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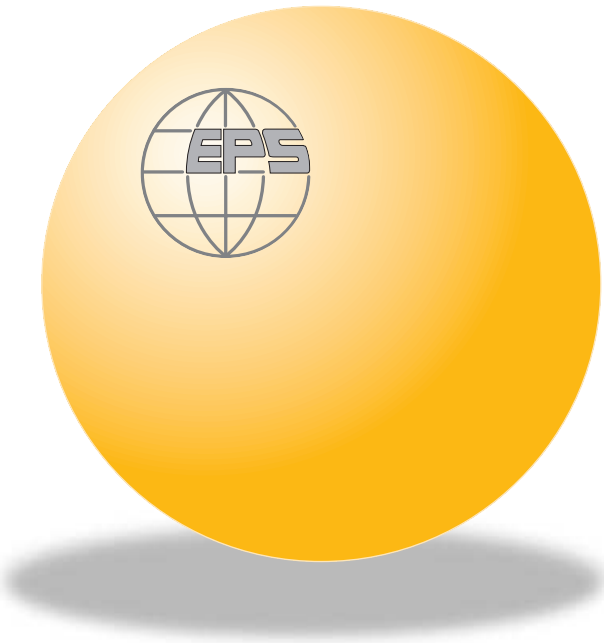

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Entanglement of $2 \times K$ quantum systems

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Abstract. – We derive an analytical expression for the lower bound of the concurrence of mixed quantum states of composite $2 \times K$ systems. In contrast to other, implicitly defined entanglement measures, the numerical evaluation of our bound is straightforward. We explicitly evaluate its tightness for general mixed states of 2×3 systems, and identify a large class of states where our expression gives the exact value of the concurrence.

Introduction. – Entanglement is a fundamental concept in the theory of quantum information, and the essential resource for (potential) modern applications of quantum mechanics [1,2]. As the cause of nonclassical correlations between measurement results on the different constituents of multipartite quantum systems, it is the key ingredient for quantum cryptography, teleportation, and quantum computing. However, the quantitative characterization of entanglement remains a largely open problem, due to the ever more intricate topology and rapidly increasing dimension of the space of admissible quantum states with the number of components of composite quantum systems. By now, only the entanglement of pure bipartite states is well understood and unambiguously quantified [3–6]. For mixed states —which we generically encounter in nature— a large variety of entanglement measures ([1]) was proposed (see, *e.g.*, [8]). Almost none of them, however, can be computed efficiently, the only exceptions (to our knowledge) being the *negativity* [9, 10], and the *entanglement of formation* [3] of two qubits [6]. For instance, to calculate the entanglement of formation in higher-dimensional spaces, one needs to perform a complicated optimization procedure over the huge space of all possible decompositions of the analyzed mixed state ρ into pure states, such as to minimize

([1])The required properties of an entanglement measure are: monotonously decreasing evolution under local operations with classical communication; convexity on state space; vanishing values for separable states alone [3, 7].

the average pure-state entanglement needed to represent ρ. By construction, such a procedure can only provide an upper bound for the degree of entanglement of ρ [11–13]. What is needed in addition is a lower bound of mixed-state entanglement, which we shall provide for $2 \times K$ systems in the present contribution. To do so, we will use the *concurrence*, originally introduced by Wootters [6] for 2×2 states, and generalized for any bipartite pure states by Rungta *et al.* [14]. (Alternative generalizations were proposed in [15,16].) We shall generalize its definition for general $2 \times K$ mixed states and derive an analytical lower bound which also implies a lower bound for the entanglement of formation. For some class of 2×3 mixed states we can establish equality between our lower bound and the exact value of the concurrence, and numerical calculations assess the tightness of our bound for general 2×3 mixed states.

Theory. – Let us start with the definition of the concurrence of a pure state on a $(N \times K)$-dimensional Hilbert space $\mathcal{H} = \mathcal{H}_N \otimes \mathcal{H}_K$ [14]. We first need the *flip operator* $\mathcal{F}$ acting on an arbitrary Hermitian operator A on $\mathcal{H}$,

$$\mathcal{F}(A) := A + (\operatorname{tr} A)\mathbb{I} - (\operatorname{tr}_N A) \otimes \mathbb{I}_K - \mathbb{I}_N \otimes (\operatorname{tr}_K A), \tag{1}$$

with $\mathbb{I}_K$ and $\mathbb{I}_N$ the identity on $\mathcal{H}_K$ and $\mathcal{H}_N$, respectively, and tr_K (tr_N) the partial trace over $\mathcal{H}_K$ ($\mathcal{H}_N$). $\mathcal{F}$ commutes with all unitary operators and preserves positivity. Moreover, the expectation value $\langle\psi|\mathcal{F}(\rho_\psi)|\psi\rangle$, where $\rho_\psi = |\psi\rangle\langle\psi|$, is non-negative for all pure states and equals zero if and only if $|\psi\rangle \in \mathcal{H}^N \otimes \mathcal{H}^K$ is a product state. This allows to define the concurrence of any arbitrary bipartite pure state as [14]

$$C(|\psi\rangle) = \sqrt{\langle\psi|\mathcal{F}(\rho_\psi)|\psi\rangle}\,, \tag{2}$$

wherefrom

$$C(|\psi\rangle) = \sqrt{2\big[|\langle\psi \mid \psi\rangle|^2 - \operatorname{tr}\left(\rho_N^2\right)\big]} \tag{3}$$

is easily deduced, with $\rho_N = \operatorname{tr}_K |\psi\rangle\langle\psi|$ the reduced density operator of dimension N. Observe that C is linear in the norm of $|\psi\rangle$. For a normalized state, $\langle\psi \mid \psi\rangle = 1$, it interpolates monotonously between zero for product states, and $\sqrt{2(N-1)/N}$ for maximally entangled states, where $N \leq K$ is assumed (without loss of generality).

We now need the generalization of this definition for mixed states. As a consequence of the generalized construction outlined in [15], any entanglement measure on the pure states can be ported to the mixed states through minimization of its average value on all possible decompositions into pure states. For instance, the *entanglement of formation* $E_{\mathrm{F}}(\rho)$ of a mixed state is defined [3] as the infimum over all possible pure state decompositions $\sum_{l=1}^{L} p_l |\psi_l\rangle\langle\psi_l|$,

$$E_{\mathrm{F}}(\rho) := \inf_{\mathcal{E}} \sum_{l=1}^{L} p_l E(|\psi_l\rangle), \tag{4}$$

with $E(|\psi\rangle) = -\operatorname{tr}(\rho_N \ln \rho_N)$ the *entropy of entanglement*. The length of the ensemble L is arbitrary, but need not exceed $(NK)^2$ [15]. In close analogy, we define the mixed-state concurrence as

$$C(\rho) := \inf_{\mathcal{E}} \sum_{l=1}^{L} p_l C(|\psi_l\rangle). \tag{5}$$

Note that, in the simplest case of 2×2 systems, the infima in (4) and (5) can be realized simultaneously, by the same optimal decomposition, and the definition (5) thus reduces to the original one [6]. However, in the general case of $N \times K$ systems, the minimum average entropy of entanglement need not be achieved with the same (optimal) decomposition as the minimum average concurrence [15].

To derive a lower bound of $C(\rho)$, we now specialize to the case $N = 2$. If a $2 \times K$ state is pure, its concurrence may be expressed in terms of unnormalized states $P^{(ij)}|\psi\rangle$, which live on a (2×2)-dimensional Hilbert space. Let $\{|k\rangle\}_{k=1,\ldots,K}$ be an arbitrary basis of $\mathcal{H}_K$, and

$$P^{(ij)} = \mathbb{I}_2 \otimes \big(|i\rangle\langle i| + |j\rangle\langle j|\big), \quad i, j \in \{1, \ldots, K\}, \tag{6}$$

denote the projections onto (2×2)-dimensional subspaces. We then obtain the squared concurrence of a $2 \times K$ pure state directly from the definition (2):

$$C^2(|\psi\rangle) = \sum_{i=1}^{K} \sum_{j=i+1}^{K} C^2\Big(P^{(ij)}|\psi\rangle\Big). \tag{7}$$

Given this expression, we can derive the desired lower bound. According to (5),

$$C(\rho) = \sum_{l=1}^{L} p_l C(|\psi_l\rangle) \tag{8}$$

for the *optimal decomposition* $\{|\psi_l\rangle\}$. Insertion of (7) yields

$$C(\rho) = \sum_{l=1}^{L} p_l \sqrt{\sum_{i>j} C^2\big(P^{(ij)}|\psi_l\rangle\big)} = \sum_{l=1}^{L} p_l \sqrt{\sum_{i>j} r_{ij} C^2\left(\frac{P^{(ij)}|\psi_l\rangle}{r_{ij}^{1/4}}\right)}, \tag{9}$$

where we introduced arbitrary coefficients $r_{ij} \geq 0$, with $\sum_{i>j} r_{ij} = 1$. Next, we use the concavity of the square root and obtain

$$C(\rho) \geq \sum_{l=1}^{L} p_l \sum_{i>j} r_{ij} \sqrt{C^2\left(\frac{P^{(ij)}|\psi_l\rangle}{r_{ij}^{1/4}}\right)} = \sum_{i>j} \sqrt{r_{ij}} \sum_{l=1}^{L} p_l C\Big(P^{(ij)}|\psi_l\rangle\Big). \tag{10}$$

The sum over l on the right-hand side can be interpreted as the average concurrence $\langle C\rangle$ of the 2×2 density matrices $\rho^{(ij)}$ obtained by projections

$$\rho^{(ij)} = P^{(ij)} \rho P^{(ij)} = \sum_{l=1}^{L} p_l P^{(ij)}|\psi_l\rangle\langle\psi_l|P^{(ij)}. \tag{11}$$

Due to the definition (2), $\langle C\rangle$ cannot be smaller than the projected concurrence $C(\rho^{(ij)})$, which is known analytically as the concurrence of a 2×2 mixed state. Hence,

$$C(\rho) \geq \sum_{i=1}^{K} \sum_{j=i+1}^{K} \sqrt{r_{ij}}\, C\big(\rho^{(ij)}\big). \tag{12}$$

Since the r_{ij} were not fixed in (9), we still can choose these coefficients r_{ij} such as to maximize the sum on the right-hand side of (12),

$$r_{ij} = \frac{C^2\big(\rho^{(ij)}\big)}{\sum_{m>n} C^2\big(\rho^{(mn)}\big)}\,, \tag{13}$$

and arrive at

$$C(\rho) \geq \sqrt{\sum_{i>j} C^2\big(\rho^{(ij)}\big)}\,. \tag{14}$$

This lower bound still depends on the choice of the basis $\{|k\rangle\}_{k=1,\ldots,K}$, of the K-dimensional subsystem. To find the tightest lower bound, we have to maximize (14) over all orthogonal basis sets, tantamount to finding the unitary $K \times K$ operator U which transforms to the optimal basis $\{U|k\rangle\}_{k=1,\ldots,K}$. Note that such a search is much faster than finding the optimal decomposition of the mixed state via a suitable unitary transformation of dimension $4K^2$.

Finally, since the entropy of entanglement of a pure state on $2 \times K$ systems is a convex function of its concurrence [6],

$$E(|\psi\rangle) = h\left(\frac{1+\sqrt{1-C(|\psi\rangle)^2}}{2}\right), \quad h(x) = -x\log_2 x - (1-x)\log_2(1-x), \tag{15}$$

the inequality (14) immediately provides a lower bound for the entanglement of formation defined in (4):

$$E_{\mathrm{F}}(\rho) \geq h\left[\frac{1}{2}\left(1+\sqrt{1-\sum_{i>j} C^2\big(\rho^{(ij)}\big)}\right)\right]. \tag{16}$$

As a matter of fact, the same bound was equally proposed in [17]. However, the proof in [17] is invalid, since it relies on the incorrect assumption that the entanglement of formation is a convex function of the *squared* concurrence C^2.

Given the above estimate, we shall now assess its tightness for the special case $K = 3$. In this case, (14) allows to distinguish between entangled and separable states, since any entangled 2×3 state also has entangled projections onto 2×2 subspaces. (This is not the case for $K > 3$, due to the existence of bound entangled states with positive partial transpose [18].) Our random mixed states were generated by partial trace $\mathrm{tr}_M(|\chi\rangle\langle\chi|)$ over pure states $|\chi\rangle$ randomly drawn (with respect to the natural Fubini-Study measure [19,20]) from a $6M$-dimensional state space, with $M = 4, 6, 10$. The larger the dimension M, the more mixed is $\rho = \mathrm{tr}_M(|\chi\rangle\langle\chi|)$, hence the smaller its concurrence. Furthermore, since $\mathrm{rank}(\rho) \leq M$, the $M = 4$ ensemble contains only states which do not have full rank. Figure 1 compares the lower bound (14) of the concurrence of the random states drawn from these three ensembles to its upper bound, which is obtained as the average concurrence with respect to a particular (numerically optimized) decomposition of the state ρ. Obviously, our lower bound comes very close to the upper bound, for the entire range from strongly entangled to almost separable states.

In many cases, in particular for all the relatively weakly entangled states drawn from the $M = 10$ ensemble, we have even found exact agreement of the lower and the upper bound of the concurrence. All these states, which are marked by dots in fig. 1, fulfill the property that there is only one entangled substate among the three (optimal) 2×2 substates, *i.e.*, $C(\rho^{(12)}) > 0$, and $C(\rho^{(13)}) = C(\rho^{(23)}) = 0$. Let us examine closer under which conditions

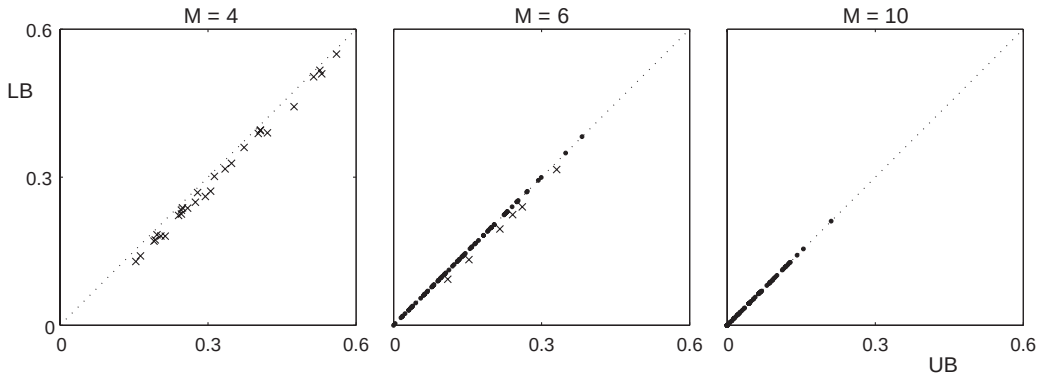

Fig. 1 – Lower bound (LB), eq. (14), *vs.* upper bound (UB), eq. (5), of the concurrence for ensembles of randomly chosen 2×3 mixed states, generated by a partial trace over pure states in a $6M$-dimensional state space, with $M = 4, 6, 10$. The deviation from the diagonal indicates the tightness of both bounds, which is obviously very good over the entire range of the three random ensembles. Dots (•) identify mixed states for which the lower bound provides the exact value.

an exact agreement of upper and lower bound may then be expected: if we re-examine (9) and (10) above, with the specific choice $r^{(12)} = 1$ and $r^{(13)} = r^{(23)} = 0$ according to (13), we conclude that the lower bound in (10) can only be exact if all the states $P^{(13)}|\psi_l\rangle$ and $P^{(23)}|\psi_l\rangle$ are product states. If so, $P^{(12)}|\psi_l\rangle$ is either a product state, or $|\psi_l\rangle$ lies in the image of $P^{(12)}$. In other words, *any* entangled $|\psi_l\rangle$ in an optimal decomposition lies in the image of $P^{(12)}$. Since for any 2×2 state there exists an optimal decomposition consisting of one entangled pure state and a separable remainder (this follows from the derivation presented in [6]), it follows that there exists an optimal decomposition of the 2×3 state ρ consisting of only *one* entangled pure state. This suggests the following procedure to test whether the lower bound (14) is saturated: if there is only one entangled 2×2 substate $\rho^{(12)}$ among the three $\rho^{(ij)}$'s, we try to find a pure state $|\psi\rangle$ with concurrence $C(|\psi\rangle) = C(\rho^{(12)})$, such that $\rho - |\psi\rangle\langle\psi|$ is positive and separable. If this succeeds, we have found the exact value of the concurrence of ρ. The dots (•) in fig. 1, where lower and upper bound coincide, have been obtained in this way.

For those mixed states for which at least two of the 2×2 states $\rho^{(ij)}$ are entangled, and equally so for some with only one entangled projection $\rho^{(ij)}$ (in particular, for the low-rank states of the $M = 4$ ensemble), the lower and the upper bound of the concurrence differ, although the difference is small in most cases. Since it is numerically quite expensive to obtain a good value of the upper bound (and there is no guarantee that the numerically found local minimum is also the global one), the actual value of the concurrence may be even closer to the lower bound.

To give an explicit example for which our lower bound can be proved to yield the exact value of the concurrence, we use the standard product basis, $|i, j\rangle = |i\rangle \otimes |j\rangle$, $i = 1, 2$, $j = 1, 2, 3$, to define the following family of states:

$$\rho_{x,y} = x|\psi_1\rangle\langle\psi_1| + y|\psi_2\rangle\langle\psi_2| + \frac{1 - x - y}{6}\mathbf{1}, \tag{17}$$

with

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\big(|11\rangle + |22\rangle\big), \qquad |\psi_2\rangle = \frac{1}{\sqrt{2}}\big(|13\rangle + |21\rangle\big), \quad x \geq y,\ x + y \leq 1. \tag{18}$$

For $y = 0$, these states may be considered as generalized Werner states [21]. By projection onto the subspace $P^{(13)}$, we obtain

$$C(\rho_{x,y}) \geq \tilde{C} = x - \frac{1}{3}\sqrt{(1-x+2y)(1-x-y)}. \tag{19}$$

On the other hand, the state $\rho - \tilde{C}|\psi_1\rangle\langle\psi_1|$ is positive and separable, provided that

$$x \leq 1 - \frac{3\sqrt{5}-1}{2}y. \tag{20}$$

Thereby, we have established $C(\rho_{x,y}) = \tilde{C}$ in this parameter regime. (If $\tilde{C} \leq 0$, which is the case for $16x \leq -2 - y + 3\sqrt{4+4y-7y^2}$, the state $\rho_{x,y}$ is separable, *i.e.*, $C(\rho_{x,y}) = 0$.)

As the simplest case which violates condition (20), let us finally consider $x = y = 1/2$. According to (7), the concurrence of an arbitrary superposition $|\psi\rangle = \cos(\theta)|\psi_1\rangle + \sin(\theta)e^{i\phi}|\psi_2\rangle$ of the states $|\psi_1\rangle$ and $|\psi_2\rangle$ reads $C^2(|\psi\rangle) = 1 - \cos^2(\theta) + \cos^4(\theta)$. The minimum $C_{\min} = \sqrt{3}/2$ is realized by the two states $(|\psi_1\rangle \pm |\psi_2\rangle)/\sqrt{2}$, which therefore form the optimal decomposition of $\rho_{1/2,1/2}$. Hence, we have shown that $C(\rho_{1/2,1/2}) = \sqrt{3}/2$. On the other hand, the lower bound (14), obtained by using the optimal basis $\{|1\rangle, |2\rangle, |3\rangle\}$, yields $C(\rho_{1/2,1/2}) \geq \sqrt{\tilde{C}^2 + \tilde{C}^2 + 0} = \sqrt{2}/2$. This proves that we cannot expect the lower bound to be exact in all cases. We conjecture that the above example with $x = y = 1/2$ realizes the largest possible difference between the lower bound and the actual value of the concurrence.

Conclusion. – In summary, combining the upper bound which follows from the very definition of mixed-state concurrence with our analytical lower bound provides a tight estimation of its exact value, for arbitrary 2×3 mixed states. Furthermore, our lower bound can be efficiently evaluated, since it involves an optimization problem on a K-dimensional rather than on a $4K^2$-dimensional space.

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