W} = \alpha \mathbb{1} - \chi \langle \chi |$, which is a typical form of witnesses. Then we have to maximize $|\chi| (U_1 \otimes U_2 |\phi\rangle)$. It is easy to see that this maximum is attained, when $|\chi\rangle$ and $(U_1 \otimes U_2 |\phi\rangle$ have the same Schmidt basis, and the Schmidt coefficients are ordered in the same way (for a detailed proof see the appendix of Ref. [7]). Hence for a system composed of two $d$-dimensional ones, we only need to vary over $d$ positive numbers with one normalization constraint (rather than $d^2$ complex amplitudes in $|\psi\rangle$). In the examples shown below this reduces the computation to a simple one parameter optimization.

**Entanglement of formation.**—The entanglement of formation $E_F$ is defined as the convex roof of the function $E_F(|\psi\rangle) = \mathbb{S} \left[ \text{Tr} \rho H - F(H) \right] = -\text{Tr} \rho \ln \rho$, the von Neumann entropy of the reduced state $|\psi\rangle$. It is one of the natural figures of merit for experimental achievements in state preparation, because it quantifies the entanglement (measured in singlet pairs) which must be invested per realization of the state. In contrast, measures like the distillable entanglement tell us about the potential further uses of the state, which may be quite low, even if the state is entanglement-expensive to make.

For small dimensions the direct computation of $\hat{E}_F$ along the lines described above is feasible. For higher dimensions it is convenient to solve (8) by an uphill iteration, which will find a maximum efficiently.

To this end we rewrite the entropy term by the Gibbs variational principle, i.e., as the Legendre transform of the free energy $F$ from statistical mechanics:

$$S(\rho) = \inf_H \left[ \text{Tr} \rho H - F(H) \right] = -\text{Tr} \rho \ln \rho, \quad (9)$$

$$F(H) = \inf_\rho \left[ \text{Tr} \rho H - S(\rho) \right] = -\ln \text{Tr} (e^{-H}). \quad (10)$$

Here the first infimum is over all Hermitian operators $H$, and the second is over all density operators $\rho$. The first infimum is attained for $H = -\ln \rho$, and the second one for $\rho = \exp(-H)/\text{Tr} (\exp(-H))$. We followed the conventions from statistical mechanics by using natural logarithms, but have set the inverse temperature $\beta = 1$ [18]. Inserting (9) into the entanglement term in (8) we get

$$\hat{E}_F(\hat{W}) = \sup_{|\phi\rangle} \sup_H \langle \psi | (\hat{W} - H \otimes \mathbb{1}) |\phi\rangle + F(H), \quad (11)$$

where the first supremum is over all unit vectors of the bipartite system, and the second over all Hermitian $H$ of the first system. The point of this way of writing $\hat{E}_F$ is that the suprema over these two variables obviously commute, and that when one of them is fixed, the supremum (in fact, the absolute maximum) over the other variable can be computed directly (without a search algorithm). Indeed, for fixed $H$ (11) requires $|\psi\rangle$ to be an eigenvector for the largest eigenvalue of $(\hat{W} - H \otimes \mathbb{1})$. On the other hand, when $|\psi\rangle$ is fixed, the variation is exactly (9) for the reduced density operator $\rho_1$ of $|\psi\rangle$, which we know to be attained at $H = -\ln \rho_1$. Hence by alternating these steps, we gain in every step, and get convergence to a local maximum. In the cases we have tried, the local maximum was always independent of the starting point, giving strong support to the claim of having found the global maximum. Therefore the algorithm is a useful tool for finding the maximum. However, a guarantee cannot be given in this algorithm, so in principle the resulting entanglement lower bound (6) could be too optimistic.

**Geometric measure of entanglement.**—This measure is an entanglement monotone for multipartite systems [10], defined via the convex roof construction and

$$E_G(|\psi\rangle) = 1 - \sup_{|\phi\rangle} \langle \phi | (\hat{W} + |\phi\rangle \langle \phi |) |\psi\rangle - 1.$$

as one minus the maximal squared overlap with the fully separable states. For pure states, the geometric measure is a lower bound on the relative entropy and one can derive from it an upper bound on the number of states which can be discriminated perfectly by local operations and classical communication [19]. We have then

$$\hat{E}_G(\hat{W}) = \sup_{|\phi\rangle} \sup_{|\psi\rangle = \{a\} |b\rangle |c\rangle \ldots} \langle \phi | (\hat{W} + |\phi\rangle \langle \phi |) |\psi\rangle - 1.$$  

To show how this optimization can be performed, let us assume for simplicity that we have three parties, i.e., $|\phi\rangle = |abc\rangle$. If $|a\rangle$, $|b\rangle$, and $|c\rangle$ are fixed, we can perform the optimization by taking $|\psi\rangle$ as an eigenvector corresponding to the maximal eigenvalue. If we fix $|\psi\rangle$ and two of the other vectors, e.g., $|b\rangle$ and $|c\rangle$, we have to find a vector $|\bar{a}\rangle$ such that $\sup_{|\bar{a}\rangle} \langle \bar{a} | a \rangle \langle b | c \rangle = -|\langle \bar{a} | a \rangle \langle b | c \rangle|^2$. If the Schmidt decomposition of $|\psi\rangle$ with respect to the $A|BC$ partition is given by $|\psi\rangle = \sum_j s_j |\eta_j^A\rangle |\eta_j^{BC}\rangle$, we have $\langle \eta_j^{BC} | a \rangle \langle a | \eta_j^A\rangle = \sum_j s_j \langle \eta_j^A a | \eta_j^{BC} | b \rangle | c \rangle$. This scalar product is maximal if the vectors are parallel. So we set

$$|\bar{a}\rangle = \mathcal{N} \sum_j s_j |\eta_j^{BC} | b \rangle | c \rangle |\eta_j^A\rangle,$$

where $\mathcal{N}$ denotes a normalization. So this optimization can be iterated, as in the case of the entanglement of formation. Note that a similar iteration also delivers a method to calculate the geometric measure $E_G(|\psi\rangle)$ for arbitrary pure states $|\psi\rangle$.

For special cases of witnesses, the Legendre transform can even be calculated analytically. Let us assume that the witness is of the form $r \hat{W} = r(a \mathbb{1} - |\chi\rangle \langle \chi |)$. Here, we have already inserted the $r$ as it is used in Eq. (6). If $r > 0$, we choose in Eq. (13) $|\phi\rangle$ orthogonal to $|\chi\rangle$, resulting in $\hat{E}(r \hat{W}) = r a$. If $r < 0$, one can directly verify that we have to choose $|\phi\rangle$ as the state with the largest overlap with $|\chi\rangle$, which results in...
where \( j \) is defined with a von Neumann in the von Neumann

\[
\hat{E}_G(r|\mathcal{W}) = \frac{1-r}{2} + \frac{1}{2}\sqrt{(1-r)^2 + 4rE_G(|\chi\rangle) + r\alpha - 1}.
\]

(15)

Hence \( \hat{E}_G \) can be computed, provided \( E_G(|\chi\rangle) \) is known.

**Application to the experiment.**—The experiment in Ref. [3] aimed at the production of the \( W \) state

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

(16)

For the entanglement verification, two witnesses have been used. The witnesses and their mean values were given by

\[
\mathcal{W}_1 = \frac{3}{2} - |W\rangle\langle W|, \quad \langle \mathcal{W}_1 \rangle = -0.197 \pm 0.018,
\]

\[
\mathcal{W}_2 = \frac{1}{2} - \langle \psi_{\text{GHZ}} \rangle, \quad \langle \mathcal{W}_2 \rangle = -0.139 \pm 0.030,
\]

where \( \langle \psi_{\text{GHZ}} \rangle = (|y^+ y^+ y^+\rangle - |y^- y^- y^-\rangle)/\sqrt{2} = i(\sqrt{3}|W\rangle - |111\rangle)/2 \) is a GHZ type state.

For the entanglement of formation, we consider the \( AB|C \) bipartition, because of the symmetry the other bipartitions are equivalent. If we apply our theory on witnesses \( \mathcal{W}_1 \) and \( \mathcal{W}_2 \) separately, we get the bounds

\[
E_F^{(1)}(\rho) \geq 0.308 \pm 0.051 \text{ from } \mathcal{W}_1 \text{ and } E_F^{(2)}(\rho) \geq 0.140 \pm 0.051 \text{ from } \mathcal{W}_2.
\]

If we use both witnesses at the same time, we get the bound

\[
E_F^{(1,2)}(\rho) \geq 0.309 \pm 0.050.
\]

(17)

For the geometric measure, using Eq. (15) and the fact that

\[
E_G(|W\rangle) = \frac{3}{2} \text{ and } E_G(|\psi_{\text{GHZ}}\rangle) = \frac{1}{2} \text{ [10]},
\]

we get the bounds

\[
E_G^{(1)}(\rho) \geq 0.199 \pm 0.022 \text{ from } \mathcal{W}_1 \text{ and } E_G^{(2)}(\rho) \geq 0.019 \pm 0.010 \text{ from } \mathcal{W}_2.
\]

Using both witnesses simultaneously, we obtain the bound

\[
E_G^{(1,2)}(\rho) \geq 0.209 \pm 0.023.
\]

(18)

The fact that the bounds from \( \mathcal{W}_1 \) are better than the ones obtained from \( \mathcal{W}_2 \) stems from the fact that \( \mathcal{W}_1 \) is by construction sensitive for detecting the \( W \) state. If the \( W \) state were produced perfectly, then the bound from \( \mathcal{W}_1 \) would give the exact value, since only the \( W \) state is compatible with \( \langle \mathcal{W}_1 \rangle = -\frac{1}{2} \). Naturally, the bounds using both witnesses are always better than the bound of the single witnesses alone, since more information on the state is available. In principle, one may still improve the bound by including all the measured coincidence probabilities from Ref. [3].

Along the same lines one can also investigate other experiments, where witnesses have been used [2,3]. In the exceptional cases where complete state tomography has been done [4], one may, of course, also try other estimation methods. Then it would be of great interest to compare these methods with our proposed one.

**Conclusion.**—We proposed a method to estimate entanglement measures in experiments. To do so, we showed how entanglement witnesses can be used to obtain lower bounds on generic entanglement measures. We have explicitly demonstrated the calculations for the entanglement of formation and the geometric measure of entanglement. Finally, we applied our results to experimental data, gaining new insights into already performed experiments. Identifying witnesses, which are not only capable to detect entanglement in noisy situations but deliver at the same time good estimates of entanglement measures is an interesting task for further study.

We thank H.J. Briegel, J. Eisert, A. Miyake, and K. Osterloh for valuable discussions. This work has been supported by the FWF, the DFG, and the EU (OLAQI, PROSECCO, QUPRODIS, QICS, SCALA).

[17] Taking the \( \mathcal{W}_i \) as witnesses with \( Tr(\rho|\mathcal{W}_i|) < 0 \) for at least one \( i \) guarantees that the bound on the entanglement measure will not be the trivial bound \( E(\rho) = 0 \).
[18] Since \( E_F(|\psi\rangle) \) is defined with a \( \log_2 \) in the von Neumann entropy, one has to rescale the obtained value at the end.