Boundary of the Set of Separable States

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Abstract

The set of all separable quantum states is compact and convex. We focus on the two-qubit quantum system and study the boundary of the set. Then we give the criterion to determine whether a separable state is on the boundary. Some straightforward geometrical interpretations for entanglement are based on the concept and presented subsequently.

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1. INTRODUCTION

Entanglement and nonlocality are some of the most emblematic concepts embodied in quantum mechanics [1,2]. Recent developments in quantum computation [3,4] and quantum information (e.g. [5–7]) evoke interest in the properties of quantum entanglement.

Now we have known that a state of a composite quantum system is called entangled (or inseparable) if it cannot be represented as a convex combination of tensor products of its subsystem states [4,8]. In the case of pure states, one has obtained a complete understanding, that is, a pure state is entangled if and only if it violates Bell’s inequality [3,11]. But the case for mixed states is much more complicated (e.g. [12,13]). Besides the above definition of entangled state, another qualitative criterion proposed by Peres [14] is more practicable to determine whether a given state is inseparable, although it is sufficient and necessary only for some simple quantum system, such as $2 \times 2$ and $2 \times 3$ systems. On the other hand, one is more interested in the quantitative measure of entangled states. Various entanglement measure has been proposed. For example, for two-party system, there are following kinds of measure: the entanglement of formation [4], the relative entropy of entanglement [15,16], and the robustness of entanglement [17], etc.

Consider the relative entropy associated with entangled state $\rho_e$ of two-qubit system. In order to obtain the relative entropy of entanglement of $\rho_e$, the crucial point is to find a separable state $\rho_s$ such that minimizes the relative entropy $S(\rho_e \parallel \rho_s)$ defined as
\[ S(\rho_e \parallel \rho_s) = tr \left\{ \rho_e \ln \frac{\rho_e}{\rho_s} \right\}. \] (1)

In general case, to find \( \rho_s \) is a laborious work.

Then recall the robustness of entanglement. It is said that given an entangled state \( \rho_e \) and a separable state \( \rho_s \) there always exists a minimal real \( s \geq 0 \) for which

\[ \rho(s) = \frac{1}{1 + s} (\rho_e + s \rho_s) \] (2)

is separable. Such minimal \( s \), denoted by \( R(\rho_e \parallel \rho_s) \), is called robustness of \( \rho_e \) relative to \( \rho_s \).

Then the entanglement embodied in \( \rho_e \) can be measured by the absolute robustness of \( \rho_e \), which is obtained by means of finding a separable state \( \rho_s' \) such that \( R(\rho_e \parallel \rho_s') \) is minimal.

We can see that both in relative entropy and in robustness, finding a specific separable state is of essence.

Additionally, let’s consider another useful tool to study entanglement, i.e., Lewenstein-Sanpera (L-S) decomposition \[\text{[18]}\]. Lewenstein et.al. have shown that any state of two-qubit system can be decomposed as

\[ \rho = \lambda \rho_s + (1 - \lambda) P_e, \quad \lambda \in [0,1], \] (3)

where \( \rho_s \) is a separable state, and \( P_e \) denotes a single pure entangled projector \( (P_e = |\Psi_e\rangle \langle \Psi_e|) \), that is, \( P_e \) represents a pure entangled state. It is known that there are many different L-S decomposition with varying values of \( \lambda \) and various \( P_e \)'s. Among them is the unique optimal decomposition, the one with the largest \( \lambda \) value in Eq. (3),

\[ \rho = S \rho_s^{(opt)} + (1 - S) P_e^{(opt)}, \] (4)

where

\[ S = \max \{\lambda\} \]

is the degree of separability possessed by \( \rho \). In other words, the entanglement possessed by \( \rho \) can be represented as \( (1 - S) E(\Psi_e) \), where \( E(\Psi_e) \) is the entanglement of its pure state.
expressed in terms of the von Neumann entropy of the reduced density matrix of either of its subsystems:

\[ E(\Psi_e) = -tr(\rho_A \log \rho_A) = -tr(\rho_B \log \rho_B). \] (5)

Here again, in the sense of maximizing or minimizing some quality, a specific separable state \( \rho_s^{(\text{opt})} \) appears.

From the above consideration, we show that there are some specific separable states playing an important role in determining the entanglement measure. Then it is meaningful to determine the properties of these separable states. A fact provokes our attention. That is, at least for two-qubit system the set of separable states, denoted by \( S \), is compact and convex [19]. Then boundary of \( S \) does exist. We argue in this paper that these special separable states mentioned above are on the boundary of \( S \). In the following, we give the criterion to determine whether a separable state is on the boundary. Taking this into account, we present more clear interpretations on some concepts concerning quantum entanglement.

II. BOUNDARY OF \( S \)

In this paper, we focus on the two-qubit quantum system. The states can be represented in the Hilbert space \( \mathbb{C}^2 \otimes \mathbb{C}^2 \). So we also call it 2×2 quantum system. We know that all 4×4 Hermitian matrices span a 16-dimensional real Hilbert space, denoted by \( \mathcal{H} \). All density matrices of states forms a subset of \( \mathcal{H} \). We choose Hilber-Schimdt metric, that is, for \( A \in \mathcal{H} \), the norm is defined as \( \|A\| = [tr(A^+A)]^{\frac{1}{2}} = [tr(A^2)]^{\frac{1}{2}} \), and for \( A, B \in \mathcal{H} \), the distance of \( A \) and \( B \) is

\[ \|A - B\| = [tr(A - B)^2]^\frac{1}{2}. \] (6)

For two-qubit system, a given state \( \rho \) is separable, i.e. \( \rho \in S \), if and only if the partial transposition of \( \rho \), denoted by \( \rho^{T_b} \) or \( \rho^{T_a} \) (\( \rho^{T_b} = (\rho^{T_a})^* \)), is also positive [14,19], or equivalently, the partial time-reversal of \( \rho \), denoted by \( \tilde{\rho} \), is positive. Consider an arbitrary separable state \( \rho_s \in S \). Mixing it with the maximal separable state \( \rho_0 = \frac{1}{4}I_{4\times 4} \), we have
\[
\rho_\varepsilon = (1 - \varepsilon) \rho_0 + \varepsilon \rho_s, \quad \varepsilon \in [0, 1].
\] (7)

Obviously, \( \rho_\varepsilon \in \mathcal{S} \) for each \( \varepsilon \). In the geometrical view, \( \rho_\varepsilon \) is on the line segment connecting \( \rho_s \) and \( \rho_0 \). Then consider another form of mixture of \( \rho_s \) and \( \rho_0 \),

\[
\rho_{\varepsilon'} = (1 - \varepsilon') \rho_0 + \varepsilon' \rho_s \quad \varepsilon' > 1.
\] (8)

At this time, \( \rho_{\varepsilon'} \) is on the extension line from \( \rho_0 \) to \( \rho_s \). From the theorems in [20], we know that \( \rho_{\varepsilon'} \) can be in the interior of \( \mathcal{S} \), on the boundary of \( \mathcal{S} \), or outside of \( \mathcal{S} \). That depends on the values of \( \varepsilon' \). So for sufficiently large \( \varepsilon' > 1 \), \( \rho_{\varepsilon'} \) may be outside of \( \mathcal{S} \).

Let us now obtain our main result, which refer to the boundary of \( \mathcal{S} \).

**THEOREM** For a given separable state \( \rho_b \in \mathcal{S} \), if and only if either of the following conditions is satisfied, \( \rho_b \) is on the boundary of \( \mathcal{S} \),

\( (i) \) there exists at least one vanishing eigenvalue for \( \rho_b \);

\( (ii) \) there exists at least one vanishing eigenvalues for \( \tilde{\rho}_b \).

or in the other words, the rank of \( \rho_b \) or \( \tilde{\rho}_b \) is no larger than 3.

**Proof** Note that \( \mathcal{S} \in \mathcal{H} \) and \( \mathcal{S} \) is compact and convex and that \( \rho_0 \) is in the interior of \( \mathcal{S} \). If \( \rho_b \) is on the boundary of \( \mathcal{S} \), let us consider the mixture with form of Eq.(8), that is,

\[
\rho_\delta = (1 - \delta) \rho_0 + \delta \rho_b, \quad \delta > 1.
\] (9)

From [20], we know that such \( \rho_\delta \) does not belong to \( \mathcal{S} \). Therefore, for a given \( \delta > 1 \), there are two possibilities for \( \rho_\delta \). That is, either \( \rho_\delta \) is positive and thus represents an entangled state, or \( \rho_\delta \) is non-positive and does not represent any physical state. In the former case, any point on the line segment from \( \rho_0 \) to \( \rho_\delta \) represents a real physical state, and particularly, all the points (except \( \rho_b \)) on the line segment from \( \rho_b \) to \( \rho_\delta \) are entangled states. Let \( \delta \to 1 \), then \( \rho_\delta \to \rho_b \). Correspondingly \( \tilde{\rho}_\delta \to \tilde{\rho}_b \). Under this condition, the distance between \( \rho_b \) and \( \rho_\delta \) can be arbitrarily small. Note that both \( \rho_b \) and \( \tilde{\rho}_b \) are clearly positive and that \( \rho_b \) is also positive. But \( \tilde{\rho}_\delta \) is non-positive. So by connectivity of the space and continuity of \( \delta \) we conclude that \( \tilde{\rho}_b \) must have vanishing eigenvalue. For the other case in which \( \rho_\delta \) is
non-positive and does not represent real state, similar analysis shows that \( \rho_b \) has at least one vanishing eigenvalue.

To prove the reverse. We first consider a separable state \( \rho_s \) the eigenvalues of which can be denoted by \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 = 0 \), that is, \( \rho_s \) has at least one vanishing eigenvalue. We assume that \( \rho_s \) is in the interior of \( S \). Due to the compactness and convexity of \( S \) and with the help of [20], we know that there always exists a \( \varepsilon' > 1 \) such that the mixture \( \rho_{\varepsilon'} \) in the form \( \rho_{\varepsilon'} = (1 - \varepsilon')\rho_0 + \varepsilon'\rho_b \ (\varepsilon' > 1) \) is also in the interior of \( S \). The eigenvalues of \( \rho_{\varepsilon'} \), denoted by \( \lambda'_i \), can be easily calculated, that is,

\[
\lambda'_i = \varepsilon'\lambda_i + \frac{1 - \varepsilon'}{4}, \quad (i = 1, \ldots, 4).
\]

(10)

Obviously, for \( \lambda_4 = 0 \), we have \( \lambda'_4 = \frac{1 - \varepsilon'}{4} < 0 \). Then \( \rho' \) is non-positive and cannot belong to \( S \). This result contradicts with the assumption made above. Hence \( \rho_s \) can not be in the interior and can only be on the boundary of \( S \), i.e. \( \rho_s = \rho_b \). On the other hand, let’s consider a separable state \( \rho_s \) such that \( \tilde{\rho}_s \) has one vanishing eigenvalue, i.e. \( \tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \tilde{\lambda}_3 > \tilde{\lambda}_4 = 0 \). Also assume that \( \rho_s \) is in the interior of \( S \). Then \( \rho_{\varepsilon'} \) is the interior point of \( S \) for some \( \varepsilon' > 1 \). So \( \tilde{\rho}_{\varepsilon'} \) is necessarily positive. Denote the eigenvalues of \( \tilde{\rho}_{\varepsilon'} \) by \( \tilde{\lambda}'_i, i = 1, \ldots, 4 \). Similar analysis will demonstrate that one of the eigenvalues of \( \tilde{\rho}_{\varepsilon'} \), which is actually \( \tilde{\lambda}_4 \), is negative. It is contrary to the assumption. So \( \rho_s = \rho_b \).

III. DISCUSSION

Having obtained the description of the boundary of \( S \), we now return to think about some concepts of quantum entanglement.

A. Relative Entropy of Entanglement

In [15][16], Vedrel et al. propose the concept of relative entropy of entanglement and give the numerical results for some examples of two-qubit entangled states. For instance, given entangled state \( \rho_e \) as
\[ \rho_e = \lambda |\Phi^+\rangle \langle \Phi^+| + (1 - \lambda) |01\rangle \langle 01|, \quad \lambda \in (0, 1), \tag{11} \]

where \(|\Phi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)\). The separable state which minimize the relative entropy \(S(\rho_e \parallel \rho_s)\) (cf. Eq.(1)) is said to be

\[ \rho_s = \frac{\lambda}{2} \left( 1 - \frac{\lambda}{2} \right) |00\rangle \langle 00| + \frac{\lambda}{2} \left( 1 - \frac{\lambda}{2} \right) |00\rangle \langle 11| + H.C. \]
\[ + \left( 1 - \frac{\lambda}{2} \right)^2 |01\rangle \langle 01| + \frac{\lambda^2}{4} |10\rangle \langle 10| + \frac{\lambda}{2} \left( 1 - \frac{\lambda}{2} \right) |11\rangle \langle 11| \tag{12} \]

Straightforward computation shows that \(\rho_s\) has a vanishing eigenvalue. Then \(\rho_s\) is on the boundary of \(\mathcal{S}\). This result also holds in the other examples mentioned in \([15,16]\). So we can say, at least for these specific cases, the relative entropy of entanglement can be achieved on the boundary of the set of separable states. It is possible to generalize this result.

**B. Robustness of Entanglement**

Recall that the robustness of entanglement proposed by Vidal et al. \([17]\). The geometrical interpretation has been obtained in \([21]\), in which the boundary of \(\mathcal{S}\) is not yet explicitly defined. The discussion in this Letter can be supplementary to \([21]\). We can say that for a given entangled state \(\rho_e\) of two-qubit system, if \(s\) in Eq.(2) is minimal among all separable states \(\rho_s\), i.e. \(s\) is the absolute robustness of \(\rho_e\), then \(\rho_s\) and \(\rho(s)\) in Eq.(2) are necessarily on the boundary of \(\mathcal{S}\).

**C. Lewenstein-Sanpera Decomposition**

Now let us give our interpretation for L-S decomposition. Recall the form of L-S decomposition represented by Eq.(3). Using Hilbert-Schmidt metric defined by Eq.(6), we can express the \(\lambda\) in Eq. (3) as

\[ \lambda = \frac{\|\rho - P_e\|}{\|\rho_s - P_e\|}. \tag{13} \]

As shown in Fig.1, \(\lambda\) can be regarded as the ratio of the length of line segment \(AB\) to that of \(AC\). With \(P_e\) (point \(A\) in Fig. 1) and \(\rho\) (point \(B\)) fixed, \(\lambda\) reaches the maximal when \(\rho_s\)
is on the boundary of $S$, i.e., the length of $AC$ is minimal. In the geometrical view, this result is straightforward. So we can always rewrite Eq. (5) as

$$\rho = \eta \rho_b + (1 - \eta) P_e, \quad \lambda \in [0, 1],$$  \hspace{1cm} (14)

where $\rho_b$ is on the boundary and $\eta$ is the maximal $\lambda$ associated with $P_e$. Obviously, for Eq.(4) $\rho_s^{(opt)}$ is on the boundary of $S$ and can be written as $\rho_b^{(opt)}$ while $S$ can be expressed as $S = \max \{\eta\}$.

In [22], Englert et al. have erred to what is involved in L-S decomposition, that is, if $\rho = S \rho_b^{(opt)} + (1 - S) P_e^{(opt)}$ is the optimal decomposition, then (a) the state $(1 + \varepsilon)^{-1}(\rho_b^{(opt)} + \varepsilon P_e^{(opt)})$ is non-separable for $\varepsilon > 0$; and (b) the state $\rho_b^{(opt)} + (\frac{1}{S} - 1)(P_e^{(opt)} - P_e')$ is either non-positive or non-separable for each $P_e' \neq P_e^{(opt)}$. It is said in [16] that their verification is rather complicated even in seemingly simple cases. But in our view, it is easy to understand. Now we give our explanation as follows.

For conclusion (a), since the optimal decomposition of $\rho$ has been obtained, $\rho_b^{(opt)}$ is necessarily on the boundary of $S$. Thus the convexity of $S$ guarantees that all points on the line segment $AD$ (cf Fig. 1) can not belong to $S$ and without choice represent entangled states. These states are expressed as the convex sum of $P_e^{(opt)}$ and $\rho_b^{(opt)}$, i.e., $(1 + \varepsilon)^{-1}(\rho_b^{(opt)} + \varepsilon P_e^{(opt)}), \varepsilon > 0$. In addition, this conclusion also holds without the “optimal” condition. That is, for any decomposition determined by Eq. (14), conclusion (a) is valid.

For conclusion (b), let

$$\rho_x = \rho_b^{(opt)} + \frac{1 - S}{S}(P_e^{(opt)} - P_e'),$$  \hspace{1cm} (15)

or equivalently,

$$S \rho_x + (1 - S) P_e' = S \rho_b^{(opt)} + (1 - S) P_e^{(opt)}.$$  \hspace{1cm} (16)

The right-handed of Eq. (16) is just the optimal decomposition of $\rho$. We already know that $S$ is the largest $\eta$ of all possible decomposition (cf Eq.(14)). If the mixture on the left-hand of Eq.(16) does represent $\rho$, the weight of $\rho_x$ must be less than $S$. In other words, the
left-hand of Eq.(16) can not be a real L-S decomposition about $\rho$. Hence $\rho_x \notin S$. Therefore, either $\rho_x$ can not be positive, or can represent a non-separable state. The conclusion (b) can be demonstrated in Fig. 2. Of course the “optimal” condition is necessary in this case.

So far we have discussed the boundary of the set of all separable states. Using this concept, we give straightforward explanations for some entanglement measure of the mixed states, mainly for L-S decomposition. We feel that introducing boundary may be helpful for better understanding of entanglement.

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REFERENCES

[1] A. Einstein, B. Podolsky and N. Rosen, Phys. Rev. 47, 777 (1935).

[2] E. Schrödinger, Proc. Cambridge Philos. Soc. 31, 555 (1935).

[3] A. Barenco, D. Deustch, A. Ekert, and R. Jozsa, Phys. Rev. Lett. 74, 4083 (1995).

[4] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin and W. K. Wootters, Phys. Rev. A54, 3824 (1996).

[5] A. Ekert, Phys. Rev. Lett. 67, 661 (1991).

[6] C. H. Bennett and S. J. Wiesner, Phys. Rev. Lett. 69, 2881 (1992).

[7] C. H. Bennett, G. Brassard, C. Crépeau, R. Jozsa, A. Peres, and W. K. Wootters, Phys. Rev. Lett. 70, 1895 (1996).

[8] R. Horodecki and M. Horodecki, Phys. Rev. A54, 1838 (1996).

[9] J. S. Bell, Physics 1, 1995 (1964).

[10] J. F. Clauser, M. A. Horne, A. Shimony and R. A. Holt, Phys. Rev. Lett. 23, 880 (1969).

[11] N. Gisin, Phys. Lett. A154, 201 (1991).

[12] S. Popescu, Phys. Rev. Lett. 72, 797 (1994).

[13] S. Popescu, Phys. Rev. Lett. 74, 2619 (1995).

[14] A. Peres, Phys. Rev. Lett. 77, 1413 (1996).

[15] V. Vedral, M. B. Plenio, M. A. Rippin and P. L. Knight, Phys. Rev. Lett. 78, 2275 (1997).

[16] V. Vedral and M. B. Plenio, Phys. Rev. A57, 1619 (1998).

[17] G. Vidal and R. Tarrach, Phys. Rev. A59, 141 (1999).

[18] M. Lewenstein and A. Sanpera, Phys. Rev. Lett. 80, 2261 (1998).
[19] M. Horodecki, P. Horodecki, R. Horodecki, Phys. Lett. A223, 1 (1996).

[20] T. Rockafellar, Convex Analysis (Princeton University Press, Princeton, 1970).

[21] J. F. Du, M. J. Shi, X.Y. Zhou and R. D. Han, Phys. Lett. A267, 244 (2000).

[22] B. Englert and N. Metwally, e-print archive: quant-ph/9912089.

Figure Caption

Fig. 1 $P_e$ (point A) denotes an entangled pure state. $\rho$ (point B) represents a given non-separable mixed state. $S$ is the set of all separable states. $\rho_s$ (point C) is in the interior of $S$ and $\rho_b$ (point D) is on the boundary of $S$.

Fig. 2 $P_{e^{(opt)}}$ and $P_{e'}$ are two different entangled pure states. $P_{e^{(opt)}}$ and $\rho_b^{(opt)}$ construct the optimal L-S decomposition of $\rho$. $\rho_x$ is outside of set $S$. $P_{e'}$ and $\rho_x$ does not construct the L-S decomposition of $\rho$. 
