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Abstract We present a set of inequalities based on mean values of quantum mechanical observables nonlinear entanglement witnesses for bipartite quantum systems. These inequalities give rise to sufficient and necessary conditions for separability of all bipartite pure states and even some mixed states. In terms of these mean values of quantum mechanical observables a measurable lower bound of the convex-roof extension of the negativity is derived.

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Entanglement is not only the characteristic trait of quantum mechanics, but also a vital resource for many aspects of quantum information processing such as quantum computation, quantum metrology, and quantum communication[1]. One of the fundamental problems in quantum entanglement theory is to determine which states are entangled and which are not, either theoretically or experimentally. The entanglement witness [2, 3] is the most useful approach to characterize quantum entanglement experimentally. In recent years there have been considerable efforts in constructing and analyzing the structure of entanglement witness (see [4, 5, 6, 7, 8] and the references therein). Generally the Bell inequalities [9, 10, 11, 12, 13, 14] can be recast as entanglement witnesses. Better entanglement witnesses can be also constructed from more effective Bell-type inequalities.

On the other side, to quantify quantum entanglement is also a significant problem in quantum information theory. A number of entanglement measures such as the entanglement of formation and distillation [15, 16, 17], negativity [18] and relative entropy [17, 19] have been proposed for bipartite systems [16] [19]-[24]. The negativity was derived from the positive partial transposition (PPT) [25]. It bounds two relevant quantities characterizing the entanglement of mixed states: the channel capacity and the distillable entanglement. The convex-roof extension of the negativity

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(CREN) [26] gives a better characterization of entanglement, which is nonzero for PPT entangled quantum states.

In this paper, similar to the non-linear entanglement witnesses and Bell-type inequalities, we present a set of inequalities based on mean values of quantum mechanical observables, which can serve as necessary and sufficient conditions for the separability of bipartite pure quantum states and the isotropic states. These inequalities are also closely related to the measure of quantum entanglement. According to the violation of these inequalities, we derive an experimentally measurable lower bound for the convex-roof extension of the negativity.

We first give a brief review of the 3-setting nonlinear entanglement witnesses enforced by the indeterminacy relation of complementary local observables for two-qubit systems [7]. For a two-level system there are three mutually complementary observables $A_i = \vec{a}_i \cdot \vec{\sigma}$, where $\vec{a}_i$, $i = 1, 2, 3$, are three normalized vectors that are orthogonal to each other, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. $\mu_A = -iA_1A_2A_3$ is the so called orientation of A_is. μ_A takes values ± 1. Similarly, one can define three mutually complementary observables $B_i = \vec{b}_i \cdot \vec{\sigma}$ ($i = 1; 2; 3$) with the corresponding orientations μ_B. It has been shown that [7]: (i) A 2-qubit state ρ is separable if and only if the following inequality holds for all sets of observables $\{A_i, B_i\}_{i=1;2;3}$ with the same orientation:

$$\sqrt{\langle A_1B_1 + A_2B_2\rangle_\rho^2 + \langle A_3 + B_3\rangle_\rho^2} - \langle A_3B_3\rangle_\rho \leq 1; \tag{1}$$

(ii) For a given entangled state the maximal violation of the above inequality is $1 - 4\lambda_{\min}$, with $\lambda_{\min}$ being the minimal eigenvalue of the partially transposed density matrix. The maximal possible violation for all states is 3, which is attainable by the maximal entangled states.

For qubit-qutrit systems, a similar inequality has been presented in [8], which detects quantum entanglement also necessarily and sufficiently. However the approaches in [7] and [8] can not be directly generalized to higher dimensional systems, since it is based on the PPT criterion that is both necessary and sufficient only for separability of two-qubit and qubit-qutrit states. For general higher dimensional $M \times N$ bipartite quantum systems a new approach has been employed in [14]. Let $\rho \in \mathcal{H}_{\mathcal{AB}}$ be any pure quantum states in vector space $\mathcal{H}_{\mathcal{AB}} = \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ with dimensions $dim\,\mathcal{H}_{\mathcal{A}} = M$ and $dim\,\mathcal{H}_{\mathcal{B}} = N$ respectively. Assume L_α^A and L_β^B be the generators of special orthogonal groups $SO(M)$ and $SO(N)$ respectively. The $M(M-1)/2$ generators L_α^A are given by $\{|j\rangle\langle k| - |k\rangle\langle j|\}$, $1 \leq j < k \leq M$, where $|i\rangle$, $i = 1, ..., M$, is the usual canonical basis of $\mathcal{H}_{\mathcal{A}}$, a column vector with the ith row 1 and the rest zeros. L_β^B can be similarly defined. The matrix operators L_α^A (resp. L_β^B) have $M-2$ (resp. $N-2$) rows and $M-2$ (resp. $N-2$) columns that are identically zero. We define the operators A_i^α (resp. B_j^β) from L_α (resp. L_β) by replacing the four entries in the positions of the two nonzero rows and two nonzero columns of L_α (resp. L_β) with the corresponding four entries of the matrix $\vec{a}_i \cdot \vec{\sigma}$ (resp. $\vec{b}_j \cdot \vec{\sigma}$), and keeping the other entries of A_i^α (resp. B_j^β) zero.

By using L_α^A and L_β^B the pure state ρ can be projected to "two-qubit" ones [14]:

$$\rho_{\alpha\beta} = \frac{L_\alpha^A \otimes L_\beta^B \rho (L_\alpha^A)^\dagger \otimes (L_\beta^B)^\dagger}{\mathrm{Tr}\{L_\alpha^A \otimes L_\beta^B \rho (L_\alpha^A)^\dagger \otimes (L_\beta^B)^\dagger\}}, \tag{2}$$

where $\alpha = 1, 2, \cdots, \frac{M(M-1)}{2}; \beta = 1, 2, \cdots, \frac{N(N-1)}{2}$. As the matrix $L_\alpha^A \otimes L_\beta^B$ has $MN - 4$ rows and $MN - 4$ columns that are identically zero, one can directly verify that there are at most $4 \times 4 = 16$ nonzero elements in each matrix $\rho_{\alpha\beta}$. For every pure state $\rho_{\alpha\beta}$ the corresponding Bell operators are defined by

$$\mathcal{B}_{\alpha\beta} = \tilde{A}_1^\alpha \otimes \tilde{B}_1^\beta + \tilde{A}_1^\alpha \otimes \tilde{B}_2^\beta + \tilde{A}_2^\alpha \otimes \tilde{B}_1^\beta - \tilde{A}_2^\alpha \otimes \tilde{B}_2^\beta, \tag{3}$$

where $\tilde{A}_i^\alpha = L_\alpha^A A_i^\alpha (L_\alpha^A)^\dagger$ and $\tilde{B}_j^\beta = L_\beta^B B_j^\beta (L_\beta^B)^\dagger$ are Hermitian operators. It has been shown that any bipartite pure quantum state is entangled if and only if at least one of the following inequalities is violated [14],

$$|\langle \mathcal{B}_{\alpha\beta} \rangle| \leq 2. \tag{4}$$

Inequalities (4) work only for general high dimensional bipartite pure states. Combining the approaches in [7] and [14], we now define the mean value of nonlinear operators $\mathcal{B}'_{\alpha\beta}$,

$$\langle \mathcal{B}'_{\alpha\beta} \rangle = \sqrt{\langle \tilde{A}_1^\alpha \tilde{B}_1^\beta + \tilde{A}_2^\alpha \tilde{B}_2^\beta \rangle_\rho^2 + \langle \tilde{A}_3^\alpha + \tilde{B}_3^\beta \rangle_\rho^2} - \langle \tilde{A}_3^\alpha \tilde{B}_3^\beta \rangle_\rho, \tag{5}$$

for high dimensional bipartite mixed states.

Theorem 1: Any bipartite quantum state $\rho \in \mathcal{H}_{\mathcal{AB}}$ is entangled if any one of the following inequalities,

$$\frac{1}{\mathrm{Tr}(L_\alpha \otimes L_\beta \rho^{T_A} L_\alpha \otimes L_\beta)} |\langle \mathcal{B}'_{\alpha\beta} \rangle| \leq 1, \tag{6}$$

is violated, where $\alpha = 1, 2, \cdots, \frac{M(M-1)}{2}, \beta = 1, 2, \cdots, \frac{N(N-1)}{2}$.

Proof: Assume that ρ is separable (not entangled) quantum state. Since the separability of a state does not change under the local operation $L_{\alpha_0}^A \otimes L_{\beta_0}^B$, one has that for any α and β, $\rho_{\alpha\beta} = \frac{L_\alpha^A \otimes L_\beta^B \rho (L_\alpha^A)^\dagger \otimes (L_\beta^B)^\dagger}{\mathrm{Tr}\{L_\alpha^A \otimes L_\beta^B \rho (L_\alpha^A)^\dagger \otimes (L_\beta^B)^\dagger\}}$, which can be treated as a two qubits state, must be also separable. According to the analysis in [7], a 2-qubit state ρ is separable if and only if (1) holds, which contradicts with the condition (6). Thus we have that if any one of the inequalities (6) is violated, ρ must be an entangled quantum state. □

It is obvious that the inequalities (6) must not be weaker than the Bell inequalities given in [14] for detecting entanglement of mixed quantum states, since (6) supplies a sufficient and necessary condition for separability of two qubits (mixed) quantum states, while violating the CHSH inequality is just a sufficient condition for two-qubit entanglement. Actually, (6) is strictly stronger, as seen from the following examples.

Example 1 We consider a 3×3 dimensional state introduced in [27] by Bennett et al. Set $|\xi_0\rangle = \frac{1}{\sqrt{2}}|0\rangle(|0\rangle - |1\rangle)$, $|\xi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)|2\rangle$, $|\xi_2\rangle = \frac{1}{\sqrt{2}}|2\rangle(|1\rangle - |2\rangle)$, $|\xi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)|0\rangle$, $|\xi_4\rangle = \frac{1}{3}(|0\rangle + |1\rangle + |2\rangle)(|0\rangle + |1\rangle + |2\rangle)$. Let

$$\rho = \frac{1}{4}(I_9 - \sum_{i=0}^{4} |\xi_i\rangle\langle\xi_i|).$$

This state is entangled according to the realignment criterion [28]. We consider the mixture of ρ and the maximal entangled singlet $P_+ = |\psi_+\rangle\langle\psi_+|$, where $|\psi_+\rangle = \frac{1}{\sqrt{3}}\sum_{i=0}^{2}|ii\rangle$:

$$\rho_p = (1-p)\rho + pP_+. \tag{7}$$

By straightforward computation, the bell inequalities (4) detect entanglement for $0.57602 \le p \le 1$, while (6) detect entanglement for $0.18221 \le p \le 1$.

Example 2 Consider the state

$$\rho_p(a) = (1-p)\rho(a) + pP_+, \tag{8}$$

where

$$\rho(a) = \frac{1}{8a+1}\begin{pmatrix} a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+a}{2} & 0 & \frac{\sqrt{1-a^2}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 \\ a & 0 & 0 & 0 & a & 0 & \frac{\sqrt{1-a^2}}{2} & 0 & \frac{1+a}{2} \end{pmatrix},$$

is the weakly inseparable state given in [29], $0 < a < 1$.

Take $a = 0.236$, which is the case that $\rho(a)$ violates the realignment criterion [28] maximally. From Fig.1 we see that the bell inequalities (4) detect entanglement for $0.26 \le p \le 1$, while (6) detect entanglement for the whole region of $0 < p \le 1$.

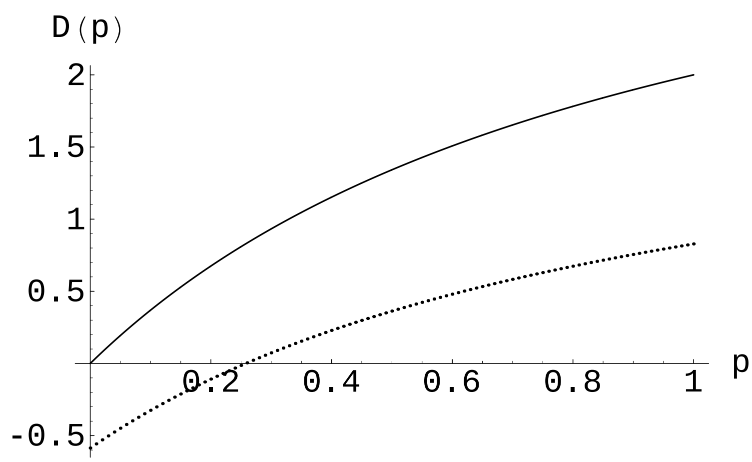

Figure 1: The differences $D(p)$ between the right and the left sides of the inequalities (6) (solid line) and the Bell inequalities (4) (doted line).

Example 3 Isotropic states [30] with dimensions $M = N = d$ can be written as the mixtures of the maximally mixed state and the maximally entangled state $|\psi_+\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |ii\rangle$,

$$\rho = \frac{1-x}{d^2} I_d \otimes I_d + x|\psi_+\rangle\langle\psi_+|. \tag{9}$$

The inequalities (6) can detect the entanglement for $x \leq \frac{1}{d+1}$ which agrees with the result in [30]. Thus (6) serves as a sufficient and necessary condition of separability for isotropic states.

The inequalities (6) not only can be used to detect entanglement, but also have some direct relations with the negativity. The negativity of a bipartite quantum states ρ with dimensions $d(H_A) = M$ and $d(H_B) = N$ $(M \leq N)$ is defined by [31]

$$\mathcal{N}(\rho) = \frac{\|\rho^{T_A}\| - 1}{M-1}, \tag{10}$$

where ρ^{T_A} is the partial transpose of ρ and $\|R\| = \mathrm{Tr}\sqrt{RR^\dagger}$ stands for the trace norm of matrix R. The negativity is defined based on the positive partial transpose criterion (PPT) [25] which can not detect the PPT bound entanglement. Thus it is not sufficient for the negativity to be a good measure of entanglement. Lee et al in [26] introduced the convex-roof extension of the negativity (CREN) $\mathcal{N}_m(\rho)$. For pure bipartite quantum states $|\psi\rangle$, $\mathcal{N}_m(|\psi\rangle)$ is exactly the negativity $\mathcal{N}(|\psi\rangle)$ defined in (10). For a mixed bipartite quantum state ρ the CREN is defined by

$$\mathcal{N}_m(\rho) = \min \sum_k p_k \mathcal{N}_m(|\psi_k\rangle), \tag{11}$$

where the minimum is taken over all the ensemble decompositions of $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$.

The CREN can detect the PPT bound entanglement, since it is zero if and only if the corresponding quantum state is separable. Lee et al also show that $\mathcal{N}_m(\rho)$ does not increase under local quantum operations and classical communication. However, generally it is very difficult to calculate CREN analytically. Here we present an experimentally measurable tight lower bound of CREN for arbitrary bipartite quantum states, in terms of the violation of the inequalities (6).

Theorem 2: For any bipartite quantum states $\rho \in \mathcal{H}_{\mathcal{AB}}$,

$$\mathcal{N}_m(\rho) \geq \frac{1}{M-1} \sum_{\alpha\beta} |C_{\alpha\beta}| \left(\frac{X(\rho_{\alpha\beta})}{2} + 1\right) - (M-1), \tag{12}$$

where $C_{\alpha\beta} = \mathrm{Tr}(L_\alpha \otimes L_\beta \rho^{T_A} L_\alpha \otimes L_\beta)$, $X(\rho_{\alpha\beta}) = \min\{0, d(\rho_{\alpha\beta})\}$, and $d(\rho_{\alpha\beta}) = \frac{1}{\mathrm{Tr}(L_\alpha \otimes L_\beta \rho^{T_A} L_\alpha \otimes L_\beta)} |\langle \mathcal{B}'_{\alpha\beta}\rangle| - 1$ stands for the difference of the left and right side of the inequalities (6).

Proof: Let $|\psi\rangle = \sum_i \sqrt{\mu_i}|ii\rangle$ be a bipartite pure state in Schmidt form. One has

$$\mathcal{N}_m(|\psi\rangle) = \frac{2}{M-1} \sum_{i<j} \sqrt{\mu_i \mu_j}. \tag{13}$$

Note that $\sum_i \mu_i = 1$. By calculating the trace norm of $L_\alpha \otimes L_\beta (|\psi\rangle\langle\psi|)^{T_A} L_\alpha \otimes L_\beta$ for each α and β, we derive that

$$\sum_{\alpha\beta} \|C_{\alpha\beta}^{|\psi\rangle} (|\psi\rangle_{\alpha\beta}\langle\psi|)^{T_A}\| = (M-1)^2 + 2\sum_{i<j} \sqrt{\mu_i \mu_j}, \tag{14}$$

where $|\psi\rangle_{\alpha\beta} = \frac{L_\alpha \otimes L_\beta |\psi\rangle}{\sqrt{C_{\alpha\beta}^{|\psi\rangle}}}$ and $C_{\alpha\beta}^{|\psi\rangle} = \mathrm{Tr}\{L_\alpha \otimes L_\beta |\psi\rangle\langle\psi| L_\alpha \otimes L_\beta\}$.

Let $\rho = \sum_k p_k \rho_k = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ be the optimal decomposition which fulfills that $\mathcal{N}_m(\rho)$ attains its minimum. In terms of (13) and (14) we get

$$\begin{aligned}
\mathcal{N}_m(\rho) &= \sum_k p_k N(\rho_k) \\
&= \frac{1}{M-1} \sum_k p_k \sum_{\alpha\beta} \| C_{\alpha\beta}^k (\rho_{\alpha\beta}^k)^{T_A} \| - (M-1) \\
&\geq \frac{1}{M-1} \sum_{\alpha\beta} \| \sum_k p_k\, C_{\alpha\beta}^k (\rho_{\alpha\beta}^k)^{T_A} \| - (M-1) \\
&= \frac{1}{M-1} \sum_{\alpha\beta} \| \sum_k p_k\, L_\alpha \otimes L_\beta \rho_k^{T_A} L_\alpha \otimes L_\beta \| - (M-1) \\
&= \frac{1}{M-1} \sum_{\alpha\beta} \| L_\alpha \otimes L_\beta \rho^{T_A} L_\alpha \otimes L_\beta \| - (M-1) \\
&= \frac{1}{M-1} \sum_{\alpha\beta} |C_{\alpha\beta}|\, \| \rho_{\alpha\beta}^{T_A} \| - (M-1) \\
&= \frac{1}{M-1} \sum_{\alpha\beta} |C_{\alpha\beta}| (\frac{X(\rho_{\alpha\beta})}{2} + 1) - (M-1),
\end{aligned}$$

where we have used that $\|\rho_{\alpha\beta}^{T_A}\|$ has at most one negative eigenvalue (see [32]) in deriving the last equation. □

Remark: For the isotropic states (9) our lower bound (12) shows that $\mathcal{N}_m(\rho) \geq \frac{4x-1}{3}$, which matches with the formula derived in [26]. Thus in this case the lower bound is exact for CREN. Moreover, our lower bound is experimentally measurable, in the sense that $C_{\alpha\beta} = \mathrm{Tr}(L_\alpha \otimes L_\beta\, \rho^{T_A} L_\alpha \otimes L_\beta) = \mathrm{Tr}(L_\alpha \otimes L_\beta\, \rho L_\alpha \otimes L_\beta)$ is the mean value of the Hermitian operator $L_\alpha L_\alpha^\dagger \otimes L_\beta L_\beta^\dagger$, and $X(\rho_{\alpha\beta}) = \min\{0, d(\rho_{\alpha\beta})\}$ is determined by the mean value of the operator $\mathcal{B}'_{\alpha\beta}$. On the other hand, according to the proof of the theorem the lower bound (12) for pure bipartite quantum states is also exact. Thus based on the continuity of the CREN, for weakly mixed quantum state ρ with $\mathrm{Tr}\{\rho^2\} \approx 1$, (12) supplies a good estimation of the CREN.

In conclusion, we have derived a set of inequalities that can detect better entanglement of quantum mixed states. These inequalities serve as sufficient and necessary conditions for separability for all bipartite pure states and the isotropic states. Nevertheless, generally bound entangled states can not be detected by these inequalities. We also find that these inequalities have close relations with the convex-roof extension of the negativity. A measurable lower bound for the convex-roof extension of the negativity has been obtained.

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