Concurrence of Arbitrary Dimensional Bipartite Quantum States

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We derive an analytical lower bound for the concurrence of a bipartite quantum state in arbitrary dimension. A functional relation is established relating concurrence, the Peres-Horodecki criterion, and the realignment criterion. We demonstrate that our bound is exact for some mixed quantum states. The significance of our method is illustrated by giving a quantitative evaluation of entanglement for many bound entangled states, some of which fail to be identified by the usual concurrence estimation method.

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Entanglement is a striking feature of quantum systems and is the key physical resource to realize quantum information tasks such as quantum cryptography, quantum teleportation, and quantum computation [1], which cannot be accounted for by classical physics. This has provided a strong motivation for the study of detection and quantification of entanglement in an operational way. Despite a great deal of effort in past years [2–13], for the moment, only partial solutions are known for generic mixed states. As for quantitative measures of entanglement, there is an elegant formula for 2 qubits in terms of *concurrence*, which is derived analytically by Wootters in Ref. [4]. This quantity has recently been shown to play an essential role in describing quantum phase transition in various interacting quantum many-body systems [14] and may affect macroscopic properties of solids significantly [15]. Furthermore, the value of concurrence will provide an estimation [13] for the entanglement of formation (EOF) [16], which quantifies the required minimally physical resources to prepare a quantum state. It is thus very important to have a precise quantitative picture of entanglement in order to get a better insight into the corresponding physical systems.

However, calculation of the concurrence is a formidable task as the Hilbert space dimension is increasing, like in the case of two parts in a real solid-state system considered for quantum computation. Good algorithms and progresses have been obtained concerning lower bounds for a qubit-qudit system [10,11] and for bipartite systems in arbitrary dimension [5,13]. Considerable progress is made in [13] to give a purely algebraic lower bound. Nevertheless, an optimized bound generally involves numerical optimization over a large number of free parameters in a level (at least $m(m-1)n(n-1)/4$ for a $m \otimes n$ bipartite system, where m, n are Hilbert space dimension for two subsystems respectively [5,11,13]). This leads to a computationally untractable problem for a realistic system with a higher dimension. In addition, these methods for evaluating concurrence cannot detect reliably *arbitrary* entangled states even if one applies all known optimization methods [13].

Our aim in this work is to improve this situation dramatically by giving an analytical lower bound for concurrence of any mixed bipartite quantum state. We find an essential quantitative relation among this measure and available strong separability criteria. A functional relation is explicitly derived to give a tightly lower bound for the concurrence. It is shown to be exact for some special class of states. Our method is further demonstrated to be better than the regular method for concurrence optimization, in the sense that it can detect and give an evaluation of entanglement for many bound entangled states (BES) which cannot be identified by the latter. This also complements a number of existing methods involving numerical optimization and provides a computational method to estimate manifestly the actual value of concurrence for any bipartite quantum state.

We start with a generalized definition [17] of concurrence for a pure state $|\psi\rangle$ in the tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$ of two (finite dimensional) Hilbert spaces $\mathcal{H}_A$, $\mathcal{H}_B$ for 2 systems A, B. The concurrence is defined by $C(|\psi\rangle) = \sqrt{2(1 - \mathrm{Tr}\rho_A^2)}$, where the reduced density matrix ρ_A is obtained by tracing over the subsystem B. The concurrence is then extended to mixed states ρ by the convex roof,

$$C(\rho) \equiv \min_{\{p_i|\psi_i\rangle\}} \sum_i p_i C(|\psi_i\rangle), \tag{1}$$

for all possible ensemble realizations $\rho = \Sigma_i p_i |\psi_i\rangle\langle\psi_i|$, where $p_i \geq 0$ and $\Sigma_i p_i = 1$. For any pure product state $|\psi\rangle$, $C(|\psi\rangle)$ vanishes according to the definition. Consequently, a state ρ is *separable* if and only if $C(\rho) = 0$ and hence can be represented as a convex combination of product states as $\rho = \Sigma_i p_i \rho_i^A \otimes \rho_i^B$ where ρ_i^A and ρ_i^B are pure state density matrices of the subsystems A and B, respectively [18].

The key point of our idea is to relate directly the concurrence and the Peres-Horodecki criterion of positivity under partial transpose (PPT criterion) [2,3] and the realignment criterion [6,7] by means of Schmidt coefficients of a pure state. Let us first consider the concurrence for a pure state. $C(|\psi\rangle)$ is invariant under a local unitary transformation (LU) [4,17]. Without loss of generality, we suppose that a pure $m \otimes n (m \leq n)$ quantum state has the standard Schmidt form

$$|\psi\rangle = \sum_i \sqrt{\mu_i}\,|a_i b_i\rangle, \tag{2}$$

where $\sqrt{\mu_i}\,(i = 1, \ldots, m)$ are the Schmidt coefficients, $|a_i\rangle$ and $|b_i\rangle$ are the orthonormal basis in $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. It is evident that the reduced density matrices ρ_A and ρ_B have the same eigenvalues of μ_i. It follows

$$C^2(|\psi\rangle) = 2\Big(1 - \sum_i \mu_i^2\Big) = 4\sum_{i<j}\mu_i\mu_j, \tag{3}$$

which varies smoothly from 0, for pure product states, to $2(m-1)/m$ for maximally entangled pure states.

In order to derive a quantitative connection with the PPT criterion and the realignment criterion, we recall some details of the two criteria. Peres made first an important step forward for separability criterion in [2] by showing that $\rho^{T_A} \geq 0$ should be satisfied for a separable state, where ρ^{T_A} stands for a partial transpose with respect to the subsystem A. $\rho^{T_A} \geq 0$ is further shown by Horodecki *et al.* [3] to be sufficient for 2×2 and 2×3 bipartite systems. $\|\rho^{T_A}\|$ is LU invariant as shown in Refs. [2,19] where $\|\cdot\|$ stands for the trace norm defined by $\|G\| = \mathrm{Tr}(GG^\dagger)^{1/2}$. Thus, it is sufficient to consider only the pure states with standard Schmidt form given by Eq. (2). It is easy to see that $\rho = |\psi\rangle\langle\psi| = \sum_{i,j}\sqrt{\mu_i\mu_j}|a_i b_i\rangle\langle a_j b_j|$ and $\rho^{T_A} = \sum_{i,j}\sqrt{\mu_i\mu_j}|a_j^* b_i\rangle\langle a_i^* b_j|$. Then we arrive at

$$\begin{aligned}\|\rho^{T_A}\| &= \|\sum_{i,j}\sqrt{\mu_i\mu_j}\,|a_j^* b_i\rangle\langle b_j a_i^*|\| \\ &= \|\sum_j \sqrt{\mu_j}\,|a_j^*\rangle\langle b_j| \otimes \sum_i \sqrt{\mu_i}\,|b_i\rangle\langle a_i^*|\| \\ &= \|G \otimes G^\dagger\| = \|G\|^2 = \Big(\sum_i \sqrt{\mu_i}\Big)^2. \end{aligned} \tag{4}$$

where $G = \sum_j \sqrt{\mu_j}|a_j^*\rangle\langle b_j|$. In this derivation we have used the unitarily invariant property of the trace norm when applying the elementary column transformation: $\langle a_i^* b_j| \to \langle b_j a_i^*|$ in the derivation of the first formula. The last formula is obtained from the observation that $GG^\dagger = \sum_{i,j}\sqrt{\mu_i\mu_j}\,|a_i^*\rangle\langle b_i| \cdot |b_j\rangle\langle a_j^*| = \sum_i \mu_i |a_i^*\rangle\langle a_i^*|$, the property of the trace norm $\|P \otimes Q\| = \|P\| \cdot \|Q\|$ and the fact that $\|G\|$ is the sum of the square root of eigenvalues μ_i of $GG^\dagger$.

Another complementary operational criterion for separability called the *realignment* criterion is very strong in detecting many of BES [6,7] and even genuinely tripartite entanglement [8]. Recently there has been considerable progress in the further analysis, and in finding stronger variants and multipartite generalizations for this criterion [9]. We recall that this criterion states that a realigned version $\mathcal{R}(\rho)$ of ρ should satisfy $\|\mathcal{R}(\rho)\| \leq 1$ for any separable state ρ. $\mathcal{R}(\rho)$ is simply $\mathcal{R}(\rho)_{ij,kl} = \rho_{ik,jl}$ where i and j are the row and column indices for the subsystem A respectively, while k and l are such indices for the subsystem B [6–8]. $\|\mathcal{R}(\rho)\|$ is also shown to be LU invariant in [7]. One has $\mathcal{R}(\rho) = \sum_{i,j}\sqrt{\mu_i\mu_j}|a_i a_j^*\rangle\langle b_i^* b_j|$ for the state Eq. (2), as follows easily from the definition. Similar to (4) one has

$$\begin{aligned}\|\mathcal{R}(\rho)\| &= \Big\|\sum_i \sqrt{\mu_i}\,|a_i\rangle\langle b_i^*| \otimes \sum_j \sqrt{\mu_j}\,|a_j^*\rangle\langle b_j|\Big\| \\ &= \|G \otimes G^*\| = \|G\|^2 = \Big(\sum_i \sqrt{\mu_i}\Big)^2. \end{aligned} \tag{5}$$

where $G = \sum_i \sqrt{\mu_i}|a_i\rangle\langle b_i^*|$. The last formula follows from the observation $GG^\dagger = \sum_{i,j}\sqrt{\mu_i\mu_j}|a_i\rangle\langle b_i^*| \cdot |b_j^*\rangle \times \langle a_j| = \sum_i \mu_i |a_i\rangle\langle a_i|$.

We now derive the main result of this Letter.

Theorem.—For any $m \otimes n (m \leq n)$ mixed quantum state ρ, the concurrence $C(\rho)$ satisfies

$$C(\rho) \geq \sqrt{\frac{2}{m(m-1)}}(\max(\|\rho^{T_A}\|, \|\mathcal{R}(\rho)\|) - 1). \tag{6}$$

Proof.—To obtain the desired lower bound, let us assume that one has already found an optimal decomposition $\sum_i p_i \rho^i$ for ρ to achieve the infimum of $C(\rho)$, where ρ^i are pure state density matrices. Then $C(\rho) = \sum_i p_i C(\rho^i)$ by definition. Noticing that $\|\rho^{T_A}\| \leq \sum_i p_i \|(\rho^i)^{T_A}\|$ and $\|\mathcal{R}(\rho)\| \leq \sum_i p_i \|\mathcal{R}(\rho^i)\|$ due to the convex property of the trace norm, one needs to show $C(\rho^i) \geq \sqrt{2/(m(m-1))}(\|(\rho^i)^{T_A}\| - 1)$ and $C(\rho^i) \geq \sqrt{2/(m(m-1))}(\|\mathcal{R}(\rho^i)\| - 1)$. For a pure state ρ^i one has $\|\mathcal{R}(\rho^i)\| = \|(\rho^i)^{T_A}\| = (\sum_k \sqrt{\mu_k})^2$ from Eqs. (4) and (5), where $\sqrt{\mu_k}$ are the Schmidt coefficients for the pure state ρ^i. From the expression of Eq. (3) it remains to prove that

$$\begin{aligned}4\sum_{i<j}\mu_i\mu_j &\geq \frac{2}{m(m-1)}\Big(\Big(\sum_k \sqrt{\mu_k}\Big)^2 - 1\Big)^2 \\ &= \frac{8}{m(m-1)}\Big(\sum_{i<j}\sqrt{\mu_i\mu_j}\Big)^2, \end{aligned} \tag{7}$$

where we have used $\sum_i \mu_i = 1$.

The verification of the inequality Eq. (7) is straightforward: by summing over all of arithmetic mean inequalities $\mu_i\mu_j + \mu_k\mu_l \geq 2\sqrt{\mu_i\mu_j\mu_k\mu_l}$ for $i < j$ and $k < l$, one gets

$$\begin{aligned}\sum_{i<j}\sum_{k<l}(\mu_i\mu_j + \mu_k\mu_l) &\geq 2\sum_{i<j}\sum_{k<l}\sqrt{\mu_i\mu_j\mu_k\mu_l} \\ &= 2\Big(\sum_{i<j}\sqrt{\mu_i\mu_j}\Big)^2. \end{aligned} \tag{8}$$

It is seen that the number of appearance times is $m(m-1)$ for the term $\mu_i\mu_j$ on the left-hand side of Eq. (8). Therefore Eq. (7) is confirmed and the conclusion, Eq. (6) is proved.

The most prominent feature of the Theorem is that it allows us to obtain an analytical lower bound for the concurrence without any numerical optimization procedure. The bound has the same range as $C(\rho)$ and goes from 0 to $\sqrt{2(m-1)/m}$ for pure product states and maximally entangled pure states, respectively. One can of course renormalizes the maximum value $C(\rho)$ to be 1 with a change of the corresponding constant factor.

We highlight some of the benefits of this new bound. First, it serves to detect and gives a lower bound of concurrence for *all* entangled states of two qubits and qubit-qutrit system. This is so because the PPT criterion is necessary and sufficient for separability in the two cases [3]. Second, it generalizes to bipartite systems of arbitrary dimension a relation given in [20] which is only valid for the two qubits case, that the concurrence is lower bounded by the negativity [19] (defined to be $\|\rho^{T_A}\| - 1$). Third, for any qubit-qudit system our bound can contribute an analytical lower bound for EOF which is a convex function of the concurrence, $E(|\psi\rangle) = H_2([1+\sqrt{1-C^2(|\psi\rangle)}]/2)$ where $H_2(\cdot)$ is the binary entropy function [11]. In fact our bound can furnish a lower bound of EOF $E(\rho)$ for the arbitrary bipartite state ρ [13]. Given any monotonously increasing, convex function $\mathcal{E}$ satisfying $\mathcal{E}[C(|\psi\rangle)] \leq -\Sigma_r \mu_r \log_2 \mu_r$, one has $E(\rho) \geq \mathcal{E}[C(\rho)]$, with the right-hand side bounded from below by our bound Eq. (6). Next we consider some examples to illustrate further the tightness and significance of our bound.

*Example 1:*Isotropic states.

Isotropic states [21,22] are a class of $U \otimes U^*$ invariant mixed states in $d \times d$ systems

$$\rho_F = \frac{1-F}{d^2-1}(I - |\Psi^+\rangle\langle\Psi^+|) + F|\Psi^+\rangle\langle\Psi^+|, \quad (9)$$

where $|\Psi^+\rangle \equiv \sqrt{1/d}\Sigma_{i=1}^d |ii\rangle$ and $F = \langle\Psi^+|\rho_F|\Psi^+\rangle$, satisfying $0 \leq F \leq 1$, is the *fidelity* of ρ_F and $|\Psi^+\rangle$. These states were shown to be separable for $F \leq 1/d$ [21]. It is shown in [6,19] that $\|\rho_F^{T_A}\| = \|\mathcal{R}(\rho_F)\| = dF$ for $F > 1/d$. The concurrence $C(\rho)$ for this class of states is recently derived in [23] to be $\sqrt{2d/(d-1)}(F - 1/d)$ by an extremization procedure. An application of our Theorem gives $C(\rho) \geq \sqrt{2/[d(d-1)]}(dF-1) = C(\rho)$. Thus, the bound gives a surprisingly exact value of the concurrence for this sort of state.

Remark.—One can see that the equality of Eq. (8) holds when $|\psi\rangle$ are product states or maximally entangled states (MES) (all μ_i are equal). Thus our bound will be tight if an optimal decomposition for achieving concurrence only involves product states and MES, and also attains the value of $\|\rho^{T_A}\|$ or $\|\mathcal{R}(\rho)\|$. Roughly speaking, the difference between our lower bound and the exact value of concurrence will be small if there are few deviations from these two types of states in the optimal ensemble decomposition. Exact estimation of this difference would be an interesting subject for future study. In the case of isotropic states, it is shown in [23] that the optimal decomposition falls exactly into this class and the concurrence is just our bound.

Example 2:3×3 BES constructed from unextendible product bases (UPB).

In [24], Bennett *et al.* introduced a 3×3 BES from the following bases:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|0\rangle(|0\rangle - |1\rangle), \qquad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)|2\rangle,$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}|2\rangle(|1\rangle - |2\rangle), \qquad |\psi_3\rangle = \frac{1}{\sqrt{2}})|1\rangle - |2\rangle)|0\rangle,$$

$$|\psi_4\rangle = \frac{1}{3}(|0\rangle + |1\rangle + |2\rangle)(|0\rangle + |1\rangle + |2\rangle),$$

from which the density matrix could be expressed as

$$\rho = \frac{1}{4}\left(Id - \sum_{i=0}^{4}|\psi_i\rangle\langle\psi_i|\right). \quad (10)$$

A simple calculation gives $\|\rho^{T_A}\| = 1$ and $\|\mathcal{R}(\rho)\| = 1.087$ [7], therefore, $C(\rho) \geq 0.05$ according to the Theorem. This shows that the state is entangled.

When BES are constructed from the UPB [24] given by $|\psi_j\rangle = |\vec{v}_j\rangle \otimes |\vec{v}_{2j\text{mod}5}\rangle$, $(j = 0, \ldots, 4)$ with $\vec{v}_j = N[\cos(2\pi j/5), \sin(2\pi j/5), h]$, with $j = 0, \ldots 4$, $h = \sqrt{1+\sqrt{5}}/2$, and $N = 2/\sqrt{5+\sqrt{5}}$, then the PPT state of Eq. (10) gives $\|\rho^{T_A}\| = 1$ and $\|\mathcal{R}(\rho)\| = 1.098$ [7], therefore, $C(\rho) \geq 0.056$ according to the Theorem, which identifies this BES.

It is conjectured by Audenaert *et al.* that the optimization method for concurrence is a necessary and sufficient for separability when one considers all possible complex linear combination of the concurrence-vectors [5]. Our numerical verification suggests a disproval for this conjecture, because of the failure to identify entanglement by applying their optimization method for the above two UPB states. Thus the direct estimation method for concurrence in [5] may not be able to detect *all* entangled states through numerical optimizations. Here our Theorem complements other existing approaches to make a quite good estimate of entanglement for BES.

*Example 3:*Horodecki's 3×3 entangled state.

A mixed two qutrits is introduced in [25]:

$$\sigma_\alpha = \frac{2}{7}|\Psi^+\rangle\langle\Psi^+| + \frac{\alpha}{7}\sigma + \frac{5-\alpha}{7}\sigma_-, \quad (11)$$

where

$$\sigma_+ = \frac{1}{3}(|0\rangle|1\rangle\langle 0|\langle 1| + |1\rangle|2\rangle\langle 1|\langle 2| + |2\rangle|0\rangle\langle 2|\langle 0|),$$

$$\sigma_- = \frac{1}{3}(|1\rangle|0\rangle\langle 1|\langle 0| + |2\rangle|1\rangle\langle 2|\langle 1| + |0\rangle|2\rangle\langle 0|\langle 2|),$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{3}}(|0\rangle|0\rangle + |1\rangle|1\rangle + |2\rangle|2\rangle). \quad (12)$$

In [25] Horodecki *et al.* demonstrate that the states Eq. (11) admit a simple characterization with respect to the parameter $2 \leq \alpha \leq 5$: separable for $2 \leq \alpha \leq 3$; bound entangled for $3 < \alpha \leq 4$; free entangled for $4 < \alpha \leq 5$. It is computed by using the realignment criterion in [6] that

$\|\mathcal{R}(\sigma_\alpha)\| = (19 + 2\sqrt{3\alpha^2 - 15\alpha + 19}/21$ and one can recognize all the entangled states for $3 < \alpha \leq 5$. One can obtain further that $\|\sigma_\alpha^{T_A}\| = 1$ for $2 \leq \alpha \leq 4$ and $\|\sigma_\alpha^{T_A}\| = (2 + \sqrt{4\alpha^2 - 20\alpha + 41}/7$ for $4 < \alpha \leq 5$. Therefore one has $C(\sigma_\alpha) \geq 1/\sqrt{3}[\|\mathcal{R}(\sigma_\alpha)\| - 1] = 2\sqrt{3}(\sqrt{3\alpha^2 - 15\alpha + 19} - 1)/63$ due to the observation that $\|\mathcal{R}(\sigma_\alpha)\|$ is always greater than $\|\sigma_\alpha^{T_A}\|$ in the entangled region $3 < \alpha \leq 5$.

However, the concurrence optimization procedure proposed in [13] can only identify the entangled states for $3.52 \lesssim \alpha \leq 5$ [13]. This suggests that Mintert *et al.*'s methods may not be necessary and sufficient for detecting entanglement. A rough comparison with the result of [13] shows that our lower bound is much better than their optimized bound in the entangled region of $3 < \alpha \lesssim 4.75$, though a little bit weaker than theirs in the region $4.75 \lesssim \alpha \leq 5$.

We remark that, like any other known approaches, there are also some drawbacks for our estimation. Our lower bound cannot detect all the entangled states due to limitation of the PPT criterion and the realignment criterion. For example, it can neither recognize the 2×4 Horodecki BES [26], which instead can be detected by the methods of [13], nor give the exact value of concurrence for 2 qubits known from [4,13].

In summary, we have provided an entirely analytical formula for a lower bound of concurrence, by making a novel connection with the known strong separability criteria. The bound leads to actual values of concurrence for some special class of quantum states. One only needs to calculate the trace norm of certain matrices, which avoids a complicated optimization procedure over a large number of free parameters in numerical approaches. The formula also permits us to furnish lower bounds of EOF for arbitrary bipartite quantum state. This complements the nice result of Wootters for 2 qubits, as well as a number of existing optimization methods for concurrence. Profiting from the strong realignment criterion, our bound can give easy entanglement evaluation for many BES, which fail to be recognized by the regular optimization methods. This shows that our method can serve as a powerful tool for investigating both static and dynamical entanglement properties in realistic quantum computing devices. Possible applications for the method could be indicating a possible quantum phase transition for a condensed matter system, and analyzing finite size or scaling behavior of entanglement in various interacting quantum many-body systems.

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