Simple algorithm for computing the geometric measure of entanglement

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We present an easy implementable algorithm for approximating the geometric measure of entanglement from above. The algorithm can be applied to any multipartite mixed state. It involves only the solution of an eigenproblem and finding a singular value decomposition; no further numerical techniques are needed. To provide examples, the algorithm was applied to the isotropic states of three qubits and the three-qubit XX model with external magnetic field.

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I. INTRODUCTION

Quantum entanglement as a fascinating nonclassical feature has attracted attention since the early days of quantum theory [1,2]. In the last decades its importance for quantum information theory has been recognized, since entanglement plays a crucial role in almost every quantum computational task [3].

A bipartite pure state is said to be entangled if it cannot be written in the product form,

$$\left|\psi_{\text{sep}}^{AB}\right\rangle = |\psi^A\rangle \otimes |\psi^B\rangle. \tag{1}$$

States which are not entangled are called separable. In general, the number of parties is $n \geqslant 2$, and fully separable pure states become

$$|\psi_{\text{sep}}\rangle = \otimes_{i=1}^{n} |\psi^{(i)}\rangle. \tag{2}$$

The theory of entanglement has also been extended to the case where the quantum state is not pure [4,5]. Then a mixed state ρ_{sep} is called separable, if it can be written as a convex combination of separable pure states,

$$\rho_{\text{sep}} = \sum_i p_i \otimes_{j=1}^{n} \left|\psi_i^{(j)}\right\rangle\left\langle\psi_i^{(j)}\right|, \tag{3}$$

with non-negative probabilities p_i, $\sum_i p_i = 1$. Quantification of entanglement is one of the main research areas in quantum information theory [5]. For bipartite pure states, the entanglement is usually quantified using the von Neumann entropy of the reduced state,

$$E(|\psi^{AB}\rangle) = -\text{Tr}[\rho^A \log_2 \rho^A], \tag{4}$$

where $\rho^A = \text{Tr}_B[|\psi^{AB}\rangle\langle\psi^{AB}|]$. For multipartite systems and mixed states many different measures of entanglement were proposed [5,6]. In general, a measure of entanglement is any continuous function E on the space of mixed states ρ which satisfies at least the following properties [5]:

(i) E is non-negative and zero if and only if the state is separable;

(ii) E does not increase under local operations and classical communication:

$$E(\Lambda(\rho)) \leqslant E(\rho),$$

where Λ is any local operations and classical communication operation.

For bipartite mixed states, an important measure of entanglement is the entanglement of formation E_f. For pure states it is defined as the von Neumann entropy of the reduced state as given in (4). The extension to mixed states is done via the convex roof construction [7,8],

$$E_f(\rho) = \min \sum_i p_i E(|\psi_i\rangle), \tag{5}$$

where the minimum is taken over all pure state decompositions of ρ.

In this paper we consider the geometric measure of entanglement. For pure states it is defined as follows [9]:

$$E_G(|\psi\rangle) = 1 - \max_{|\phi\rangle \in S} |\langle\psi|\phi\rangle|^2, \tag{6}$$

where the maximization is done over the set of separable states S. For mixed states ρ the geometric measure of entanglement was originally defined via the convex roof construction, in the same way as was done for the entanglement of formation [9]:

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

with minimization over all pure state decompositions of ρ. Similar measures of entanglement were also considered earlier in [10,11].

If ρ is a two-qubit state, general expressions for E_f and E_G are known [9,12,13]:

$$E_f(\rho) = h\left(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - C(\rho)^2}\right), \tag{8}$$

$$E_G(\rho) = \tfrac{1}{2}\left(1 - \sqrt{1 - C(\rho)^2}\right). \tag{9}$$

The concurrence $C(\rho)$ is given by

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{10}$$

where λ_i are the square roots of the eigenvalues of $\rho \cdot \tilde{\rho}$ in decreasing order, and $\tilde{\rho}$ is defined as $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\, \rho^\star (\sigma_y \otimes \sigma_y)$.

For most quantum states no exact expression for any measure of entanglement is known, and thus numerical algorithms must be used. One of the first algorithms computing entanglement has been presented in [14]. There the entanglement of formation was approximated using a random walk algorithm on the space of the decompositions of the given

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mixed state. A much faster algorithm for the entanglement of formation was presented in [15]. This algorithm made use of the conjugate gradient method. In [16] the authors extended and improved the algorithm. The authors also applied the algorithm to the convex roof extension of the multipartite Meyer-Wallach measure [17]. We also note that the geometric measure of entanglement for some bound entangled states was computed numerically in Ref. [18].

In this paper we present an algorithm for the geometric measure of entanglement. The algorithm is easy to implement, since every step is either the solution of an eigenproblem or finding a singular value decomposition of a matrix, and no further numerical techniques are needed.

This paper is organized as follows. In Sec. II we present the algorithm for pure and mixed states. We also discuss its properties and convergence. In Sec. III we test our algorithm on bipartite and multipartite mixed states with the known value of the geometric measure of entanglement. Further, we compute an approximation of the geometric measure of entanglement for the isotropic states of three qubits, and the three-qubit XX model with a constant magnetic field. We conclude in Sec. IV.

II. ALGORITHM

Before we present our algorithm for general multipartite states, we begin with bipartite and multipartite pure states.

A. Pure states

1. Bipartite states

For bipartite pure states $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ the geometric measure of entanglement is given by [10]

$$E_G(|\psi\rangle) = 1 - \lambda_{\max}^2, \tag{11}$$

where $\lambda_{\max}$ is the largest Schmidt coefficient of $|\psi\rangle$. Note that $\lambda_{\max}^2$ is also the maximal eigenvalue of $\mathrm{Tr}_1[|\psi\rangle\langle\psi|]$ and $\mathrm{Tr}_2[|\psi\rangle\langle\psi|]$. Further, let $|\phi_1\rangle \in \mathcal{H}_1$ and $|\phi_2\rangle \in \mathcal{H}_2$ be the eigenstate corresponding to the maximal eigenvalue of $\mathrm{Tr}_2[|\psi\rangle\langle\psi|]$ and $\mathrm{Tr}_1[|\psi\rangle\langle\psi|]$ respectively. Then the state $|\phi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$ is a closest separable state to $|\psi\rangle$.

2. Multipartite states

If we consider pure states $|\psi\rangle$ on an n-partite Hilbert space $\mathcal{H} \in \otimes_{i=1}^n \mathcal{H}_i$ with $n > 2$, the geometric measure of entanglement is only known for a few special cases [9,19]. In Refs. [20,21] the authors presented an algorithm for an approximation of E_G for pure states. For simplicity we discuss the algorithm from [20,21] for a pure state of three qubits, a generalization to arbitrary systems is done at the end of this section.

Let $|\psi\rangle$ be the given state of three qubits. The algorithm starts with a random product state $|\phi_0\rangle = |0_0^{(1)}\rangle|0_0^{(2)}\rangle|0_0^{(3)}\rangle$ of three qubits, where the lower index will be used for counting the steps of the algorithm and the upper index denotes the "number" of the qubit. Now we consider $|\tilde{\psi}\rangle = (\langle 0_0^{(2)}|\langle 0_0^{(3)}|)|\psi\rangle$, which is a pure un-normalized state on the space of the first qubit. If we want to maximize the overlap $|\langle\phi_0|\psi\rangle|$ for fixed states $|0_0^{(2)}\rangle$ and $|0_0^{(3)}\rangle$, we have to replace $|0_0^{(1)}\rangle$ with the state $|0_1^{(1)}\rangle = \frac{1}{\sqrt{\langle\tilde{\psi}|\tilde{\psi}\rangle}}|\tilde{\psi}\rangle$. The procedure is repeated for the second qubit, starting in the product state $|0_1^{(1)}\rangle|0_0^{(2)}\rangle|0_0^{(3)}\rangle$ and resulting in the state $|0_1^{(1)}\rangle|0_1^{(2)}\rangle|0_0^{(3)}\rangle$. Finally, the same maximization is done for the third qubit with the final state $|\phi_1\rangle = |0_1^{(1)}\rangle|0_1^{(2)}\rangle|0_1^{(3)}\rangle$. In the same way we define the product state $|\phi_n\rangle = |0_n^{(1)}\rangle|0_n^{(2)}\rangle|0_n^{(3)}\rangle$ to be the result of n iterations of the algorithm. In the following we prove some properties of the algorithm.

Proposition 1. Let $|000\rangle = \lim_{n\to\infty}|\phi_n\rangle$ be the product state after an infinite number of steps of the algorithm, giving

$$\langle 100|\psi\rangle = \langle 010|\psi\rangle = \langle 001|\psi\rangle = 0. \tag{12}$$

Proof. If $\langle 100|\psi\rangle \neq 0$, then there exists a product state of the form $|\phi\rangle = |\phi^{(1)}\rangle|00\rangle$ such that $|\langle\phi|\psi\rangle| > |\langle 000|\psi\rangle|$. This means that $|000\rangle \neq \lim_{n\to\infty}|\phi_n\rangle$, which is a contradiction to the definition of $|000\rangle$. Using the same argument it can be seen that $\langle 010|\psi\rangle = \langle 001|\psi\rangle = 0$ also holds. ■

From Proposition 1 we see that the state $|\psi\rangle$ can be written as follows:

$$|\psi\rangle = \lambda_1|000\rangle + \lambda_2|110\rangle + \lambda_3|101\rangle + \lambda_4|011\rangle + \lambda_5|111\rangle, \tag{13}$$

where four of the coefficients λ_i can be chosen real and non-negative, and $\sum_i |\lambda_i|^2 = 1$. The form (13) is also known as *generalized Schmidt decomposition* [22,23]. For a general multipartite pure state $|\psi\rangle$ it is defined [23] as an expansion in the product basis $\{|\psi_{i_1}^{(1)}\rangle \cdots |\psi_{i_n}^{(n)}\rangle\}$,

$$|\psi\rangle = \sum_{i_1,\ldots,i_n} c_{i_1,\ldots,i_n}\left|\psi_{i_1}^{(1)}\right\rangle \cdots \left|\psi_{i_n}^{(n)}\right\rangle, \tag{14}$$

where the coefficients $c_{i_1,\ldots,i_n}$ have the property $c_{jii,\ldots,i} = c_{iji,\ldots,i} = \cdots = c_{ii,\ldots,ij} = 0$ if $1 \leqslant i < j \leqslant d$, where d is the dimension of a subsystem.

Proposition 2. The algorithm computes a generalized Schmidt decomposition of an arbitrary multipartite pure state with an arbitrary given precision.

Proof. For simplicity we give the proof for a pure state of three qubits. Generalization to an arbitrary system is given below. In order to find a generalized Schmidt decomposition with a given precision ε we need to find five parameters μ_i with $\sum_{i=1}^5 |\mu_i|^2 = 1$ and a product basis $\{|ijk\rangle\}$ such that the state

$$\begin{aligned}|\psi_{\mathrm{approx}}\rangle = {} & \mu_1|000\rangle + \mu_2|110\rangle + \mu_3|101\rangle \\ & + \mu_4|011\rangle + \mu_5|111\rangle\end{aligned} \tag{15}$$

is closer to $|\psi\rangle$ than ε; that is, $D(|\psi\rangle,|\psi_{\mathrm{approx}}\rangle) \leqslant \varepsilon$ with the trace distance $D(|\psi\rangle,|\phi\rangle) = \sqrt{1 - |\langle\psi|\phi\rangle|^2}$. This is accomplished by the state

$$|\psi_n\rangle = \frac{1}{N}\sum_{i,j,k} b_{ijk}|ijk\rangle_n, \tag{16}$$

where $|ijk\rangle_n = |i_n^{(1)}\rangle|j_n^{(2)}\rangle|k_n^{(3)}\rangle$ are the basis states after n iterations of the algorithm. The coefficients b_{ijk} are defined as follows: $b_{100} = b_{010} = b_{001} = 0$, and $b_{ijk} = (\langle\psi|ijk\rangle_n)^\star$ otherwise. N assures normalization of $|\psi_n\rangle$. The trace distance between $|\psi\rangle$ and $|\psi_n\rangle$ becomes $D(|\psi\rangle,|\psi_n\rangle) = \sqrt{|\langle\psi|100\rangle_n|^2 + |\langle\psi|010\rangle_n|^2 + |\langle\psi|001\rangle_n|^2}$. Using Proposition 1 we see that $\lim_{n\to\infty} D(|\psi\rangle,|\psi_n\rangle) = 0$. The wanted

approximation $|\psi_{\text{approx}}\rangle$ is obtained by a state $|\psi_n\rangle$ such that $D(|\psi\rangle,|\psi_n\rangle) \leqslant \varepsilon$. ■

Thus, we showed that the algorithm presented in the beginning of this section computes a generalized Schmidt decomposition of the given pure state. As the generalized Schmidt decomposition is, in general, not unique [22,23], the result of the computation may depend on the choice of the initial product state $|\phi_0\rangle$. In particular, the final overlap $1 - |\langle 000|\psi\rangle|^2$ does not have to be the geometric measure of entanglement, even for an infinite number of iterations.

Finally, we note that all results presented in this section can be extended to an arbitrary number of qubits. Then the equations have to be changed accordingly. For four qubits, Eq. (12) becomes $\langle 1000|\psi\rangle = \langle 0100|\psi\rangle = \langle 0010|\psi\rangle = \langle 0001|\psi\rangle = 0$. Moreover, the results even hold if the subsystems are not qubits, but have arbitrary dimensions. For simplicity, we consider a pure state of three qutrits in the following. Again, $|000\rangle = \lim_{n\to\infty}|\phi_n\rangle$ denotes the product state which is achieved after infinite number of iterations. Using the same arguments as in the proof of Proposition 1 we see

$$\langle 100|\psi\rangle = \langle 010|\psi\rangle = \langle 001|\psi\rangle = 0, \tag{17}$$

$$\langle 200|\psi\rangle = \langle 020|\psi\rangle = \langle 002|\psi\rangle = 0, \tag{18}$$

where $|1\rangle$ and $|2\rangle$ are arbitrary states orthogonal to $|0\rangle$ on the corresponding subspace. In order to find a generalized Schmidt decomposition we also have to find specific states $|1\rangle$ and $|2\rangle$ for each subspace. Let $|\psi\rangle = \sum_{i=0}^{2}\sum_{j=0}^{2}\sum_{k=0}^{2} a_{ijk}|ijk\rangle$ be the expansion of the state in a product basis containing $|000\rangle$. Then consider the un-normalized state $|\tilde{\psi}\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{k=1}^{2} a_{ijk}|ijk\rangle$. Since in the present stage of the algorithm we only have the knowledge about the state $|000\rangle = |0^{(1)}\rangle|0^{(2)}\rangle|0^{(3)}\rangle$, the state $|\tilde{\psi}\rangle$ can be computed as follows. Starting from the state $|\psi\rangle$ we compute the un-normalized state $|\alpha\rangle = |\psi\rangle - |000\rangle\langle 000|\psi\rangle$. In the second step we compute $|\beta\rangle = |\alpha\rangle - \sum_{i<j}|0^{(i)}0^{(j)}\rangle\langle 0^{(i)}0^{(j)}|\alpha\rangle$. In the final step we get $|\tilde{\psi}\rangle = |\beta\rangle - \sum_i |0^{(i)}\rangle\langle 0^{(i)}|\beta\rangle$. The state $|\tilde{\psi}\rangle$ is an un-normalized pure state of three qubits, and according to Proposition 1 applying the algorithm to it will give us the desired product basis $\{|ijk\rangle\}$ with the property $\langle 211|\psi\rangle = \langle 121|\psi\rangle = \langle 112|\psi\rangle = 0$. The expansion of the state $|\psi\rangle$ in the final product basis $\{|ijk\rangle\}$ is a generalized Schmidt decomposition of $|\psi\rangle$ [23]. Let $\{|ijk\rangle_n\}$ be the computed product basis after n iterations of the algorithm. The approximated generalized Schmidt decomposition of $|\psi\rangle$ becomes

$$|\psi_n\rangle = \frac{1}{N}\sum_{i,j,k} b_{ijk}|ijk\rangle_n, \tag{19}$$

with $b_{iij} = b_{iji} = b_{jii} = 0$ for $i < j$ and $b_{ijk} = a_{ijk}$ otherwise. N assures normalization of $|\psi_n\rangle$. The precision of the approximation is then given by $D(|\psi\rangle,|\psi_n\rangle) = \sqrt{\sum_{i<j}(|\langle iij|\psi\rangle|^2 + |\langle iji|\psi\rangle|^2 + |\langle jii|\psi\rangle|^2)}$. In the same way we can find a generalized Schmidt decomposition for any multipartite pure state with an arbitrary precision.

B. Mixed states

The main idea of the algorithm for mixed states is a consequence of the fact, that the geometric measure of entanglement may also be written as [24]

$$E_G(\rho) = 1 - \max_{\sigma\in S} F(\rho,\sigma), \tag{20}$$

where S denotes the set of separable states and $F(\rho,\sigma) = (\text{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$ is the fidelity. Let $|\psi\rangle \in \mathcal{H}\otimes\mathcal{H}_a$ be a purification of ρ. It can be written as

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

with probabilities p_i and $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$. According to Uhlmann's theorem [3, p. 410] and using (20) we can also write

$$E_G(\rho) = 1 - \max_{\text{Tr}_a[|\phi\rangle\langle\phi|]\in S} |\langle\psi|\phi\rangle|^2, \tag{22}$$

where the maximization is done over all states $|\phi\rangle \in \mathcal{H}\otimes\mathcal{H}_a$ which are purifications of a separable state. Note that any $|\phi\rangle$ can be written in the form

$$|\phi\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle\otimes U^\dagger|j\rangle, \tag{23}$$

with pure separable states $|\phi_j\rangle \in S$, probabilities q_j, a unitary U acting on the Hilbert space $\mathcal{H}_a$, and $\langle i|j\rangle = \delta_{ij}$.

From (22) we see, that we can get an approximation of E_G by maximizing the overlap $|\langle\psi|\phi\rangle|$ over all states $|\phi\rangle$ of the form (23). Our approach for this maximization is the following.

(1) For fixed q_i and $|\phi_i\rangle$ we find a unitary U in (23) such that the overlap $|\langle\psi|\phi\rangle|$ is maximal.

(2) For fixed U and q_i we find states $|\phi_i\rangle$ in (23) such that the overlap $|\langle\psi|\phi\rangle|$ is maximal. Note that this is, in general, only possible for bipartite states. For multipartite states we compute $|\phi_i\rangle$ such that the overlap $|\langle\psi|\phi\rangle|$ does not decrease.

(3) For fixed U and $|\phi_i\rangle$ we find probabilities q_i in (23) such that the overlap $|\langle\psi|\phi\rangle|$ is maximal.

Steps (1)–(3) are iterated until the increase of the overlap $|\langle\psi|\phi\rangle|$ is smaller than a small parameter $\varepsilon > 0$. When the algorithm stops, the approximation of the geometric measure of entanglement is given by $\tilde{E}_G(\rho) = 1 - |\langle\psi|\tilde{\phi}\rangle|^2$, where $|\tilde{\phi}\rangle$ is the final state of the form (23).

In the following section we discuss the properties of the algorithm. Note that the order of the steps presented above can also be changed without changing these properties.

C. Properties

In the following we discuss some properties of the algorithm presented above. In the first step the probabilities q_i and the separable pure states $|\phi_i\rangle$ are fixed. The product $|\langle\psi|\phi\rangle|$ can be maximized using Uhlmann's theorem [3, p. 410]; it is maximal if U is chosen such that the following holds:

$$A = \sqrt{AA^\dagger}U^\dagger, \tag{24}$$

where A is a matrix defined as $A = \sum_{i,j}\sqrt{p_i q_j}\langle\phi_j|\psi_i\rangle|i\rangle\langle j|$. Note that Eq. (24) is the polar decomposition of A, which can be computed efficiently for any matrix A [25].

In the second step of the algorithm we fix U, which was found in the step before. The probabilities q_i are also unchanged. In order to maximize the overlap $|\langle\psi|\phi\rangle|$ the separable states $|\phi_i\rangle$ have to be changed to the states $|\phi_i'\rangle$ for which holds

$$\langle\psi_i'|\phi_i'\rangle = \sqrt{F_s(|\psi_i'\rangle)}, \tag{25}$$

with the states $|\psi_i'\rangle = \frac{1}{\sqrt{p_i'}}\sum_j u_{ij}\sqrt{p_j}|\psi_j\rangle$, where $u_{ij} = \langle i|U|j\rangle$ are elements of U in the computational basis, and $p_i' > 0$ is chosen such that $|\psi_i'\rangle$ is normalized. For bipartite states $|\psi_i'\rangle$ this step is evaluated according to the discussion in Sec. II A 1. If $|\psi_i'\rangle$ is multipartite, the closest separable state $|\phi_i'\rangle$ cannot be found in general. However, there is a way to circumvent this problem as follows. We apply the algorithm described in Sec. II A 2 to the state $|\psi_i'\rangle$ with the initial product state $|\phi_i\rangle$, thus getting a final product state $|\phi_i'\rangle$. The state $|\phi_i'\rangle$ is not necessarily the closest separable state to $|\psi_i'\rangle$; however, it will be closer to $|\psi_i'\rangle$ than the initial product state $|\phi_i\rangle$. However, if we replace $|\phi_i\rangle$ by $|\phi_i'\rangle$, we get a better approximation of the geometric measure of entanglement. This can be seen by noting that for the overlaps of the purifications holds: $|\langle\psi|\phi'\rangle| \geqslant |\langle\psi|\phi\rangle|$, where in $|\phi'\rangle$ all product states $|\phi_i\rangle$ were replaced with $|\phi_i'\rangle$.

In the last step of the iteration we fix U which was found in the first step, and the separable states $|\phi_i'\rangle$ which were found in the second step. Using the method of Lagrange multipliers we find the optimal probabilities:

$$q_i' = \frac{p_i'|\langle\psi_i'|\phi_i'\rangle|^2}{\sum_k p_k'|\langle\psi_k'|\phi_k'\rangle|^2}. \tag{26}$$

Let $\tilde{E}_n(\rho)$ be the approximation of the geometric measure of entanglement after n iterations of the algorithm. We now prove the main property of the algorithm.

Proposition 3. The approximated value of the geometric measure of entanglement never increases in a step of the iteration:

$$\tilde{E}_{n+1}(\rho) \leqslant \tilde{E}_n(\rho). \tag{27}$$

Proof. It is sufficient to show that the overlap of the purifications $|\langle\psi|\phi\rangle|$ does not decrease in any step of the algorithm. This is seen directly from the definition of the algorithm in Sec. II B. ■

D. Implementation

First we set a small parameter $\varepsilon > 0$. The algorithm starts with a random decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^{d^2}$ into d^2 elements of the state $\rho = \sum_{i=1}^{d^2} p_i|\psi_i\rangle\langle\psi_i|$ and a separable decomposition $\{q_i, |\phi_i\rangle\}_{i=1}^{d^2}$ of a random separable state $\sigma = \sum_{i=1}^{d^2} q_i|\phi_i\rangle\langle\phi_i|$, where we demand that $p_i > 0$ and $q_i > 0$ for all $1 \leqslant i \leqslant d^2$. The steps (1)–(3) from the Sec. II B can be implemented as follows,

(1) Find the singular value decomposition of the matrix $A = \sum_{i,j}\sqrt{p_i q_j}\langle\phi_j|\psi_i\rangle|i\rangle\langle j|$, that is, $A = VDW$ with unitary matrices V, W and diagonal non-negative matrix D. Define $U = W^\dagger V^\dagger$, noting that (24) is fulfilled.

(2) Define un-normalized states

$$|\alpha_i\rangle = \sum_{j=1}^{d^2} u_{ij}\sqrt{p_j}|\psi_j\rangle, \tag{28}$$

with $u_{ij} = \langle i|U|j\rangle$. Compute $p_i' = \langle\alpha_i|\alpha_i\rangle$ and $|\psi_i'\rangle = \frac{1}{\sqrt{p_i'}}|\alpha_i\rangle$ for all i. For bipartite states compute separable pure states $|\phi_i'\rangle \in S$ such that $\langle\psi_i'|\phi_i'\rangle = \sqrt{F_s(|\psi_i'\rangle)}$. For multipartite states find product states $|\phi_i'\rangle$ which are closer to $|\psi_i'\rangle$ than the states $|\phi_i\rangle$ computed in the step before. This can be done applying the algorithm presented in Sec. II A 2 to the state $|\psi_i'\rangle$ with the initial product state $|\phi_i\rangle$.

(3) Compute $q_i' = \frac{p_i'|\langle\psi_i'|\phi_i'\rangle|^2}{\sum_k p_k'|\langle\psi_k'|\phi_k'\rangle|^2}$.

After performing steps (1)–(3) define a new separable state $\sigma' = \sum_i q_i'|\phi_i'\rangle\langle\phi_i'|$, which is an approximation of the closest separable state to ρ. If $F(\rho,\sigma') - F(\rho,\sigma) > \varepsilon$, set $|\psi_i\rangle = |\psi_i'\rangle$, $|\phi_i\rangle = |\phi_i'\rangle$, $p_i = p_i'$ and $q_i = q_i'$ for all i and go back to step (1); otherwise stop. The computed approximation is $\tilde{E}_G(\rho) = 1 - F(\rho,\sigma')$.

E. Convergence

One of the most important questions regarding algorithms computing entanglement is whether the algorithm converges to the exact value of the entanglement measure, at least for infinite number of steps. For a general multipartite state with more than two parties the algorithm will converge to the wrong value with some nonzero probability, depending on the initial separable state. This is due to the fact that the algorithm for pure multipartite states presented in Sec. II A 2 does not necessarily compute the correct value, since it can converge to a local minimum [21,26].

For bipartite mixed states there is no full answer to this question, and testing the algorithm on bipartite states with known geometric measure of entanglement we did not observe convergence to a wrong value. However, it can be shown that for some states and some special choice of the purifications $|\psi\rangle$ and $|\phi\rangle$ the algorithm does not compute the correct value even after an infinite number of iterations. To see this we consider a separable state $\rho \in S$ with rank r such that any separable decomposition of ρ has more elements than r. The existence of such states is assured [5]. Let now $\{p_i, |\psi_i\rangle\}_{i=1}^r$ be a decomposition of ρ which is optimal among all decompositions with r elements; that is, the average entanglement $\sum_{i=1}^r p_i E_G(|\psi_i\rangle)$ is minimal among all decompositions into r elements. Further, let $|\phi_i\rangle$ be the closest separable state to $|\psi_i\rangle$ and we also choose $q_i = \frac{p_i|\langle\psi_i|\phi_i\rangle|^2}{\sum_k p_k|\langle\psi_k|\phi_k\rangle|^2}$. Now we start the algorithm with the decompositions $\{p_i, |\psi_i\rangle\}_{i=1}^r$ and $\{q_i, |\phi_i\rangle\}_{i=1}^r$, as described in the previous section. Then the unitary U which maximizes the overlap of the purifications $|\psi\rangle = \sum_i\sqrt{p_i}|\psi_i\rangle\otimes|i\rangle$ and $|\phi\rangle = \sum_j\sqrt{q_j}|\phi_j\rangle\otimes U^\dagger|j\rangle$ is given by $U = \mathbb{1}$. In the second step the algorithm will maximize the overlaps $\langle\phi_i|\psi_i\rangle$, which are already optimal. The same is true for the last step of the algorithm, where the probabilities q_j are optimized. Thus, the algorithm preserves the initial separable state and does not compute the correct value even for infinite number of steps.

To avoid the problem mentioned above the algorithm should always start with a separable state chosen at random, that is, with random initial probabilities q_i and random separable

pure states $|\phi_i\rangle$. Moreover, the number of initial nonzero probabilities q_i should be at least $(\dim \mathcal{H})^2$.

In the following section we test the algorithm and present some applications for states with unknown geometric measure of entanglement.

III. APPLICATIONS

A. Testing the algorithm

1. Two qubits

If ρ is a two-qubit state, the geometric measure of entanglement is given by (9). We applied our algorithm with $\varepsilon = 10^{-15}$ to 10^3 random states of two qubits and tested the computed value $\tilde{E}_G$ against the exact value given in (9). The maximal deviation $\tilde{E}_G - E_G$ from the exact value was 6×10^{-11}. The average number of steps made by the algorithm was 291.

2. Isotropic states

We also tested our algorithm on the isotropic states in dimension $d \times d$; these are states of the form

$$\rho = p|\Phi^+\rangle\langle\Phi^+| + \frac{1-p}{d^2}\mathbb{1}, \tag{29}$$

with the maximally entangled state $|\Phi^+\rangle = \frac{1}{\sqrt{d}}\sum_{i=1}^{d}|ii\rangle$. For these states an exact expression for the geometric measure of entanglement was given in [9]; the states are entangled if and only if $p > \frac{1}{1+d}$. We applied our algorithm to the state (29) for $2 \leqslant d \leqslant 3$ with the parameter $\varepsilon = 10^{-15}$ for $p = 0.01n$ and $0 \leqslant n \leqslant 99$. The difference between the approximated value $\tilde{E}_G$ and the exact value E_G was always less than 10^{-10}.

In order to do the test for $d = 4$ within a reasonable time some modifications had to be applied. First, we minimized only over decompositions into $d^2 = 16$ instead of $d^4 = 256$ pure states. Further, for $d = 4$ the test was done on entangled states only, that is, for $p = 0.01n$ with $20 < n \leqslant 99$. The difference between the approximation $\tilde{E}_G$ and the exact value E_G never exceeded 10^{-13}. The results are summarized in Table I. There $\bar{N}$ denotes the average number of steps made by the algorithm.

For the cases tested above the algorithm always converged into the correct value of E_G within the precision given in Table I with a single run of the algorithm. Note that in general more than one run with different initial parameters should be done to avoid convergence into a wrong value. Further, we see from Table I that the parameter ε should not be used directly to quantify the precision of the approximation, although the deviation from the exact value is very small.

TABLE I. Precision of the approximation $\tilde{E}_G - E_G$ and the average number of steps $\bar{N}$ for the isotropic states (29) with parameter $\varepsilon = 10^{-15}$.

d	2	3	4
$\tilde{E}_G - E_G$	$<10^{-13}$	$<10^{-10}$	$<10^{-13}$
$\bar{N}$	80	516	2259

3. Four qubits

In Ref. [27] the authors computed the geometric measure of entanglement for a class of mixed states of four qubits. We tested our algorithm on the state $\rho(t)$, which for $t = 0$ is defined as the four-qubit cluster state

$$|\mathrm{CL}_4\rangle = \tfrac{1}{2}(|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle). \tag{30}$$

For $t > 0$ the diagonal terms of ρ are left invariant, and the off-diagonal components decay exponentially with t; that is,

$$\rho_{kl}(t) = \begin{cases} \rho_{kl}(0) & \text{for} \quad k = l, \\ e^{-t}\rho_{kl}(0) & \text{for} \quad k \neq l \end{cases}. \tag{31}$$

We applied our algorithm with parameter $\varepsilon = 10^{-15}$ on the states $\rho(t)$ with $t = 0.01n$ for all $1 \leqslant n \leqslant 100$. The discrepancy between the approximated value and the exact value given in [27] was always smaller than 10^{-14}.

The same test was done for the state $\tilde{\rho}(t)$, which for $t = 0$ is defined as the four-qubit W state

$$|W_4\rangle = \tfrac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle), \tag{32}$$

and for $t > 0$ the off-diagonal components decay exponentially as given in (31). There the discrepancy between the approximation and the exact value was always smaller than 10^{-11}.

Finally, we tested our algorithm on the four-qubit state $\bar{\rho}(t)$, which for $t = 0$ is defined as the symmetrized Dicke state,

$$|D_4\rangle = \frac{1}{\sqrt{6}}(|0011\rangle + |0101\rangle + |1001\rangle + |1100\rangle + |0110\rangle + |1010\rangle). \tag{33}$$

Again, for $t > 0$ the off-diagonal components decay as in (31). The test was done with $t = 0.01n$ for all $1 \leqslant n \leqslant 100$, the difference $\tilde{E}_G - E_G$ was always smaller than 10^{-12}. The results are summarized in Table II. There $\bar{N}$ denotes the average number of iterations made by the algorithm.

Note that the optimizations above were done over pure state decompositions into 2^4 elements instead of 2^8. This reduction was needed in order to do the computation within a reasonable time. Moreover, we note that for very small parameter $t = 0.01$ we sometimes observed convergence into a wrong value. This is due to the fact that for small t the state $\rho(t)$ is almost pure. As was mentioned in Sec. II E the algorithm can converge to wrong values for pure multipartite states. In these cases the algorithm was started again with random initial parameters. To get an impression we mention that for the last example $\bar{\rho}(0.01)$ the algorithm sometimes converged to $\tilde{E}_G - E_G \approx 8 \times 10^{-4}$.

We also mention that the examples given here were computed on a standard computer. The computation time

TABLE II. Precision of the approximation $\tilde{E}_G - E_G$ and the average number of steps $\bar{N}$ for the four-qubit states presented in the text with parameter $\varepsilon = 10^{-15}$.

$\rho(0)$	$\|\mathrm{CL}_4\rangle$	$\|W_4\rangle$	$\|D_4\rangle$
$\tilde{E}_G - E_G$	$<10^{-14}$	$<10^{-11}$	$<10^{-12}$
$\bar{N}$	12	173	126

for a single state of three and four qubits was on the order of 1 min. If in the four-qubit case the optimization is done over decompositions into 2^8 instead of 2^4 pure states, the computation time increases at least by the factor 2^4. In general, for an n-partite system of qudits with dimensions d, the computation time scales at least with the number of pure states in the decomposition, given by d^{2n}.

4. Comparison with other algorithms

A significant difference between our algorithm and the algorithms presented in [15,16] is the fact that our algorithm implies only the solution of the eigenproblem and finding a singular value decomposition. For both problems efficient numerical algorithms exist [25], implying that each step of our algorithm can be done efficiently. The algorithms based on conjugate gradients usually imply a line search [15]. It is not known to us whether a line search can in general be done efficiently for the problem considered here.

As noted in Sec. III A 1, the average number of iterations made by our algorithm for random two-qubit states with parameter $\varepsilon = 10^{-15}$ was 291. This is comparable to the performance of the conjugate gradient algorithm; for comparison, see Fig. 1 in [16].

B. On additivity of entanglement

A measure of entanglement E is called additive, if for any two states ρ^{AB} and σ^{AB} holds [6]:

$$E(\rho^{AB} \otimes \sigma^{AB}) = E(\rho^{AB}) + E(\sigma^{AB}), \tag{34}$$

where the entanglement between the parties A and B is considered.

For pure states $|\psi^{AB}\rangle$ and $|\phi^{AB}\rangle$ we see that

$$F_s(|\psi^{AB}\rangle \otimes |\phi^{AB}\rangle) = F_s(|\psi^{AB}\rangle) F_s(|\phi^{AB}\rangle), \tag{35}$$

with $F_s(\rho) = \max_{\sigma \in s} F(\rho,\sigma)$ and the fidelity $F(\rho,\sigma) = (\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$. From (35) we see that the geometric measure of entanglement is not additive. Note that for the entanglement of formation nonadditivity has also been proved [28].

We consider the *logarithmic entanglement*

$$E_{\log}(\rho) = -\log_2 F_s(\rho), \tag{36}$$

which is additive for pure bipartite states, as is seen from (35). In general, $F_s(\rho^{AB} \otimes \sigma^{AB}) \geqslant F_s(\rho^{AB}) F_s(\sigma^{AB})$ holds, and thus the logarithmic entanglement is subadditive:

$$E_{\log}(\rho^{AB} \otimes \sigma^{AB}) \leqslant E_{\log}(\rho^{AB}) + E_{\log}(\sigma^{AB}). \tag{37}$$

We use our algorithm to test the inequality (37). Note that for two-qubit states ρ we get $F_s(\rho) = \frac{1}{2}(1 + \sqrt{1 - C(\rho)^2})$. We take ρ^{AB} and σ^{AB} to be random states of two qubits and apply the algorithm to $\rho^{AB} \otimes \sigma^{AB}$ with parameter $\varepsilon = 10^{-7}$. This procedure is repeated 100 times; each time the computed approximation $\tilde{F}_s(\rho^{AB} \otimes \sigma^{AB})$ was slightly below $F_s(\rho^{AB}) F_s(\sigma^{AB})$, which means that we could not disprove additivity of logarithmic entanglement in this way. The difference $F_s(\rho^{AB}) F_s(\sigma^{AB}) - \tilde{F}_s(\rho^{AB} \otimes \sigma^{AB})$ was always smaller than 10^{-5}.

C. Applications to three qubits

In this section we apply our algorithm to three-qubit states with unknown value of E_G. If d is the dimension of the total Hilbert space, then for any ρ there always exists an optimal decomposition with at most d^2 elements [24]. A decomposition $\{p_i, |\psi_i\rangle\}$ of a state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is called optimal if its average entanglement is equal to the geometric measure of entanglement: $\sum_i p_i E_G(|\psi_i\rangle) = E_G(\rho)$. In order to make sure that the algorithm always has the chance to find the optimal decomposition, all minimizations in this section were done over decompositions into $d^2 = 2^6 = 64$ pure states. In order to do the computation within a reasonable time we used the parameter $\varepsilon = 10^{-7}$.

1. Isotropic states

Isotropic states of three qubits have the form

$$\rho = p|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}| + \frac{1-p}{8}\mathbb{1}, \tag{38}$$

with $|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. They are known to be fully separable if and only if $p \leqslant \frac{1}{5}$ [29]. We apply our algorithm to these states with parameter $\varepsilon = 10^{-7}$ for $p > \frac{1}{5}$. The result is shown in Fig. 1 (solid line). The plot can be compared to the geometric measure of entanglement of the isotropic states of two qubits; see the dashed line in Fig. 1. In the limit $p \to 1$ the state becomes the pure GHZ state with $E_G(|\mathrm{GHZ}\rangle) = \frac{1}{2}$ [9].

2. XX model

As a final example we apply our algorithm to the isotropic XX model of three qubits in a constant magnetic field. The corresponding Hamiltonian is given by [30,31]

$$H = \frac{B}{2}\sum_{i=1}^{3}\sigma_i^z + J\sum_{i=1}^{3}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y), \tag{39}$$

with periodic boundary conditions $\sigma_4^x = \sigma_1^x$ and $\sigma_4^y = \sigma_1^y$. In thermal equilibrium the system is found in the mixed state $\rho = \frac{e^{-\frac{H}{kT}}}{Z}$ with $Z = \mathrm{Tr}[e^{-\frac{H}{kT}}]$. In the following we set $k = 1$.

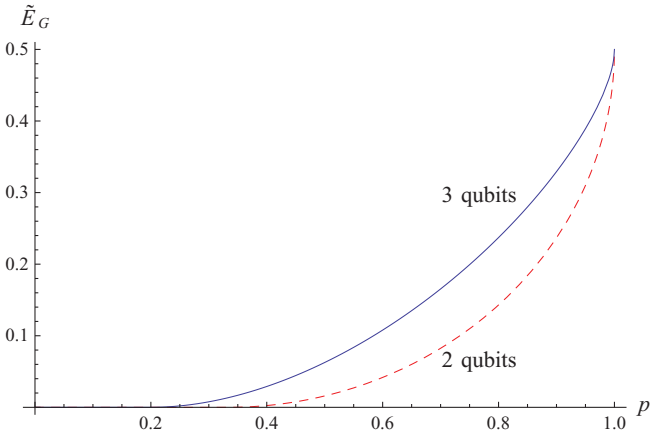

FIG. 1. (Color online) Approximation of the geometric measure of entanglement $\tilde{E}_G$ for isotropic states of three qubits given in (38) as a function of p (solid line) compared to the two-qubit case (dashed line).

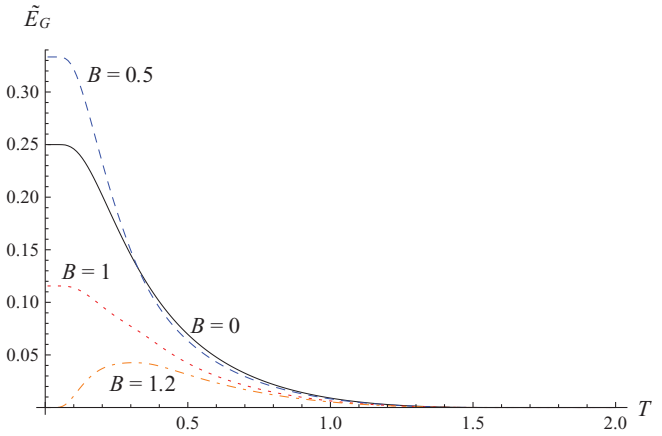

FIG. 2. (Color online) Approximation of the geometric measure of entanglement $\tilde{E}_G$ plotted as function of the temperature T for $\rho = \frac{e^{-\frac{H}{kT}}}{Z}$ with H given in (39). The parameter J is set to $\frac{1}{2}$ and $k = 1$.

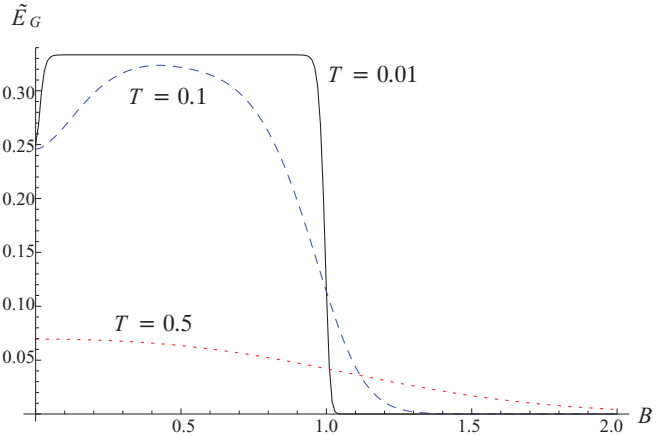

FIG. 3. (Color online) Approximation of the geometric measure of entanglement $\tilde{E}_G$ for fixed values of T plotted as a function of the magnetic field B. The parameter J is set to $\frac{1}{2}$ and $k = 1$.

The results of the approximation with parameter $\varepsilon = 10^{-7}$ are shown in Fig. 2. They can be compared to the results for two qubits in ([32], Fig. 4). For different values of the magnetic field B we observe a different behavior of the system in the low temperature limit. This behavior is explained in the following.

Note that the Hamiltonian (39) has four nondegenerate eigenvalues $\pm\frac{3}{2}B$, and $4J \pm \frac{1}{2}B$. Further, the following two eigenvalues are degenerated twice: $-2J \pm \frac{1}{2}B$. For vanishing magnetic field the ground state of the system is a mixture of the four eigenstates corresponding to the eigenvalue $-2J$ with equal probabilities. In this case we get $\tilde{E}_G \approx \frac{1}{4}$ for $T \to 0$;see the solid curve in Fig. 2. For small nonzero magnetic field $0 < B < 2J$ the ground state of the system is the mixture of the eigenstates corresponding to the eigenvalue $-2J - \frac{1}{2}B$. As can be seen from the dashed curve in Fig. 2, for $T \to 0$ the approximation becomes $\tilde{E}_G \approx \frac{1}{3}$ in this case. In the case $B = 2J$, there are three eigenstates corresponding to the smallest eigenvalue $-3J$. The approximated value for $T \to 0$ in this case becomes $\tilde{E}_G \approx 0.116$; see the dotted curve in Fig. 2. Finally, for $B > 2J$ the ground state is the product state $|111\rangle$, and the entanglement vanishes for $T \to 0$, as is seen from the dot-dashed curve in Fig. 2.

In Fig. 3 we show the plot of $\tilde{E}_G$ as a function of the magnetic field B for three different temperatures T. For $T \to 0$ we observe that $\tilde{E}_G$ becomes a nonanalytic function of B for two different values of the magnetic field, namely for $B = 0$ and $B = 2J$. This is a significant difference to the two-qubit case, where such behavior occurred only for a single value of B ([32], Fig. 5).

IV. CONCLUDING REMARKS

In this paper we presented an algorithm for approximating the geometric measure of entanglement for arbitrary multipartite mixed states. The algorithm is based on a connection between the geometric measure of entanglement and the fidelity [24]. It is easily implementable, since it implies only the solution of an eigenproblem and finding a singular value decomposition. We tested our algorithm on bipartite and multipartite mixed states, where an exact formula for the geometric measure of entanglement is known. In all cases we found convergence to the exact value. For two qubits, the performance of our algorithm is comparable to the performance of the algorithms based on conjugate gradients. We also applied our algorithm to the isotropic state of three qubits, and the three-qubit XX model with external magnetic field.

In our tests on bipartite mixed states with known value of the geometric measure of entanglement our algorithm always converged to the correct value within a given precision. It remains an open question whether this is always the case. For quantum states with more than two parties the algorithm can converge to wrong values with nonzero probability. In general, more than one run of the algorithm with different initial parameters should be performed.

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