Estimating Entanglement Monotones with a Generalization of the Wootters Formula

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(Received 23 July 2012; published 16 November 2012)

Entanglement monotones, such as the concurrence, are useful tools to characterize quantum correlations in various physical systems. The computation of the concurrence involves, however, difficult optimizations and only for the simplest case of two qubits a closed formula was found by Wootters [Phys. Rev. Lett. **80**, 2245 (1998)]. We show how this approach can be generalized, resulting in lower bounds on the concurrence for higher dimensional systems as well as for multipartite systems. We demonstrate that for certain families of states our results constitute the strongest bipartite entanglement criterion so far; moreover, they allow us to recognize novel families of multiparticle bound entangled states.

DOI: 10.1103/PhysRevLett.109.200503 PACS numbers: 03.67.Mn, 03.65.Ud

Entanglement has proven to be a fundamental concept in physics, with applications spanning virtually all areas of quantum science: These include antipodal topics such as the black hole information paradox and industrial realizations of quantum cryptographic devices. By definition, entanglement between two or more particles is given by those quantum correlations which cannot be created by local operations and classical communication. For the case of more than two particles, also different classes of entanglement can be distinguished. For the quantification of entanglement and also for the discrimination between entanglement classes, one can use so-called *entanglement measures* or *entanglement monotones*—parameters that indeed are nonincreasing under local operations and classical communication. The concurrence and the entanglement of formation are important parameters of this kind [1].

A central problem for the quantification of entanglement is the fact that nearly all entanglement monotones are extremely difficult to compute. Indeed, most definitions of entanglement monotones contain nontrivial optimizations, such as the optimization over all possible local operations and classical communication protocols or the minimization over all possible decompositions of a given density matrix. This difficulty is an important issue for the application of monotones to real world problems or experiments.

A milestone in the theory of entanglement measures was the derivation of a closed formula for the concurrence of two qubits by Wootters in 1998 [2]. In this work, it was shown how the minimization over all state decompositions can be done for such a special case. Consequently, the Wootters formula has led to many applications of the concurrence, e.g., for characterizing phase transitions in spin models [3]. In the following years, the formula has been shown to work also for a special type of multipartite measures by Uhlmann [4]. Furthermore, the concurrence can also be computed for some special states with high symmetries [5].

In the present Letter, we generalize the idea of Wootters to compute lower bounds on the concurrence. Our methods work for higher dimensional bipartite systems as well as for multipartite systems. Compared with the large amount of research about lower bounds on entanglement measures [6–8], our approach has substantial advantages: For the bipartite case, we discuss a family of bound entangled states and show that our result gives the strongest separability criterion so far; for the multipartite examples, our estimates give the precise value of the multipartite concurrence, and allow us to identify a novel and simple family of bound entangled states. Finally, our approach can also be used to estimate other quantities besides the concurrence, which might be useful to deal with entanglement monotones based on antilinear operators and combs [9]. It should be noted that lower bounds on the concurrence based on Wootters' idea have appeared in the literature before [8]; as we will see, however, the existing approaches are fundamentally limited.

Setting the stage.—To start, let us recall the main definitions. For a general $(m \times n)$-dimensional bipartite pure quantum state $\varrho_{AB} = |\psi\rangle\langle\psi|$ on $\mathcal{H}_A \otimes \mathcal{H}_B$, the *concurrence* [1,10] can be defined as

$$C(|\psi\rangle) = \sqrt{2(1 - \mathrm{Tr}\varrho_A^2)}, \tag{1}$$

where $\varrho_A = \mathrm{Tr}_B(|\psi\rangle\langle\psi|)$ is the reduced density matrix of the first particle [11]. A pure state is separable if and only if its concurrence is zero. The above definitions are extended to mixed states via the so-called *convex roof construction*

$$C(\varrho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i C(|\psi_i\rangle), \quad (2)$$

where the minimization is meant as an optimization over all possible ensemble realizations $\varrho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, where $p_i \geq 0$ and $\sum_i p_i = 1$. The decomposition attaining the minimum is said to be the *optimal decomposition*. Clearly, this is a difficult optimization problem, and different estimates have been obtained [6–8].

The bipartite bound.—For our approach, we first need to reformulate the definition of the concurrence. The pure state $|\psi\rangle$ can be expressed in a product basis as $|\psi\rangle = \sum_{i=1}^m \sum_{j=1}^n \psi_{ij} |ij\rangle$. Furthermore, we can define on $\mathcal{H}_A$ the generators of the group $SO(m)$ as $L_\alpha = |i\rangle\langle j| - |j\rangle\langle i|$. There are $m(m-1)/2$ generators of this type; similarly, there are $n(n-1)/2$ generators S_β of $SO(n)$ on $\mathcal{H}_B$. Then, a direct calculation for the ψ_{ij} shows that one can express the concurrence as (see also Ref. [12])

$$C^2(|\psi\rangle) = 2(1 - \mathrm{Tr}\varrho_A^2) = \sum_{\alpha,\beta} |\langle\psi| L_\alpha \otimes S_\beta |\psi^*\rangle|^2, \quad (3)$$

where $|\psi^*\rangle$ denotes the complex conjugation. In the following, it is convenient to use a single index for the matrices $L_\alpha \otimes S_\beta$, and we define $J_t = L_\alpha \otimes S_\beta$, where the index t runs from 1 to $N = [mn(m-1)(n-1)]/4$.

In order to formulate our bound, we first fix an integer k. We then choose a subset of indices $\vec{t} = \{t_1, \ldots, t_k\} \subset \{1, \ldots, N\}$, where we use the ordering $t_i < t_{i+1}$. Moreover, we can choose k complex numbers $\vec{u} = \{u_s\}$ for which the absolute values are bounded via $|u_s| \leq 1$. Then, we consider the quantity

$$\Delta_k(\varrho, \vec{t}, \vec{u}) = \max\left\{0, \lambda_{mn}^{(1)} - \sum_{i>1} \lambda_{mn}^{(i)}\right\}; \quad (4)$$

here the numbers $\lambda_{mn}^{(j)}$ are the square roots of the eigenvalues of

$$\mathcal{X} = \varrho\left(\sum_{s=1}^k u_s J_{t_s}\right)\varrho^*\left(\sum_{s=1}^k u_s^* J_{t_s}\right) \quad (5)$$

in nonincreasing order. Alternatively, one can say that the $\lambda_{mn}^{(j)}$ are the eigenvalues of the Hermitian matrix

$$\mathcal{Y} = \sqrt{\sqrt{\varrho}\left(\sum_s u_s J_{t_s}\right)\varrho^*\left(\sum_s u_s^* J_{t_s}\right)\sqrt{\varrho}}. \quad (6)$$

For our given k, we consider the set of *all* possible $\vec{t}$ and choose for any of them a different vector $\vec{u}$ and compute the corresponding $\Delta_k(\varrho, \vec{t}, \vec{u})$. This leads to $\binom{N}{k}$ numbers, and for these we can state our first main result.

Observation 1.—Let ϱ be a density matrix acting on an $(m \times n)$-dimensional bipartite quantum system and consider for fixed k all the possible $\vec{t}$ and a possible choice of $\vec{u}$ as discussed above. Then, a lower bound on the concurrence is given by

$$C(\varrho)^2 \geq \frac{N}{k^2\binom{N}{k}} \sum_{\vec{t}} [\Delta_k(\varrho, \vec{t}, \vec{u})]^2. \quad (7)$$

Especially if ϱ is separable, then $\Delta_k(\varrho, \vec{t}, \vec{u}) = 0$ for any choice of k, $\vec{t}$, and $\vec{u}$.

Before proving this theorem, let us discuss some of its implications. Equation (7) is a lower bound for the concurrence for any given choice of the $\vec{u}$. In order to obtain a good bound, the set of the $\vec{u}$ has to be optimized for the given state ϱ. Often this has to be done numerically, but we will also present examples where a good choice of the J_{t_s} is given analytically.

Second, for the case of two qubits there is only one possible generator, namely, $L_\alpha = S_\beta = |0\rangle\langle 1| - |1\rangle\langle 0| = i\sigma_y$. This implies that the only possibility in Observation 1 is $k = N = 1$, and then Eq. (7) reduces to the well known formula for the concurrence of mixed states. Of course, obtaining a closed formula for the concurrence is a significantly more advanced result, as one has to prove in addition that equality holds. In Refs. [2,4], this has been achieved by writing down an explicit decomposition. This is, however, beyond the scope of the present Letter; we focus on the problem of deriving lower bounds.

Finally, one should add that other researchers have obtained lower bounds on the concurrence by using the formulation of Eq. (3) and ideas similar to the original construction [8]. In these works, the terms $|\langle\psi| L_\alpha \otimes S_\beta |\psi^*\rangle|^2$ are estimated separately. A single observable $L_\alpha \otimes S_\beta$, however, acts on a 2×2 subspace only, and for these subspaces the criterion of the positivity of the partial transpose is a necessary and sufficient criterion for entanglement [1]. This implies that the approaches in Ref. [8] can never detect weak forms of entanglement, such as bound entanglement which is not detected by the positivity of the partial transpose criterion [13]. On the other side, Observation 1 represents a strong criterion for bound entanglement, as we will see below.

Proof of Observation 1.—First we prove that for a fixed k and fixed vector $\vec{t}$ we have that

$$\min_{\{p_i, |\psi_i\rangle\}} \left\{\sum_i p_i \left|\langle\psi_i| \sum_{s=1}^k u_s J_{t_s} |\psi_i^*\rangle\right|\right\} \geq \Delta_k(\varrho, \vec{t}, \vec{u}), \quad (8)$$

where the minimum is taken over all decompositions $\varrho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. Let λ_i and $|\chi_i\rangle$ be the eigenvalues and the eigenvectors, respectively, of ϱ. It is known that any decomposition of ϱ is connected to the eigenvalue decomposition via a unitary matrix U_{ij}; namely, one has $\sqrt{p_i}|\psi_i\rangle = \sum_{j=1}^{mn} U_{ij}^* (\sqrt{\lambda_j}|\chi_j\rangle)$ [14]. Therefore, we have $\sqrt{p_i p_j}\langle\psi_i| \sum_{s=1}^k u_s J_{t_s} |\psi_j^*\rangle = (UYU^T)_{ij}$, where the matrix Y is defined by $Y_{\alpha\beta} = \sqrt{\lambda_\alpha \lambda_\beta}\langle\chi_\alpha| \sum_{s=1}^k u_s J_{t_s} |\chi_\beta^*\rangle$. Since the J_k are symmetric, the matrix $Y = Y^T$ is complex and symmetric, and we can use Takagi's factorization [15] to write $Y = VDV^T$ with a real diagonal matrix D. The entries of D are non-negative and given by the square roots of the eigenvalues of $YY^\dagger$. Then, following directly the argumentation of Ref. [2], we have

$$\min_{\{p_i,|\psi_i\rangle\}}\Big\{\sum_i p_i|\langle\psi_i|\sum_{s=1}^{k}u_s J_{t_s}|\psi_i^*\rangle|\Big\}$$
$$= \min_{W=UV}\Big\{\sum_i|[WDW^T]_{ii}|\Big\} \geq \lambda_{mn}^{(1)} - \sum_{i>1}\lambda_{mn}^{(i)}$$
$$= \Delta_k(\varrho,\vec{t},\vec{u}), \tag{9}$$

where $\lambda_{mn}^{(j)}$ are the entries of D in decreasing order. These quantities are, however, nothing but the eigenvalues of $\mathcal{X}$ in Eq. (5). Therefore, if a state ϱ is separable, then a decomposition into pure states without concurrence exists. Due to Eq. (3), all the mean values of J_k vanish, which implies already that $\Delta_k(\varrho,\vec{t},\vec{u}) = 0$.

It remains to show that $\Delta_k(\varrho,\vec{t},\vec{u})$ can give a lower bound on the concurrence also for entangled states. Suppose that $\varrho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ is an optimal decomposition of ϱ. Then $C(\varrho) = \sum_i p_i C(|\psi_i\rangle) = \sum_i p_i\sqrt{\sum_{t=1}^{N}|\langle\psi_i|J_t|\psi_i^*\rangle|^2}$. From the argumentation above, we know that for fixed k and $\vec{t}$ and fixed $t_1,\ldots,t_k$ the estimates $\Delta_k(\varrho,\vec{t},\vec{u}) \leq \sum_i p_i\sum_{s=1}^{k}|\langle\psi_i|u_s J_{t_s}|\psi_i^*\rangle| \leq \sum_i p_i\sum_{s=1}^{k}|\langle\psi_i|J_{t_s}|\psi_i^*\rangle|$ hold.

Finally, using the rule $(\sum_{j=1}^{k}x_j)^2 \leq k\sum_j x_j^2$ and the Cauchy-Schwartz inequality, we can directly estimate the right-hand side of Eq. (7) as

$$\sum_{\vec{t}}[\Delta_k(\varrho,\vec{t},\vec{u})]^2 \leq \frac{k^2}{N}\binom{N}{k}C(\varrho)^2. \tag{10}$$

The details of this calculation are given in Appendix A1 [16]. This concludes the proof of Observation 1.

Before proceeding to the examples, let us discuss the properties of the concurrence that were used in the proof. The starting point was Eq. (3), and the only further requirement needed was the fact that the $J_t = J_t^T$ were symmetric [17]. Moreover, if $A_t = -A_t^T$ were antisymmetric, then one has for any state $|\langle\psi|A_t|\psi^*\rangle|^2 = 0$, so restricting to symmetric J_t can be done without losing generality. In summary, the convex roof of any quantity $E(|\psi\rangle)$, which can be written as

$$E^2(|\psi\rangle) = \sum_t \pm m_t|\langle\psi|M_t|\psi^*\rangle|^2, \tag{11}$$

can be estimated with our methods: One can split each M_t into a symmetric and an antisymmetric part and estimate the contributions from the symmetric part. The fact that some of the coefficients m_t can be negative does not matter: Using the relation $\sum_t|\langle\psi|G_t|\psi^*\rangle|^2 = 1$ (where the G_t form an orthonormal basis of the operator space), one can rewrite $E^2(|\psi\rangle)$ as a sum with only positive coefficients minus a constant term.

Bound entangled states as an example.—In order to show that Observation 1 results in a stronger separability criterion than the best methods that are currently known, we consider the family of 3×3 bound entangled states introduced by Horodecki [18]. This family of states ϱ_a^{PH} is not detected by positivity of the partial transpose criterion but is nevertheless entangled for any $0 < a < 1$. The detailed form of these states is given in Appendix A2 [16]. We consider a mixture of these states with white noise, $\varrho_a(p) = p\varrho_a^{PH} + (1-p)\mathbb{1}/9$, and ask for the minimal p, so that the entanglement in $\varrho_a(p)$ is still detected. First, we use Observation 1 with the purpose of detecting entanglement and find the optimal J_t via numerical optimization. We finally compare our values with the values obtained via different known criteria: the Zhang-Zhang-Zhang-Guo (ZZZG) criterion [19], the Ma and Bao (MB) criterion [20], and the method based on symmetric extensions and semidefinite programming (SDP) [21,22]. We also used the algorithm proposed in Ref. [23] to prove separability of quantum states. This allows us to compute values of p, for which $\varrho_a(p)$ is provably separable.

The results are given in Fig. 1. One clearly sees that Observation 1 provides the best criterion, but the comparison with the separability algorithm also suggests that Observation 1 does not detect all states.

Estimating the multipartite concurrence.—For simplicity, we discuss only the three-particle case, but our results can be directly generalized to arbitrary N-partite states. Let us consider a pure state $|\psi\rangle$ in a $d\times d\times d$ system. Its concurrence is given by

$$C^\tau(|\psi\rangle) = \sqrt{[3 - (\mathrm{Tr}\varrho_1^2 + \mathrm{Tr}\varrho_2^2 + \mathrm{Tr}\varrho_3^2)]}, \tag{12}$$

where $\varrho_1 = \mathrm{Tr}_{23}(\varrho)$, etc., are the reduced one-particle states. For this definition, it directly follows that for pure states $C^\tau(|\psi\rangle)^2 = \frac{1}{2}([C^{(1|23)}(|\psi\rangle)]^2 + [C^{(2|13)}(|\psi\rangle)]^2 + [C^{(3|12)}(|\psi\rangle)]^2)$, where $C^{(1|23)}(|\psi\rangle)$, etc., are the corresponding bipartite concurrences. This definition is

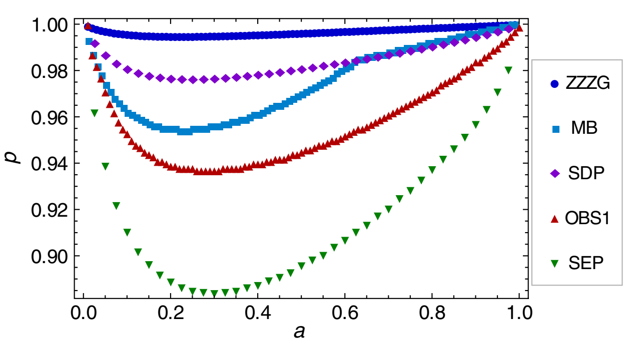

FIG. 1 (color online). Detecting entanglement in the Horodecki 3×3 bound entangled state mixed with white noise. The criterion of Observation 1 (points denoted by OBS1) is stronger than previously known criteria. For values of p smaller than the values given by SEP, the states $\varrho_a(p)$ are proven to be separable. See the text for further details.

extended to mixed states via the convex roof construction. Clearly, $C^\tau(\varrho) = 0$ if and only if ϱ is a fully separable state.

A first possibility to estimate the multipartite concurrence is to start with an estimate of the bipartite concurrence for each bipartition (as in Observation 1) and then estimate the total concurrence C^τ from it. This is indeed a viable way; in Appendix A3 [16], we present and discuss a corresponding theorem. The disadvantage of this approach is that there are states which are separable for any bipartition but not fully separable [24]. For them, this method will not succeed, since all the bipartite concurrences vanish.

To overcome this limitation, one should note that $C^\tau(|\psi\rangle)^2$ is of the same structure as Eq. (11): We define the operators J_t as before, but separately for any bipartition, and write $J_t^{1|23} = L_\alpha^1 \otimes S_\beta^{23}$ and similarly for the other bipartitions. Then we have the expression $C^\tau(|\psi\rangle)^2 := \frac{1}{2}\sum_t[|\langle\psi|J_t^{1|23}|\psi^*\rangle|^2 + |\langle\psi|J_t^{2|13}|\psi^*\rangle|^2 + |\langle\psi|J_t^{3|12}|\psi^*\rangle|^2]$. So we have to consider

$$\Delta_k^{tot}(\varrho, \vec{t}, \vec{x}) = \max\Big(0, \lambda_{mn}^{(1)} - \sum_{i>1} \lambda_{mn}^{(i)}\Big), \tag{13}$$

where the $\lambda_{mn}^{(j)}$ are the square roots of eigenvalues of

$$\mathcal{X}^{\text{tot}} = \varrho \sum_{s=1}^{k} (u_s J_{t_s}^{1|23} + v_s J_{t_s}^{2|13} + w_s J_{t_s}^{3|12}) \times \varrho^* \sum_{s=1}^{k} (u_s^* J_{t_s}^{1|23} + v_s^* J_{t_s}^{2|13} + w_s^* J_{t_s}^{3|12}) \tag{14}$$

in decreasing order. Here, $\vec{x} = (\vec{u}, \vec{v}, \vec{w})$ denotes a triple of complex vectors which are normalized as in Observation 1 and $\vec{t} = \{t_1, \ldots, t_k\}$. For this quantity we can state the following.

Observation 2.—For any arbitrary mixed state on $\mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H}$ and for every fixed k and for arbitrary $\vec{x}$, we have

$$\frac{N}{6k^2\binom{N}{k}} \sum_{\vec{t}} [(\Delta_k^{tot}(\varrho, \vec{t}, \vec{x}))^2] \leq C^\tau(\varrho)^2. \tag{15}$$

A proof is given in Appendix A4 [16].

Multipartite examples.—We will consider two simple examples for three qubits, but these already demonstrate two interesting points: First, they give an idea how the observables J_t and the coefficients $\vec{x}$ can be chosen; second, it turns out that the entanglement criterion in Observation 2 is strong and allows us to identify a novel family of bound entangled states.

As the first example, we consider the three-qubit Greenberger-Horne-Zeilinger (GHZ) state $|\text{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ and mix it with white noise, $\varrho^G(p) = p|\text{GHZ}\rangle\langle\text{GHZ}| + (1-p)\mathbb{1}/8$. Then we take the single-qubit operator $S^{(a)} = |0\rangle\langle 1| - |1\rangle\langle 0|$ and the two-qubit operator $L^{(bc)} = |00\rangle\langle 11| - |11\rangle\langle 00|$, and from them we form the operators $J^{i|jk} = S^{(i)} \otimes L^{(jk)}$ for all three bipartitions. Applying Observation 2 for the choice $k = 1$ and $u_1 = v_1 = w_1 = 1$, one finds already from a single term in the sum of Eq. (15) that the three-qubit concurrence is bounded by

$$(C^\tau[\varrho^G(p)])^2 \geq \frac{1}{6}\Big(\frac{3}{4}[5p - 1]\Big)^2. \tag{16}$$

For $p = 1$, this reproduces exactly concurrence of the pure GHZ state. Moreover, this bound shows that the state $\varrho^G(p)$ is entangled for $p > 1/5$. This means that Observation 2 provides a necessary and sufficient criterion for entanglement for the family of states $\varrho^G(p)$, since it is known that for $p \leq 1/5$ these states are separable [25]. In fact, Eq. (16) gives a linear lower bound on the convex function $C^\tau[\varrho^G(p)]$, and this bound coincides with the exact value on the points $p = 1/5$ and $p = 1$. This means that the bound equals the exact value on the whole interval $p \in [1/5; 1]$, and for them we have $C^\tau[\varrho^G(p)] = (\frac{3}{4}[5p - 1])/\sqrt{6}$.

As the second example, we consider the three-qubit W state $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ mixed with white noise, $\varrho^W(p) = p|W\rangle\langle W| + (1-p)\mathbb{1}/8$. In this case, we use again the operator $S^{(a)} = |0\rangle\langle 1| - |1\rangle\langle 0|$, but for two qubits we use the $L^{(bc)} = |00\rangle\langle 10| - |10\rangle\langle 00|$, and from them we form the operators $J^{i|jk} = S^{(i)} \otimes L^{(jk)}$. Applying Observation 2 for $k = 1$ and $u_1 = v_1 = w_1 = 1$, we find that $(C^\tau[\varrho^W(p)])^2 \geq (1/96)[p(8 + \sqrt{3}) - \sqrt{3}]^2$; especially, the state $\varrho^W(p)$ is entangled for $p > p_s = \sqrt{3}/(8 + \sqrt{3}) \approx 0.178$.

This is a remarkable value for several reasons. First, using the separability algorithm from Ref. [23], one can prove that the states $\varrho^W(p)$ are fully separable for $p \leq 0.177$, giving strong evidence that Observation 2 provides a necessary and sufficient criterion for the family of states $\varrho^W(p)$.

Second, these calculations show that the states $\varrho^W(p)$ exhibit quite peculiar entanglement properties: One can directly check that for $p \leq 3(8\sqrt{2} - 3)/119 \approx 0.2096$ the states have a positive partial transpose for any bipartition, and using the separability algorithm [23] one finds that for $p \leq 0.2095$ the states are indeed separable for any bipartition. Hence, for $p \in [p_s; 0.2095]$ the states $\varrho^W(p)$ are separable for any bipartition but not fully separable. This implies that they are bound entangled: No entanglement can be distilled from them, even if two of the three parties join. It was known that such states exist [24]; however, the existing examples required a sophisticated construction. It is surprising that the simple family $\varrho^W(p)$ includes bound entangled states, and it underlines the power of our approach that these states can be detected with Observation 2. Finally, the bound entanglement in the family $\varrho^W(p)$ can easily be generated experimentally (contrary to other known examples of bound entangled states), since adding noise to a pure state is easy in practically any experimental implementation.

Conclusion.—We have provided a general method to bound entanglement monotones by extending in a nontrivial way the original construction of Wootters [2], an approach that works for both bipartite and multipartite concurrence. We leave open the problem of determining for which states our method gives the exact value of the concurrence. It would also be interesting to broaden our approach to the general classification of invariants of quantum states [9], since this may help to understand the different entanglement classes for multiparticle systems.

We thank M. Hofmann for discussions. This work has been carried on while Z. M. was visiting the Department of Computer Science and the Department of Physics at University College London. Z. C. is supported by NSF of China (11201427), Z. M. is supported by the NSF of China (10901103), O. G. is supported by the EU (Marie Curie CIG 293993/ENFOQI) and the BMBF (Chist-Era Project QUASAR), and S. S. is supported by the Royal Society.

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