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Linking a distance measure of entanglement to its convex roof

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Abstract. An important problem in quantum information theory is the quantification of entanglement in multipartite mixed quantum states. In this work, a connection between the geometric measure of entanglement and a distance measure of entanglement is established. We present a new expression for the geometric measure of entanglement in terms of the maximal fidelity with a separable state. A direct application of this result provides a closed expression for the Bures measure of entanglementof two qubits. We also prove that the number of elements in an optimal decomposition w.r.t. the geometric measure of entanglement is bounded from above by the Caratheodory bound, and we find necessary conditions for the structure of an optimal decomposition.

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1. Introduction

Entanglement [1] is one of the most fascinating features of quantum mechanics, and allows a new view on information processing. In spite of the central role of entanglement there does not yet exist a complete theory for its quantification. Various entanglement measures have been suggested—for an overview see [2, 3].

A composite pure quantum state $|\psi\rangle$ is called entangled iff it cannot be written as a product state. A composite mixed quantum state ρ on a Hilbert space $\mathcal{H} = \otimes_{j=1}^{n} \mathcal{H}_j$ is called entangled iff it cannot be written in the form [2, 4]

$$\rho = \sum_i p_i \left(\otimes_{j=1}^{n} |\psi_i^{(j)}\rangle \psi_i^{(j)}| \right) \tag{1}$$

with $p_i > 0$, $\sum_i p_i = 1$, and where $n \geqslant 2$ and $|\psi_i^{(j)}\rangle \in \mathcal{H}_j$.

The degree of entanglement can be captured in a function $E(\rho)$ that should fulfil at least the following criteria [2]:

- $E(\rho) \geqslant 0$ and equality holds iff ρ is separable[1],
- E cannot increase under local operations and classical communication (LOCC), i.e. $E(\Lambda(\rho)) \leqslant E(\rho)$ for any LOCC map Λ.

[1] Note that the distillable entanglement E_D does not satisfy this criterion, i.e. it can be zero on entangled states. However it is also accepted as a measure of entanglement [2].

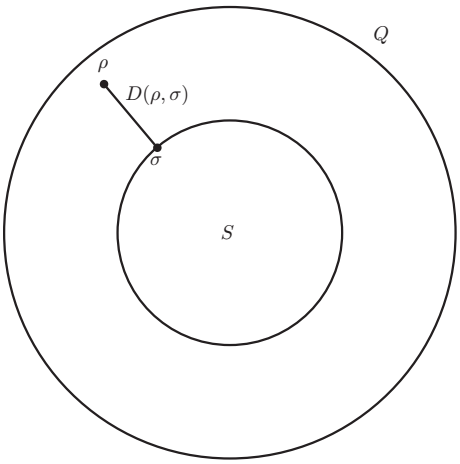

Figure 1. S denotes the set of separable states within the set of all quantum states Q. The state σ is the closest separable state to ρ, w.r.t. the distance D.

These criteria are satisfied by all measures of entanglement presented in this paper. One possibility to define an entanglement measure for a mixed quantum state ρ is via its *distance* to the set of separable states [5]; for an illustration see figure 1. Another possibility to define an entanglement measure for a mixed quantum state ρ is the *convex roof* extension, in which the entanglement is quantified by the weighted sum of the entanglement measure of the pure states in a given decomposition of ρ, minimized over all possible decompositions. There is no *a priori* reason why these two types of entanglement measures should be related. In this paper, we will establish a link between them, by showing the equality between the convex roof extension of the geometric measure of entanglement for pure states and the corresponding distance measure based on the fidelity with the closest separable state. Using this result, we will also study the properties of the optimal decompositions of the given state ρ and its closest separable state.

Our paper is organized as follows: in section 2, we provide the definitions of the used entanglement measures. In section 3, we derive the main result of this paper, namely the equality between the convex roof extension of the geometric measure of entanglement and the fidelity-based distance measure. In section 4, we study the simplest composite quantum system, namely two qubits, give an analytical expression for the Bures measure of entanglement and consider other measures that are based on the geometric measure of entanglement. In section 5, we characterize the optimal decomposition of ρ (i.e. the one that reaches the minimum in the convex roof construction) from knowledge of the closest separable state and vice versa. Finally, in section 6, we derive a necessary criterion that the states in an optimal decomposition have to fulfil. We conclude in section 7.

2. Definitions

Two classes of entanglement measures are considered in this paper. The first class consists of measures based on a distance [5, 6],

$$E_D(\rho) = \inf_{\sigma \in S} D(\rho, \sigma), \tag{2}$$

where $D(\rho,\sigma)$ is the 'distance' between ρ and σ and S is the set of separable states. This concept is illustrated in figure 1. Following [2], we do not require a distance to be a metric. In this paper, we will consider for example the Bures measure of entanglement [6]

$$E_{\mathrm{B}}(\rho) = \min_{\sigma\in S}(2-2\sqrt{F(\rho,\sigma)}), \tag{3}$$

where $F(\rho,\sigma) = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]\right)^2$ is Uhlmann's fidelity [7]. A very similar measure is the Groverian measure of entanglement [8, 9], defined as

$$E_{\mathrm{Gr}}(\rho) = \min_{\sigma\in S}\sqrt{1-F(\rho,\sigma)}. \tag{4}$$

As it can be expressed as a simple function of E_{B}, we will not consider it explicitly. Another important representative of the first class is the relative entropy of entanglement defined as [6]

$$E_{\mathrm{R}}(\rho) = \min_{\sigma\in S} S(\rho\|\sigma), \tag{5}$$

where $S(\rho\|\sigma)$ is the relative entropy,

$$S(\rho\|\sigma) = \mathrm{Tr}\left[\rho\log_2\rho\right] - \mathrm{Tr}\left[\rho\log_2\sigma\right]. \tag{6}$$

The second class of entanglement measures consists of convex roof measures [10]

$$E(\rho) = \min\sum_i p_i E(|\psi_i\rangle), \tag{7}$$

where $\sum_i p_i = 1$, $p_i \geqslant 0$, and the minimum is taken over all pure state decompositions of $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. An important example of the second class is the geometric measure of entanglement E_{G}, defined as follows [11]:

$$E_{\mathrm{G}}(|\psi\rangle) = 1 - \max_{|\phi\rangle\in S}|\langle\phi|\psi\rangle|^2, \tag{8}$$

$$E_{\mathrm{G}}(\rho) = \min\sum_i p_i E_{\mathrm{G}}(|\psi_i\rangle), \tag{9}$$

where the minimum is taken over all pure state decompositions of ρ. Entanglement measures of this form were considered earlier in [12, 13]. Another important representative of the second class for bipartite states ρ^{AB} is the entanglement of formation E_{F}, which is for pure states $\rho = |\psi\rangle\langle\psi|$ defined as the von Neumann entropy of the reduced density matrix,

$$E_{\mathrm{F}}(|\psi\rangle) = -\mathrm{Tr}\left[\rho^A\log_2\rho^A\right], \tag{10}$$

where $\rho^A = \mathrm{Tr}_{\mathrm{B}}[|\psi\rangle\langle\psi|]$. For mixed states this measure is again defined via the convex roof construction [14]:

$$E_{\mathrm{F}}(\rho) = \min_{\{p_i,|\psi_i\rangle\}}\sum_i p_i E_{\mathrm{F}}(|\psi_i\rangle). \tag{11}$$

For two-qubit states analytic formulae for E_{F} and E_{G} are known; both are simple functions of the concurrence [11, 15].

Remember that the concurrence for a two-qubit state ρ is given by [15]

$$C(\rho) = \max\{\xi_1-\xi_2-\xi_3-\xi_4, 0\}, \tag{12}$$

where ξ_i, with $i\in\{1,2,3,4\}$, are the square roots of the eigenvalues of $\rho\cdot\tilde{\rho}$ in decreasing order, and $\tilde{\rho}$ is defined as $\tilde{\rho} = (\sigma_y\otimes\sigma_y)\rho^*(\sigma_y\otimes\sigma_y)$.

The entanglement of formation for a two-qubit state ρ as a function of the concurrence is expressed as [15]

$$E_{\mathrm{F}}(\rho) = h(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - C(\rho)^2}), \tag{13}$$

where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the Shannon entropy. The geometric measure of entanglement for a two-qubit state ρ as a function of the concurrence was shown in [11] to be

$$E_{\mathrm{G}}(\rho) = \tfrac{1}{2}(1 - \sqrt{1 - C(\rho)^2}). \tag{14}$$

This formula was already found in [16] in a different context. For bipartite states, it is furthermore known that [6]

$$E_{\mathrm{F}}(\rho) \geqslant E_{\mathrm{R}}(\rho), \tag{15}$$

where for bipartite pure states the equal sign holds [6].

The geometric measure of entanglement plays an important role in the research on fundamental properties of quantum systems. Recently it has been used to show that most quantum states are too entangled to be used for quantum computation [17]. In [18] the authors have shown how a lower bound on the geometric measure of entanglement can be estimated in experiments. A connection to Bell inequalities for graph states has also been reported [19].

3. Geometric measure of entanglement for mixed states

In this section, we will show the main result of our paper: the geometric measure of entanglement, defined via the convex roof, see equation (9), is equal to a distance-based alternative.

We introduce the *fidelity of separability*

$$F_s(\rho) = \max_{\sigma \in S} F(\rho, \sigma), \tag{16}$$

where the maximum is taken over all separable states of the form (1).

Theorem 1. *For a multipartite mixed state ρ on a finite dimensional Hilbert space $\mathcal{H} = \otimes_{j=1}^{n}\mathcal{H}_j$ the following equality holds:*

$$F_s(\rho) = \max_{\{p_i, |\psi_i\rangle\}} \sum_i p_i F_s(|\psi_i\rangle), \tag{17}$$

where the maximization is done over all pure state decompositions of $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

Proof. Remember that according to Uhlmann's theorem [20, p 411],

$$F(\rho, \sigma) = \max_{|\phi\rangle} |\langle\psi|\phi\rangle|^2 \tag{18}$$

holds for two arbitrary states ρ and σ, where $|\psi\rangle$ is a purification of ρ and the maximization is done over all purifications of σ, which are denoted by $|\phi\rangle$.

We start the proof with equation (16). In order to find $F_s(\rho)$, we have to maximize $|\langle\psi|\phi\rangle|^2$ over all purifications $|\phi\rangle$ of all separable states $\sigma = \sum_j q_j |\phi_j\rangle\langle\phi_j|$, where all $|\phi_j\rangle$ are separable.

The purifications of ρ and σ can in general be written as

$$|\psi'\rangle = \sum_i \sqrt{p_i'}\,|\psi_i'\rangle \otimes |i\rangle, \tag{19}$$

$$\left|\phi'\right\rangle = \sum_j \sqrt{q_j}\,\left|\phi_j\right\rangle \otimes U^\dagger\,|j\rangle\,, \tag{20}$$

where $\{p_i', |\psi_i'\rangle\}$ is a fixed decomposition of ρ, $\langle k|l\rangle = \delta_{kl}$ and U is a unitary on the ancillary Hilbert space spanned by the states $\{|i\rangle\}$. To see whether all purifications of a separable state $\sigma = \sum_j q_j|\phi_j\rangle\langle\phi_j|$ are of the form given by $|\phi'\rangle$, we start with an arbitrary purification $|\phi''\rangle = \sum_k \sqrt{r_k}\,|\alpha_k\rangle \otimes |k\rangle$, such that $\sigma = \sum_k r_k\,|\alpha_k\rangle\,\langle\alpha_k|$ and $\langle k|l\rangle = \delta_{k,l}$. Further the following holds $\sqrt{r_k}\,|\alpha_k\rangle = \sum_j u_{kj}\sqrt{q_j}|\phi_j\rangle$, with u_{kj} being elements of a unitary matrix [21]. Using the last relation we get $|\phi''\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle \otimes |j'\rangle$, with $|j'\rangle = \sum_k u_{kj}\,|k\rangle$. Thus we brought an arbitrary purification of σ to the form given by $|\phi'\rangle$.

In order to find $F_s(\rho)$ in the above parametrization we have to maximize the overlap $|\langle\psi'|\phi'\rangle|^2$ over all unitaries U, all probability distributions $\{q_i\}$ and all sets of separable states $\{|\phi_i\rangle\}$.

We will now show that we can also achieve $F_s(\rho)$ by maximizing the overlap $|\langle\psi|\phi\rangle|^2$ of the purifications

$$|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle \otimes |i\rangle\,, \tag{21}$$

$$|\phi\rangle = \sum_j \sqrt{q_j}\,\left|\phi_j\right\rangle \otimes |j\rangle\,, \tag{22}$$

where now the maximization has to be done over all decompositions $\{p_i, |\psi_i\rangle\}$ of the given state ρ, all probability distributions $\{q_i\}$ and all sets of separable states $\{|\phi_i\rangle\}$. To see how this works we write the matrix U in its elements, $U = \sum_{kl} u_{kl}\,|k\rangle\,\langle l|$, and apply it in the overlap $|\langle\psi'|\phi'\rangle|^2$, thus noting that the action of the unitary is equivalent to a transformation of the set of unnormalized states $\{\sqrt{p_i'}|\psi_i'\rangle\}$ into the new set $\{\sqrt{p_i}|\psi_i\rangle\}$. The connection between the two sets is given by the unitary: $\sqrt{p_i}|\psi_i\rangle = \sum_j u_{ij}\sqrt{p_j'}|\psi_j'\rangle$, which is a transformation between two decompositions of the state ρ, see also [20, p 103f]. The advantage of this parametrization is that now both purifications have the same orthogonal states on the ancillary Hilbert space.

We now do the maximization of the overlap

$$|\langle\psi|\phi\rangle| = \left|\sum_i \sqrt{q_i}\sqrt{p_i}\,\langle\psi_i|\phi_i\rangle\right| \tag{23}$$

starting with the separable states $\{|\phi_i\rangle\}$. The optimal states can be chosen such that all terms $\langle\psi_i|\phi_i\rangle$ are real, positive and equal to $\sqrt{F_s\,(|\psi_i\rangle)} = \max_{|\phi\rangle\in S}\,|\langle\psi_i|\phi\rangle|$; it is obvious that this choice is optimal. We also used the fact that for pure states $|\psi\rangle$ it is enough to maximize over pure separable states: $F_s(|\psi\rangle) = \max_{|\phi\rangle\in S}\,|\langle\psi|\phi\rangle|^2$. To see this, note that $F(|\psi\rangle\,\langle\psi|\,,\sigma) = \langle\psi|\sigma|\psi\rangle$. Suppose now the closest separable state to $|\psi\rangle$ is the mixed state σ with the separable decomposition $\sigma = \sum_j q_j|\phi_j\rangle\langle\phi_j|$, all $|\phi_j\rangle$ being separable. Without loss of generality let $|\langle\psi|\phi_1\rangle| \geqslant |\langle\psi|\phi_j\rangle|$ be true for all j. Then the following holds: $F\,(|\psi\rangle\,\langle\psi|\,,\sigma) = \langle\psi|\sigma|\psi\rangle = \sum_j q_j|\langle\psi|\phi_j\rangle|^2 \leqslant \sum_j q_j\,|\langle\psi|\phi_1\rangle|^2 = |\langle\psi|\phi_1\rangle|^2$, and thus $|\phi_1\rangle$ is a closest separable state to $|\psi\rangle$.

The maximization over $\{|\phi_i\rangle\}$ gives us

$$\max_{\{|\phi_j\rangle\}}\,|\langle\psi|\phi\rangle| = \sum_i \sqrt{q_i}\sqrt{p_i}\sqrt{F_s\,(|\psi_i\rangle)}. \tag{24}$$

Now we do the optimization over q_i. Using Lagrange multipliers we obtain

$$\sqrt{q_i} = \frac{\sqrt{p_i}\sqrt{F_s\left(|\psi_i\rangle\right)}}{\sqrt{\sum_k p_k F_s\left(|\psi_k\rangle\right)}}, \tag{25}$$

with the result

$$\max_{\{q_j,|\phi_j\rangle\}} |\langle\psi|\phi\rangle|^2 = \sum_i p_i F_s\left(|\psi_i\rangle\right). \tag{26}$$

It is easy to understand that this choice of $\{q_i\}$ is optimal when one interprets the right-hand side of equation (24) as a scalar product between a vector with entries $(\sqrt{p_1}\sqrt{F_s\left(|\psi_1\rangle\right)}, \sqrt{p_2}\sqrt{F_s\left(|\psi_2\rangle\right)}, \ldots)$ and a vector with entries $(\sqrt{q_1}, \sqrt{q_2}, \ldots)$. The scalar product of two vectors with given length is maximal when they are parallel.

In the last step, we do the maximization over all decompositions $\{p_i, |\psi_i\rangle\}$ of the given state ρ which leads to the end of the proof, namely

$$F_s\left(\rho\right) = \max |\langle\psi|\phi\rangle|^2 = \max_{\{p_i,|\psi_i\rangle\}} \sum_i p_i F_s\left(|\psi_i\rangle\right). \tag{27}$$

□

We can generalize theorem 1 for arbitrary convex sets; the result can be found in appendix A. Using theorem 1 it follows immediately that the geometric measure of entanglement is not only a convex roof measure, but also a distance-based measure of entanglement:

Proposition 1. *For a multipartite mixed state ρ on a finite dimensional Hilbert space $\mathcal{H} = \otimes_{j=1}^n \mathcal{H}_j$ the following equality holds:*

$$E_{\mathrm{G}}\left(\rho\right) = 1 - \max_{\sigma\in S} F(\rho,\sigma). \tag{28}$$

Proposition 1 establishes a connection between E_{G} and distance-based measures such as the Bures measure E_{B} and Groverian measure E_{Gr}. All of them are simple functions of each other.

In [22] the authors found the following connection between E_{R} and E_{G} for pure states:

$$E_{\mathrm{R}}\left(|\psi\rangle\right) \geqslant -\log_2(1 - E_{\mathrm{G}}\left(|\psi\rangle\right)). \tag{29}$$

This inequality can be generalized to mixed states as follows:

$$E_{\mathrm{R}}\left(\rho\right) \geqslant \max\{0, -\log_2(1 - E_{\mathrm{G}}\left(\rho\right)) - S\left(\rho\right)\}, \tag{30}$$

where $S(\rho) = -\mathrm{Tr}[\rho\log_2\rho]$ is the von Neumann entropy of the state. Inequality (30) is a direct consequence of the following proposition.

Proposition 2. *For two arbitrary quantum states ρ and σ holds*

$$S\left(\rho||\sigma\right) \geqslant \mathrm{Tr}\left[\rho\log_2\rho\right] - \log_2 F(\rho,\sigma). \tag{31}$$

Proof. With $\rho = \sum_i p_i\,|\psi_i\rangle\langle\psi_i|$ we will estimate $-\mathrm{Tr}[\rho\log_2\sigma]$ from below:

$$-\mathrm{Tr}\left[\rho\log_2\sigma\right] = -\sum_i p_i\langle\psi_i|\log_2\sigma|\psi_i\rangle \tag{32}$$

$$\geqslant -\sum_i p_i\log_2\langle\psi_i|\sigma|\psi_i\rangle. \tag{33}$$

Here we used concavity of the log function

$$\log_2 \langle\psi_i|\sigma|\psi_i\rangle \geqslant \langle\psi_i|\log_2 \sigma|\psi_i\rangle. \tag{34}$$

Using concavity again we obtain $\sum_i p_i \log_2 \langle\psi_i|\sigma|\psi_i\rangle \leqslant \log_2 \sum_i p_i \langle\psi_i|\sigma|\psi_i\rangle$ and thus

$$-\mathrm{Tr}\left[\rho \log_2 \sigma\right] \geqslant -\log_2 \sum_i p_i \langle\psi_i|\sigma|\psi_i\rangle \tag{35}$$

$$= -\log_2 \mathrm{Tr}\left[\rho\sigma\right]. \tag{36}$$

The fidelity can be bounded from below as follows:

$$F(\rho,\sigma) = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]\right)^2 = \left(\sum_i \lambda_i\right)^2 \tag{37}$$

$$\geqslant \sum_i \lambda_i^2 = \mathrm{Tr}\left[\sqrt{\rho}\sigma\sqrt{\rho}\right] = \mathrm{Tr}\left[\rho\sigma\right], \tag{38}$$

where λ_i are the eigenvalues of the positive operator $\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}$. □

Inequality (30) becomes trivial for states with high entropy. As a nontrivial example we consider the two-qubit state

$$\rho = p|\psi\rangle\langle\psi| + (1-p)|01\rangle\langle 01|, \tag{39}$$

with $|\psi\rangle = \sqrt{a}\,|01\rangle + \sqrt{1-a}\,|10\rangle$. This state was called the generalized Vedral–Plenio state in [23], where the authors showed that the closest separable state σ w.r.t. the relative entropy of entanglement is given by

$$\sigma = (1-p+pa)\,|01\rangle\langle 01| + p\,(1-a)\,|10\rangle\langle 10|. \tag{40}$$

In figures 2 and 3, we show the plot of E_{F} (dotted curve), E_{R} (solid curve) and $\mathcal{E} = \max\{0, -\log_2(1-E_{\mathrm{G}}(\rho)) - S(\rho)\}$ (dashed curve) as a function of a for $p = \frac{99}{100}$ and $p = \frac{9}{10}$, respectively. It can be seen that $\mathcal{E}$ drops quickly with increasing entropy of the state and thus is nontrivial only for states close to pure states with high entanglement.

In [24, 25], the authors gave lower bounds for the relative entropy of entanglement in terms of the von Neumann entropies of the reduced states, which provide better lower bounds for E_{R} than (30). Thus, the inequality (30) should be seen as a connection between the two entanglement measures E_{R} and E_{G}, and not as an improved lower bound for E_{R}.

4. Entanglement measures for two qubits

4.1. Bures measure of entanglement

We can use proposition 1 to evaluate entanglement measures for two qubit states. From [11, 16] we know the geometric measure for two-qubit states as a function of the concurrence, see equation (14). Using this together with equation (28), we find the fidelity of separability as a function of the concurrence:

$$F_{\mathrm{s}}(\rho) = \max_{\sigma\in S} F(\rho,\sigma) = \frac{1}{2}\left(1+\sqrt{1-C(\rho)^2}\right). \tag{41}$$

Now we are able to give an expression for the Bures measure of entanglement for two-qubit states, remember its definition in equation (3).

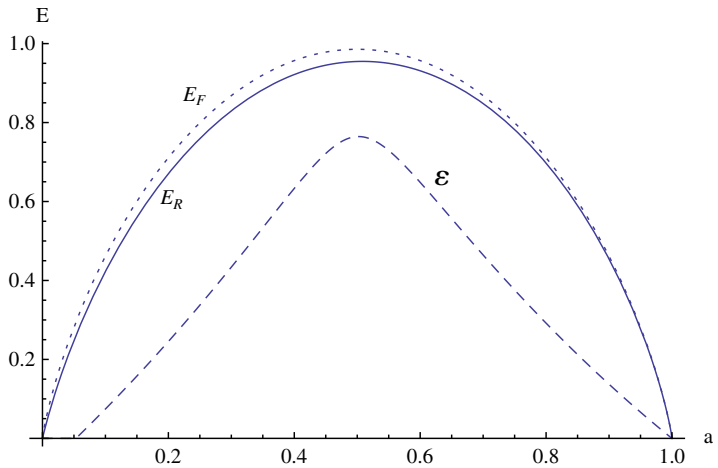

Figure 2. Entanglement of formation E_{F} (dotted curve), relative entropy of entanglement E_{R} (solid curve) and $\mathcal{E} = \max\{0, -\log_2(1 - E_{\mathrm{G}}(\rho)) - S(\rho)\}$ (dashed curve) of the state $\rho = p\,|\psi\rangle\langle\psi| + (1-p)\,|01\rangle\langle 01|$ with $|\psi\rangle = \sqrt{a}\,|01\rangle + \sqrt{1-a}\,|10\rangle$ for $p = \frac{99}{100}$ as a function of a.

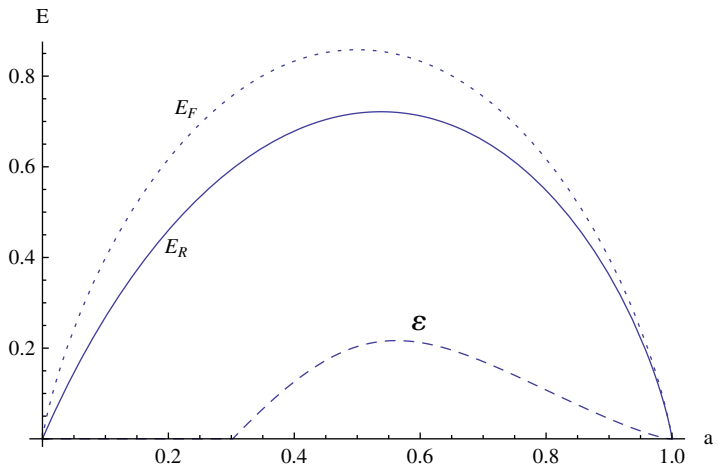

Figure 3. Entanglement of formation E_{F} (dotted curve), relative entropy of entanglement E_{R} (solid curve) and $\mathcal{E} = \max\{0, -\log_2(1 - E_{\mathrm{G}}(\rho)) - S(\rho)\}$ (dashed curve) of the state $\rho = p\,|\psi\rangle\langle\psi| + (1-p)\,|01\rangle\langle 01|$ with $|\psi\rangle = \sqrt{a}\,|01\rangle + \sqrt{1-a}\,|10\rangle$ for $p = \frac{9}{10}$ as a function of a.

Proposition 3. *For any two-qubit state ρ the Bures measure of entanglement is given by*

$$E_{\mathrm{B}}(\rho) = 2 - 2\sqrt{\frac{1 + \sqrt{1 - C(\rho)^2}}{2}}. \tag{42}$$

Note that for a maximally entangled state, $E_{\mathrm{G}} = \frac{1}{2}$ and $E_{\mathrm{B}} = 2 - \sqrt{2}$. In order to compare these measures we renormalize them such that each of them becomes equal to 1 for maximally entangled states. We show the result in figure 4. There we also plot the Groverian measure of entanglement, see equation (4).

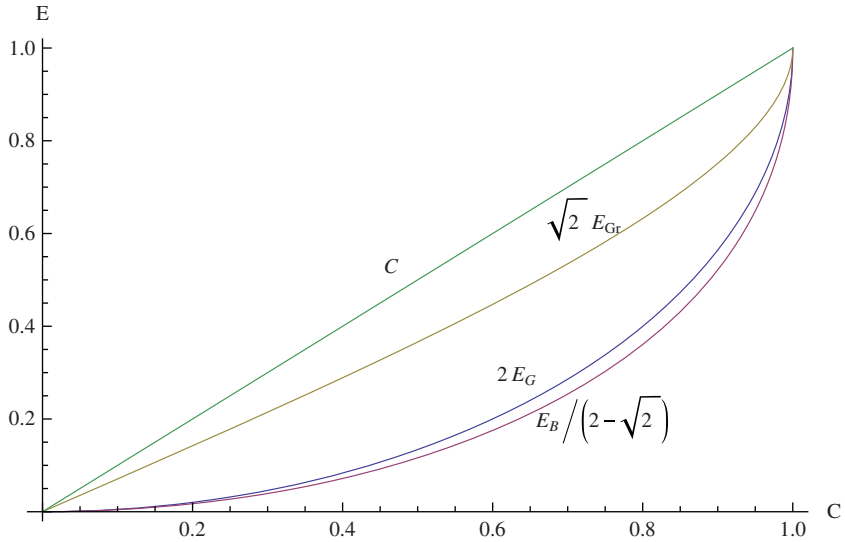

Figure 4. Plot of the geometric measure of entanglement E_{G}, Bures measure of entanglement E_{B} and Groverian measure of entanglement E_{Gr} as a function of the concurrence C for two qubit states. All measures were renormalised such that they reach 1 for maximally entangled states.

4.2. Measures induced by the geometric measure of entanglement

We consider now any generalized measure of entanglement for two-qubit states ρ which can be written as a function of the geometric measure of entanglement:

$$E_f(\rho) = f\left(E_{\mathrm{G}}(\rho)\right). \tag{43}$$

Proposition 4. *Let $f(x)$ be any convex function that is non-negative for $x \geqslant 0$ and obeys $f(0) = 0$. Then for two qubits $E_f(\rho) = f(E_{\mathrm{G}}(\rho))$ is equal to its convex roof, that is,*

$$E_f(\rho) = \min \sum_i p_i E_f(|\psi_i\rangle) = f\left(\frac{1}{2}\left(1 - \sqrt{1 - C(\rho)^2}\right)\right), \tag{44}$$

where the minimization is done over all pure state decompositions of ρ.

Proof. From [11] we know that the geometric measure of entanglement is a convex non-negative function of the concurrence, see also (14) and figure 4. As shown in [11], from convexity follows that E_{G} and E_{F} have identical optimal decompositions, and every state in this optimal decomposition has the same concurrence. This observation led directly to expression (14) for E_{G} of two qubit states.

As f is convex, E_f also is a convex function of the concurrence. To see this we note that convexity of E_{G} implies

$$E_{\mathrm{G}}\left(\sum_i p_i C_i\right) \leqslant \sum_i p_i E_{\mathrm{G}}(C_i), \tag{45}$$

where we defined $E_{\mathrm{G}}(C) = \frac{1}{2}(1-\sqrt{1-C^2})$. As $f(x)$ is convex, non-negative and $f(0)=0$, it also must be monotonically increasing for $x \geqslant 0$. Thus we have

$$f\left(E_{\mathrm{G}}\left(\sum_i p_i C_i\right)\right) \leqslant f\left(\sum_i p_i E_{\mathrm{G}}(C_i)\right). \tag{46}$$

Now we can use convexity of f to obtain

$$f\left(E_{\mathrm{G}}\left(\sum_i p_i C_i\right)\right) \leqslant \sum_i p_i f(E_{\mathrm{G}}(C_i)). \tag{47}$$

Defining $E_f(C) = f(E_{\mathrm{G}}(C)) = f(\frac{1}{2}(1-\sqrt{1-C^2}))$ the inequality above becomes

$$E_f\left(\sum_i p_i C_i\right) \leq \sum_i p_i E_f(C_i). \tag{48}$$

This proves that $E_f(C)$ is a convex function of the concurrence. Using the same argumentation as was used in [11] to prove expression (14) we see that (44) must hold. □

As an example consider the Bures measure of entanglement, which can be written as $E_{\mathrm{B}}(\rho) = E_f(\rho)$ with the convex function $f = 2-2\sqrt{1-E_{\mathrm{G}}(\rho)}$. Using proposition 4, we see that for two qubits the Bures measure of entanglement is equal to its convex roof.

However, this might not be the case for a general higher-dimensional state ρ. To see this assume that $E_{\mathrm{B}}(\rho)$ is equal to $\min \sum_i p_i E_{\mathrm{B}}(|\psi_i\rangle)$. This means that $\sqrt{F_s(\rho)}$ is equal to $\max \sum_i p_i \sqrt{F_s(|\psi_i\rangle)}$. On the other hand, from theorem 1 we know that

$$F_s(\rho) = \max \sum_i p_i F_s(|\psi_i\rangle), \tag{49}$$

and using monotonicity and concavity of the square root, we find

$$\sqrt{F_s(\rho)} = \max \sqrt{\sum_i p_i F_s(|\psi_i\rangle)} \geqslant \max \sum_i p_i \sqrt{F_s(|\psi_i\rangle)}. \tag{50}$$

The Bures measure of entanglement is equal to its convex roof if and only if the inequality (50) becomes an equality for all states ρ.

Finally we note that any entanglement measure E_h defined as $E_h(\rho) = \min_{\sigma\in S} h(F(\rho,\sigma))$ with a monotonically decreasing non-negative function h, $h(1)=0$, becomes $E_h(\rho) = h(F_s(\rho))$, and can be evaluated exactly for two qubits using proposition 1. An example of such a measure is the Bures measure of entanglement.

5. Optimal decompositions w.r.t. geometric measure of entanglement and consequences for closest separable states

Let ρ be an n-partite quantum state acting on a finite-dimensional Hilbert space $\mathcal{H} = \otimes_{i=1}^n \mathcal{H}_i$ of dimension d. A decomposition of a mixed state ρ is a set $\{p_i, |\psi_i\rangle\}$ with $p_i > 0$, $\sum_i p_i = 1$ and $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. Throughout this paper, we will call a decomposition optimal if it minimizes the geometric measure of entanglement, i.e. if $E_{\mathrm{G}}(\rho) = \sum_i p_i E_{\mathrm{G}}(|\psi_i\rangle)$. A separable state σ is a closest separable state to ρ if $E_{\mathrm{G}}(\rho) = 1 - F(\rho,\sigma)$. In the following, we will show how to find an optimal decomposition of ρ, given a closest separable state.

5.1. Equivalence between closest separable states and optimal decompositions

In the maximization of $F(\rho,\sigma)$, we can restrict ourselves to separable states σ acting on the same Hilbert space $\mathcal{H}$. To see this, note that this is obviously true for pure states, as we can always find a pure separable state $|\phi\rangle \in \mathcal{H}$ such that $|\langle\psi|\phi\rangle|^2$ is maximal. (Extra dimensions cannot increase the overlap with the original state.) Let now $\sigma = \sum_i q_i\,|\phi_i\rangle\,\langle\phi_i|$ be the closest separable state with purification $|\phi\rangle$ such that $F_s(\rho) = |\langle\psi|\phi\rangle|^2$, where $|\psi\rangle$ is a purification of ρ. We can again write the purifications as

$$|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle|i\rangle\,, \tag{51}$$

$$|\phi\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle\,|j\rangle\,, \tag{52}$$

with separable pure states $|\phi_j\rangle$ such that $\sqrt{F_s\,(|\psi_i\rangle)} = \langle\psi_i|\phi_i\rangle$. As the states $|\phi_j\rangle$ are elements of $\mathcal{H}$, the reduced state $\sigma = \mathrm{Tr_a}[|\phi\rangle\,\langle\phi|]$ is a bounded operator acting on the same Hilbert space $\mathcal{H}$, $\mathrm{Tr_a}$ denotes partial trace over the ancillary Hilbert space spanned by the orthonormal basis $\{|i\rangle\}$.

Now we are in a position to prove the following result:

Proposition 5. *Let ρ be an n-partite quantum state acting on $\mathcal{H} = \otimes_{i=1}^n \mathcal{H}_i$. The separable state $\sigma = \sum_{j=1}^s q_j|\phi_j\rangle\langle\phi_j|$ with $s \geqslant d$ separable pure states $|\phi_j\rangle$ and $\sum_{j=1}^s q_j = 1$, $q_i \geqslant 0$, is the closest separable state if and only if there exists an optimal decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$ with $s \geqslant d$ elements such that the following holds: $\sqrt{F_s\,(|\psi_i\rangle)} = \langle\psi_i|\phi_i\rangle$ and $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$.*

Proof. In the following, $\{|i\rangle\}$ denotes a basis on the ancillary Hilbert space $\mathcal{H}_\mathrm{a}$. The closest separable state $\sigma = \sum_{j=1}^s q_j|\phi_j\rangle\langle\phi_j|$ can be purified by

$$|\phi\rangle = \sum_{j=1}^s \sqrt{q_j}|\phi_j\rangle\,|j\rangle. \tag{53}$$

We write a purification of the state ρ as

$$|\psi\rangle = \sum_{i=1}^s \sqrt{\lambda_i}\,|\lambda_i\rangle\,U\,|i\rangle, \tag{54}$$

where λ_i are the eigenvalues and $|\lambda_i\rangle$ are the corresponding eigenstates of ρ, with $\lambda_i = 0$ for $i \geqslant d$, and U is a unitary acting on the ancillary Hilbert space $\mathcal{H}_\mathrm{a}$. According to Uhlmann's theorem [7, 20] it holds

$$|\langle\psi|\phi\rangle|^2 \leqslant F\,(\rho,\sigma) = F_s\,(\rho). \tag{55}$$

In the following, let U be a unitary such that equality is achieved in (55); its existence is assured by Uhlmann's theorem. Writing $U = \sum_{k,l=1}^s u_{kl}|k\rangle\langle l|$ in (54), we obtain

$$|\psi\rangle = \sum_{k,l=1}^s u_{kl}\sqrt{\lambda_l}\,|\lambda_l\rangle\,|k\rangle = \sum_{k=1}^s \sqrt{p_k}\,|\psi_k\rangle\,|k\rangle \tag{56}$$

with $\sqrt{p_k}\,|\psi_k\rangle = \sum_{l=1}^s u_{kl}\sqrt{\lambda_l}\,|\lambda_l\rangle$. Note that $\{p_k, |\psi_k\rangle\}_{k=1}^s$ is a decomposition of ρ.

We will now show that $\{p_k, |\psi_k\rangle\}_{k=1}^s$ is an optimal decomposition by showing that $|\langle\psi|\phi\rangle|^2 = \sum_i p_i F_s(|\psi_i\rangle)$. As we chose the purifications such that $|\langle\psi|\phi\rangle|^2 = F_s(\rho)$, this will complete the proof. Computing the overlap $|\langle\psi|\phi\rangle|^2$ using (53) and (56) we obtain

$$|\langle\psi|\phi\rangle|^2 = \left|\sum_i \sqrt{p_i q_i}\,\langle\psi_i|\phi_i\rangle\right|^2. \tag{57}$$

As in the proof of theorem 1, maximality of (57) implies that $|\langle\psi_i|\phi_i\rangle| = \sqrt{F_s(|\psi_i\rangle)}$ and $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$. Then we immediately see that $\{p_k, |\psi_k\rangle\}_{k=1}^s$ is optimal, because $F_s(\rho) = |\langle\psi|\phi\rangle|^2 = \sum_{i=1}^s p_i F_s(|\psi_i\rangle)$, which is exactly the optimality condition.

So far, we proved the existence of an optimal decomposition $\{p_i, |\psi_i\rangle\}$ with the property $\sqrt{F_s(|\psi_i\rangle)} = \langle\psi_i|\phi_i\rangle$ starting from the existence of the closest separable state $\sigma = \sum_{j=1}^s q_j |\phi_j\rangle\langle\phi_j|$. Now we will prove the inverse direction. Given an optimal decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$, we will find the closest separable state. We again define the purifications of ρ and σ as

$$|\psi\rangle = \sum_{i=1}^s \sqrt{p_i}\,|\psi_i\rangle \otimes |i\rangle, \tag{58}$$

$$|\phi\rangle = \sum_{j=1}^s \sqrt{q_j}\,|\phi_j\rangle \otimes |j\rangle, \tag{59}$$

where we define the states $|\phi_j\rangle$ to be separable and to have maximal overlap with $|\psi_j\rangle$, i.e. $\langle\psi_j|\phi_j\rangle = \sqrt{F_s(|\psi_j\rangle)}$. The real numbers q_j are defined as follows: $q_j = \frac{p_j F_s(|\psi_j\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$. Now we note that $|\langle\psi|\phi\rangle|^2 = F_s(\rho)$ because the decomposition $\{p_i, |\psi_i\rangle\}$ was defined to be optimal. Thus, we see that there exists no purification $|\phi'\rangle$ such that $|\langle\psi|\phi'\rangle| > |\langle\psi|\phi\rangle|$. Together with Uhlmann's theorem this implies that $F(\rho, \sigma) = F_s(\rho)$. □

5.2. Caratheodory bound

Now we are in a position to show that the number of elements in an optimal decomposition (w.r.t. the geometric measure of entanglement) is bounded from above by the Caratheodory bound.

Corollary 1. *For any state ρ acting on a Hilbert space of dimension d there always exists an optimal (w.r.t. the geometric measure of entanglement) decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$ such that $s \leqslant d^2$.*

Proof. Let σ be the closest separable state. From Caratheodory's theorem [6, 26] follows that σ can be written as a convex combination of $s \leqslant d^2$ pure separable states. According to proposition 5 the state σ can be used to find an optimal decomposition with s elements. □

6. Structure of optimal decomposition w.r.t. geometric measure of entanglement

In this section, we will show that the optimal decomposition of ρ w.r.t. the geometric measure of entanglement has a certain symmetric structure.

6.1. *n*-partite states

First, we derive the structure of an optimal decomposition $\{p_i, |\psi_i\rangle\}$ for a general n-partite state.

Proposition 6. *Every optimal decomposition* $\{p_i, |\psi_i\rangle\}_{i=1}^{s}$ *must have the following structure,*

$$\sqrt{F_s(|\psi_k\rangle)}\,\langle\psi_i|\phi_k\rangle = \sqrt{F_s(|\psi_i\rangle)}\,\langle\phi_i|\psi_k\rangle \tag{60}$$

for all $1 \leqslant i, k \leqslant s$. *Here the states* $|\phi_i\rangle$ *are separable and have the property* $\langle\phi_i|\psi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$.

Equation (60) represents a nonlinear system of equations. Finding all solutions of it is equivalent to computing the optimal decomposition of ρ. For pure states our result reduces to the nonlinear eigenproblem given in equations (5*a*) and (5*b*) in [11].

Proof. Let the states $|i\rangle$ denote an orthonormal basis on the ancillary Hilbert space $\mathcal{H}_\mathrm{a}$. Let $|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle\,|i\rangle$ and $|\phi\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle\,|j\rangle$ be purifications of ρ and σ, respectively, such that $\{p_i, |\psi_i\rangle\}$ is an optimal decomposition of ρ, $\langle\psi_i|\phi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$ and $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$. This implies that

$$F_s(\rho) = |\langle\psi|\phi\rangle|^2 = \sum_i |\langle\psi|\,(|\phi_i\rangle \otimes |i\rangle)|^2\,. \tag{61}$$

Optimality implies that $|\langle\psi|\phi\rangle|^2$ is stationary under unitaries acting on the ancillary Hilbert space $\mathcal{H}_\mathrm{a}$ (for stationarity under unitaries acting on the original space see subsection 6.5), that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_\mathrm{a}}|\phi\rangle|^2_{t=0} = 0 \tag{62}$$

for any Hermitian $H_\mathrm{a} = H_\mathrm{a}^\dagger$ acting on $\mathcal{H}_\mathrm{a}$ and the derivative is taken at $t = 0$. Using (61) we can write

$$|\langle\psi|\mathrm{e}^{\mathrm{i}tH_\mathrm{a}}|\phi\rangle|^2 = \sum_k |\langle\psi|\,(|\phi_k\rangle\,\mathrm{e}^{\mathrm{i}tH_\mathrm{a}}\,|k\rangle)|^2. \tag{63}$$

The derivative at $t = 0$ becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_\mathrm{a}}|\phi\rangle|^2_{t=0} = \mathrm{Tr}_\mathrm{a}\left[H_\mathrm{a}\cdot\mathrm{Tr}_{\bar{\mathrm{a}}}\left[\sum_k\left(A_k + A_k^\dagger\right)\right]\right] \tag{64}$$

with $A_k = \mathrm{i}(|\phi_k\rangle\langle\phi_k| \otimes |k\rangle\langle k|)\,|\psi\rangle\langle\psi|$ and $\mathrm{Tr}_{\bar{\mathrm{a}}}$ means partial trace over all parts except for the ancillary space $\mathcal{H}_\mathrm{a}$. Using $(\langle\phi_k|\langle k|)|\psi\rangle = \sqrt{p_k}\sqrt{F_s(|\psi_k\rangle)}$, we can write A_k as

$$A_k = \mathrm{i}\sqrt{p_k F_s(|\psi_k\rangle)}\,|\phi_k\rangle|k\rangle\langle\psi|\,. \tag{65}$$

Expression (64) has to be zero for all Hermitians H_a, which can only be true if $\mathrm{Tr}_{\bar{\mathrm{a}}}[\sum_k (A_k + A_k^\dagger)] = 0$, which is equivalent to

$$\sum_k \mathrm{Tr}_{\bar{\mathrm{a}}}\left[\sqrt{p_k F_s(|\psi_k\rangle)}\,|\phi_k\rangle\,|k\rangle\,\langle\psi|\right] = \sum_k \mathrm{Tr}_{\bar{\mathrm{a}}}\left[\sqrt{p_k F_s(|\psi_k\rangle)}\,|\psi\rangle\,\langle k|\,\langle\phi_k|\right]. \tag{66}$$

With $|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle\,|i\rangle$ we obtain

$$\sum_{i,k}\sqrt{p_k p_i F_s(|\psi_k\rangle)}\,\langle\psi_i|\phi_k\rangle\,|k\rangle\,\langle i| = \sum_{i,k}\sqrt{p_i p_k F_s(|\psi_k\rangle)}\,\langle\phi_k|\psi_i\rangle\,|i\rangle\,\langle k|\,. \tag{67}$$

Using orthogonality of $\{|i\rangle\}$ completes the proof. □

6.2. Bipartite states

Let us illustrate the structure of an optimal decomposition with the example of bipartite states. We consider expression (60) for a bipartite mixed state ρ with optimal decomposition $\{p_i, |\psi_i\rangle\}$. In this case it is possible to write the Schmidt decomposition of the pure states $|\psi_i\rangle$ as follows:

$$|\psi_i\rangle = \sum_j \lambda_{i,j} |j_i^{(1)}\rangle |j_i^{(2)}\rangle \tag{68}$$

with $\sum_j \lambda_{i,j}^2 = 1$, and the Schmidt coefficients are in decreasing order, i.e. $\lambda_{i,1} \geqslant \lambda_{i,2} \geqslant \cdots > 0$. The separable states $|\phi_i\rangle$ that have the highest overlap with $|\psi_i\rangle$ are given by

$$|\phi_i\rangle = |1_i^{(1)}\rangle |1_i^{(2)}\rangle,$$

and $\sqrt{F_s(|\psi_i\rangle)} = \lambda_{i,1}$. With this in mind, expression (60) reduces to

$$\lambda_{k,1} \langle\psi_i|1_k^{(1)}\rangle |1_k^{(2)}\rangle = \lambda_{i,1} \langle 1_i^{(1)}| \langle 1_i^{(2)}|\psi_k\rangle \tag{69}$$

for all i, k.

6.3. Qubit–qudit states

Let now the first system be a qubit, that is, $d_1 = 2$. In this case, we can set $\lambda_{k,1} = \cos\alpha_k$ and $\lambda_{k,2} = \sin\alpha_k$, with $\cos\alpha_k \geqslant \sin\alpha_k$. With $|\psi_k\rangle = \cos\alpha_k\,|11\rangle + \sin\alpha_k\,|22\rangle$, we get from equation (69)

$$\cos\alpha_k \sin\alpha_i (\langle 2_i^{(1)}|1_k^{(1)}\rangle \langle 2_i^{(2)}|1_k^{(2)}\rangle) = \cos\alpha_i \sin\alpha_k (\langle 1_i^{(1)}|2_k^{(1)}\rangle \langle 1_i^{(2)}|2_k^{(2)}\rangle). \tag{70}$$

Noting that $|\langle 2_i^{(1)}|1_k^{(1)}\rangle| = |\langle 1_i^{(1)}|2_k^{(1)}\rangle|$ it follows that

$$\frac{\tan\alpha_i}{\tan\alpha_k} = \left| \frac{\langle 1_i^{(2)}|2_k^{(2)}\rangle}{\langle 2_i^{(2)}|1_k^{(2)}\rangle} \right|. \tag{71}$$

It is interesting to mention that in the case $d_2 = 2$, we can simplify (71) to $\tan\alpha_i = \tan\alpha_k$. This means that in the optimal decomposition $\{p_i, |\psi_i\rangle\}$ of a two-qubit state all states $|\psi_i\rangle$ have the same Schmidt coefficients, a result already known from [15].

6.4. Nonoptimal stationary decompositions

Note that expression (60) is necessary, but not sufficient for a decomposition to be optimal. To prove this we will give two nonoptimal decompositions that satisfy (60).

6.4.1. Bell diagonal states. Consider the state

$$\rho = \tfrac{1}{2}\,|\psi^+\rangle\,\langle\psi^+| + \tfrac{1}{2}\,|\phi^+\rangle\,\langle\phi^+|\,, \tag{72}$$

with $|\psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ and $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. It is well known that the state (72) is separable, and thus the decomposition into Bell states cannot be optimal. On the other hand, it is easy to see that this decomposition satisfies (60).

6.4.2. Separable states. Now we will give a more complicated example. We call a decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$ s-optimal if for a given number of terms s there is no decomposition

$\{q_i, |\phi_i\rangle\}_{i=1}^s$ such that $\sum_{i=1}^s q_i E_G(|\phi_i\rangle) < \sum_{i=1}^s p_i E_G|\psi_i\rangle$. It is known [2] that there exist separable states ρ of dimension d with the property that any d-optimal decomposition is not separable and thus not optimal. Let $\{p_i, |\psi_i\rangle\}_{i=1}^d$ be a d-optimal decomposition of such a state ρ.

We write a purification of ρ as $|\psi\rangle = \sum_{i=1}^d \sqrt{p_i}\,|\psi_i\rangle|i\rangle$. Further, we define separable states $|\phi_i\rangle$ such that $\langle\psi_i|\phi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$, $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$ and $|\phi\rangle = \sum_{j=1}^d \sqrt{q_j}\,|\phi_j\rangle|j\rangle$. Then it holds

$$|\langle\psi|\phi\rangle|^2 = \sum_{i=1}^d p_i F_s(|\psi_i\rangle)^2 . \tag{73}$$

From d-optimality of $|\langle\psi|\phi\rangle|^2$ it follows that for all Hermitian matrices acting on a d-dimensional Hilbert space $\mathcal{H}_a$

$$\frac{d}{dt}|\langle\psi|e^{itH_a}|\phi\rangle|^2_{t=0} = 0 \tag{74}$$

holds. We will now show that $\frac{d}{dt}|\langle\psi|e^{itH_a}|\phi\rangle|^2_{t=0} = 0$ also holds for $\dim(\mathcal{H}_a) \geqslant d$. This means that adding more dimensions to the ancillary Hilbert space will not help. Performing the same calculation as in the proof of proposition 6 we obtain

$$\frac{d}{dt}|\langle\psi|e^{itH_a}|\phi\rangle|^2_{t=0} = \mathrm{Tr}_a\left[H_a \cdot \mathrm{Tr}_{\bar{a}}\left[\sum_{k=1}^{d(\mathcal{H}_a)}\left(A_k + A_k^\dagger\right)\right]\right] \tag{75}$$

with $A_k = i\sqrt{p_k F_s(|\psi_k\rangle)}\,|\phi_k\rangle|k\rangle\langle\psi|$. Note that A_k is non-zero only for $k \leqslant d$, because $p_k = 0$ otherwise. Thus, we can restrict ourselves to $k \leqslant d$ in the calculation, which is equivalent to setting $\dim(\mathcal{H}_a) = d$. Then (74) implies $\mathrm{Tr}_{\bar{a}}[\sum_{k=1}^{d(\mathcal{H}_a)}(A_k + A_k^\dagger)] = 0$ and it follows that (74) holds for arbitrary $d(\mathcal{H}_a) \geqslant d$.

6.5. *Stationarity on the original subspace*

In proposition 6, we used the argument that in the optimal case $|\langle\psi|\phi\rangle|^2$ has to be stationary under unitaries acting on the ancillary Hilbert space $\mathcal{H}_a$. In (61), we could rewrite this expression as

$$F_s(\rho) = |\langle\psi|\phi\rangle|^2 = \sum_i |\langle\psi|\phi_i\rangle|i\rangle|^2 ,$$

where all $|\phi_i\rangle$ are separable. We can also demand $\sum_i |\langle\psi|\phi_i\rangle\,|i\rangle|^2$ to be stationary under (separable) unitaries acting on the original Hilbert space of the states $|\phi_i\rangle$. From this procedure we will gain stationary equations describing the states $|\phi_i\rangle$. However, we already know that in the optimal case we can choose $|\phi_i\rangle$ to be the closest separable state to $|\psi_i\rangle$, that is, $\langle\psi_i|\phi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$, such that this method does not give new results.

7. Concluding remarks

We have shown in this paper that the geometric measure of entanglement belongs to two classes of entanglement measures. Namely it is a convex roof measure and also a distance measure of entanglement. As an application we gave a closed formula for the Bures measure of

entanglement for two qubits. We also note that the revised geometric measure of entanglement defined in [27] is equal to the original geometric measure of entanglement.

We furthermore proved that the problems of finding a closest separable state and finding an optimal decomposition are equivalent. We used this insight to bound the number of elements in an optimal decomposition (w.r.t. the geometric measure of entanglement). It turns out that the bound is exactly given by the Caratheodory bound.

Finally, we obtained stationary equations that ensure optimality of a decomposition. For the case of two qubits these equations lead to the known fact that each constituting state of an optimal decomposition has equal concurrence. Our equations hold for any dimension. However, they are only necessary, not sufficient for a decomposition to be optimal. Given an arbitrary decomposition, they provide a simple test whether the decomposition may be optimal.

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Appendix A. Geometric measure of a convex set

In theorem 1 we stated that if S is the set of separable states it holds

$$F_s(\rho) = \max \sum_i p_i F_s(|\psi_i\rangle), \tag{A.1}$$

where F_s is the maximal fidelity between ρ and the set of separable states: $F_s(\rho) = \max_{\sigma\in S} F(\rho,\sigma)$ and the maximization is done over all pure state decompositions of ρ. In the following, we will generalize this result to arbitrary convex sets.

Let X be a set of states $\{\sigma_k\}$ and C be a set containing all convex combinations of the elements of X, these are states σ such that it holds

$$\sigma = \sum_k q_k \sigma_k \tag{A.2}$$

with $q_k \geqslant 0$, $\sum_k q_k = 1$. We define the quantities $F_X(\rho)$ and $F_C(\rho)$ to be the maximal fidelity between ρ and an element of X and C, respectively,

$$F_X(\rho) = \max_{\sigma\in X} F(\rho,\sigma), \tag{A.3}$$

$$F_C(\rho) = \max_{\sigma\in C} F(\rho,\sigma). \tag{A.4}$$

Theorem 2. *For an arbitrary quantum state ρ and a convex set of states C it holds*

$$F_C(\rho) = \max_{\rho=\sum_k p_k\rho_k} \sum_i p_i F_X(\rho_i), \tag{A.5}$$

where the maximization is done over all decompositions of $\rho = \sum_i p_i\rho_i$, $p_i \geqslant 0$.

Proof. The proof is a modification of the proof of theorem 1. According to Uhlmann's theorem [20, p 411] it holds

$$F(\rho,\sigma) = \max_{|\phi\rangle} |\langle\psi|\phi\rangle|^2, \tag{A.6}$$

where $|\psi\rangle$ is a purification of ρ and the maximization is done over all purifications of σ denoted by $|\phi\rangle$.

In order to find $F_C(\rho)$ we have to maximize $|\langle\psi|\phi\rangle|^2$ over purifications $|\phi\rangle$ of all states of the form $\sigma = \sum_k q_k\sigma_k$, $\sigma_k \in X$. Using similar arguments as in the proof of the theorem 1, we see that the purifications can always be written as

$$|\psi\rangle = \sum_i \sqrt{p_i}\left(\sum_j \sqrt{p_{i,j}}|\psi_{i,j}\rangle \otimes |i, j\rangle\right), \tag{A.7}$$

$$|\phi\rangle = \sum_k \sqrt{q_k}\left(\sum_l \sqrt{q_{k,l}}|\phi_{k,l}\rangle \otimes |k, l\rangle\right), \tag{A.8}$$

with $\langle i, j|k, l\rangle = \delta_{ik}\delta_{jl}$. In the maximization of $|\langle\psi|\phi\rangle|^2$ we are free to choose the states $|\phi_{k,l}\rangle$ under the restriction that $\sum_l \sqrt{q_{k,l}}|\phi_{k,l}\rangle \otimes |k, l\rangle$ purifies $\sigma_k \in X$, the probabilities $q_k > 0$ are restricted only by $\sum_k q_k = 1$. We are also free to choose $\{|\psi_{i,j}\rangle\}$, $\{p_i\}$ and $\{p_{i,j}\}$ under the restriction $\rho = \sum_{i,j} p_i p_{ij}|\psi_{i,j}\rangle\langle\psi_{i,j}|$. With this in mind we obtain

$$|\langle\psi|\phi\rangle| = \left|\sum_{i,k} \sqrt{p_i q_k} a_{i,k}\right|, \tag{A.9}$$

with $a_{i,k}$ being the product of the purifications of ρ_i and σ_k:

$$a_{i,k} = \left(\sum_j \sqrt{p_{i,j}}\langle\psi_{i,j}| \otimes \langle i, j|\right)\left(\sum_l \sqrt{q_{k,l}}|\phi_{k,l}\rangle \otimes |k, l\rangle\right).$$

Now we optimize over $\{q_{k,l}, |\phi_{k,l}\rangle\}$ with the result

$$a_{i,k} = \sqrt{F_X(\rho_i)}\delta_{ik} \tag{A.10}$$

and thus

$$\max_{\{q_{k,l},|\phi_{k,l}\rangle\}} |\langle\psi|\phi\rangle| = \sum_i \sqrt{q_i p_i}\sqrt{F_X(\rho_i)}. \tag{A.11}$$

Now we do the optimization over q_i. Using Lagrange multipliers we obtain

$$\sqrt{q_i} = \frac{\sqrt{p_i}\sqrt{F_X(\rho_i)}}{\sqrt{\sum_k p_k F_X(\rho_k)}}, \tag{A.12}$$

with the result

$$\max_{\{q_j,q_{k,l},|\phi_{k,l}\rangle\}} |\langle\psi|\phi\rangle|^2 = \sum_i p_i F_X(\rho_i). \tag{A.13}$$

In the last step we do the maximization over all decompositions $\{p_i, \rho_i\}$ of the given state ρ, which leads to the final result

$$F_C(\rho) = \max|\langle\psi|\phi\rangle|^2 = \max\sum_i p_i F_X(\rho_i). \tag{A.14}$$

□

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