Characterization of maximally entangled two-qubit states via the Bell-Clauser-Horne-Shimony-Holt inequality

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Maximally entangled states should maximally violate the Bell inequality. In this paper, it is proved that all two-qubit states that maximally violate the Bell-Clauser-Horne-Shimony-Holt inequality are exactly Bell states and the states obtained from them by local unitary transformations. The proof is obtained by using the certain algebraic properties that Pauli’s matrices satisfy. The argument is extended to the three-qubit system. Since all states obtained by local unitary transformations of a maximally entangled state are equally valid entangled states, we thus give the characterizations of maximally entangled states in both the two-qubit and three-qubit systems in terms of the Bell inequality.

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The Bell inequality [1] was originally designed to rule out various kinds of local hidden variable theories. Precisely, the Bell inequality indicates that certain statistical correlations predicted by quantum mechanics for measurements on two-qubit ensembles cannot be understood within a realistic picture based on Einstein, Podolsky, and Rosen’s (EPR’s) notion of local realism [2]. However, this inequality also provides a test to distinguish entangled from nonentangled quantum states. In fact, Gisin’s theorem [3] asserts that all entangled two-qubit states violate the Bell inequality [11] are exactly GHZ states and the states obtained from them by local unitary transformations. This was conjectured by Gisin and Bechmann-Pasquinucci [8]. Since all states obtained by local unitary transformations of a maximally entangled state are equally valid entangled states, we thus give the characterizations of maximally entangled states in the two-qubit and three-qubit systems via the Bell-CHSH and Bell-Klyshko inequalities, respectively.

Let us consider a system of two qubits labelled by 1 and 2. Let $A, A'$ denote spin observables on the first qubit, and $B, B'$ on the second. For $A^{(i)} = \vec{\sigma}^{(i)} \cdot \vec{\sigma}_1$ and $B^{(i)} = \vec{b}^{(i)} \cdot \vec{\sigma}_2$, we write

$$(A, A') = (\vec{a}, \vec{a}') , A \times A' = (\vec{a} \times \vec{a}') \cdot \vec{\sigma}_1 ,$$

and similarly, $(B, B')$ and $B \times B'$. Here $\vec{\sigma}_1$ and $\vec{\sigma}_2$ are the Pauli matrices for qubits 1 and 2, respectively; the norms of real vectors $\vec{a}^{(i)}, \vec{b}^{(i)}$ in $\mathbb{R}^3$ are equal to 1. We write $AB$, etc., as shorthand for $A \otimes B$ and $A = AI_2$, where $I_2$ is the identity on qubit 2. Recall that the Bell-CHSH inequality is that

$$\langle AB + AB' + A'B - A'B' \rangle \leq 2, \quad (1)$$

which holds true when assuming EPR’s local realism [2]. We define the two-qubit Bell operator [10]

$${\mathcal B}_2 = AB + AB' + A'B - A'B' . \quad (2)$$
Since
\[ AA' = (A, A') + iA \times A', A'A = (A, A') - iA \times A', \]
\[ BB' = (B, B') + iB \times B', B'B = (B, B') - iB \times B', \]
a simple computation yields that
\[ B_2^2 = 4 - [A, A'][B, B'] = 4 + 4(A \times A')(B \times B'). \quad (3) \]

Since
\[ \| A \times A' \|^2 = 1 - (A, A')^2, \| B \times B' \|^2 = 1 - (B, B')^2, \]
it concludes that \( B_2^2 \leq 8 \) and \( \| B_2^2 \| = 8 \) if and only if
\[ (A, A') = (B, B') = 0. \quad (5) \]

Accordingly, the Bell-CHSH inequality can be violated by quantum states by a maximal factor of \( \sqrt{2} \) [13]. In particular, one concludes that Eq. (5) is a necessary and sufficient condition that there exists a two-qubit state that maximally violates the Bell-CHSH inequality, i.e.,
\[ \langle \psi | B_2 | \psi \rangle = 2\sqrt{2} \quad (6) \]
for some state \( \psi \).

As follows, we show that every state \( | \psi \rangle \) satisfying (6) can be obtained by a local unitary transformation of the Bell states. Indeed, let \( A'' = A \times A' \) and \( B'' = B \times B' \). Since Eq. (5) holds true, it concludes that both \( (\tilde{a}, \tilde{a}', \tilde{a}'') \) and \( (\tilde{b}, \tilde{b}', \tilde{b}'') \) are triads in \( S^2 \), the unit sphere in \( \mathbb{R}^3 \). Then, it is easy to check that
\[ AA' = -A'A = iA'', \quad (7) \]
\[ A'A'' = -A''A' = iA, \quad (8) \]
\[ A''A = -AA'' = iA'; \quad (9) \]
\[ A^2 = (A')^2 = (A'')^2 = 1. \quad (10) \]
Hence, \( \{ A, A', A'' \} \) satisfy the algebraic identities that Pauli’s matrices satisfy [14] and similarly, \( \{ B, B', B'' \} \). Therefore, choosing \( A''\)-representation \( \{ |0\rangle_A, |1\rangle_A \} \), i.e.,
\[ A''|0\rangle_A = |0\rangle_A, A''|1\rangle_A = -|1\rangle_A, \quad (11) \]
we have that
\[ A|0\rangle_A = e^{-i\alpha}|1\rangle_A, A|1\rangle_A = e^{i\alpha}|0\rangle_A, \quad (12) \]
\[ A'|0\rangle_A = i e^{-i\alpha}|1\rangle_A, A'|1\rangle_A = -i e^{i\alpha}|0\rangle_A, \quad (13) \]
\[ (0 \leq \alpha \leq 2\pi). \]

Similarly, we have that
\[ B|0\rangle_B = e^{-i\beta}|1\rangle_B, B|1\rangle_B = e^{i\beta}|0\rangle_B, \quad (14) \]
\[ B'|0\rangle_B = i e^{-i\beta}|1\rangle_B, B'|1\rangle_B = -i e^{i\beta}|0\rangle_B, \quad (15) \]
\[ B''|0\rangle_B = |0\rangle_B, B''|1\rangle_B = -|1\rangle_B, \quad (16) \]
for the \( B''\)-representation \( \{ |0\rangle_B, |1\rangle_B \} \) \( (0 \leq \beta \leq 2\pi) \).

We write \( |00\rangle_{AB} \), etc., as shorthand for \( |0\rangle_A \otimes |0\rangle_B \). Since \( \{ |00\rangle_{AB}, |01\rangle_{AB}, |10\rangle_{AB}, |11\rangle_{AB} \} \) is an orthogonal basis of the two-qubit system, we can uniquely write
\[ |\psi \rangle = \lambda_{00}|00\rangle_{AB} + \lambda_{01}|01\rangle_{AB} + \lambda_{10}|10\rangle_{AB} + \lambda_{11}|11\rangle_{AB}, \]
where
\[ |\lambda_{00}|^2 + |\lambda_{01}|^2 + |\lambda_{10}|^2 + |\lambda_{11}|^2 = 1. \]

Since \( \psi \) maximize \( B_2 \), it also maximize \( B_2^2 = 4 + 4A''B'' \) and so
\[ A''B''|\psi \rangle = |\psi \rangle. \quad (17) \]

By Eqs. (11) and (16) we have that \( \lambda_{01} = \lambda_{10} = 0 \). Hence \( |\psi \rangle \) is of the form
\[ |\psi \rangle = a|00\rangle_{AB} + b|11\rangle_{AB} \]
with \( |a|^2 + |b|^2 = 1 \).

On the other hand, we conclude by Eq. (6) that
\[ (AB + AB' + A'B - A'B') |\psi \rangle = 2\sqrt{2}|\psi \rangle. \quad (18) \]

By using Eqs. (12)-(15) we have that
\[ be^{i(\alpha + \beta)}(1 - i) = \sqrt{2}a, \quad ae^{-i(\alpha + \beta)}(1 + i) = \sqrt{2}b, \]

and so
\[ a = \frac{1}{\sqrt{2}}e^{i(\alpha + \beta - \frac{\pi}{4})}, b = \frac{1}{\sqrt{2}}e^{i\beta}, \]

where \( 0 \leq \beta \leq 2\pi \). Thus,
\[ |\psi \rangle = e^{i\theta} \frac{1}{\sqrt{2}} \left( e^{i(\alpha + \beta - \frac{\pi}{4})}|00\rangle_{AB} + |11\rangle_{AB} \right). \]

Let \( U_1 \) be the unitary transform from the original \( \sigma_z \)-representation to \( A''\)-representation on the first qubit, i.e., \( U_1|0\rangle = |0\rangle_A \) and \( U_1|1\rangle = |1\rangle_A \), and similarly \( U_2 \) on the second qubit. Define
\[ U_A = e^{i\beta}U_1, \quad U_B = U_2 \left( \begin{array}{cc} e^{i(\alpha + \beta - \frac{\pi}{4})} & 0 \\ 0 & 1 \end{array} \right). \]

Then \( U_A \) and \( U_B \) are unitary operators on the first qubit and the second respectively, so that
\[ |\psi \rangle = (U_AU_B) \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle), \]
i.e., $|\psi\rangle$ can be obtained by a local unitary transformation of the Bell state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$.

For the three-qubit system, let us consider a system of three qubits labeled by 1, 2, and 3. Let $A, A'$ denote spin observables on the first qubit, $B, B'$ on the second, and $C, C'$ on the third. Recall that the Bell-Klyshko inequality [11] for three qubits reads that

$$(A'B'C + A'BC' + AB'C' - ABC) \leq 2,$$  \hspace{1cm} (19)$$

Accordingly, by Eq.(4) we have $\|B_3^2\| \leq 16$ and so $\|B_3\| \leq 4$. As follows, we will prove that a state $|\psi\rangle$ maximally violates the Bell-Klyshko inequality Eq.(19), i.e.,

$$\langle \psi | B_3 | \psi \rangle = 4,$$  \hspace{1cm} (22)$$

if and only if it is of the form

$$|\psi\rangle = (U_A U_B U_C) \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$$  \hspace{1cm} (23)$$

where $U_A, U_B$, and $U_C$ are unitary operators respectively on the first qubit, second one and third one. Therefore, the GHZ state

$$|GHZ\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$$

and the states obtained from it by local unitary transformations are the unique states that violate maximally the Bell-Klyshko inequality of three qubit, as conjectured by Gisin and Bechmann-Pasquinucci [8].

It is easy to check that all states of the form Eq.(23) maximally violate Eq.(19). In this case, we only need to choose that

$$A = U_A \sigma_1^A \sigma_2^A \sigma_3^A U_A^*, A' = U_A \sigma_1^A \sigma_2^A \sigma_3^A U_A^*;$$

$$B = U_B \sigma_1^B U_B^*, B' = U_B \sigma_1^B U_B^*;$$

and

$$C = U_C \sigma_1^C U_C^*, C' = U_C \sigma_1^C U_C^*.$$  \hspace{1cm} (24)$$

This is so, because of that $|GHZ\rangle$ satisfies Eq.(22) for the Bell operator

$$B_3 = (\sigma_1^A \sigma_2^A \sigma_3^A) \sigma_1^B \sigma_2^C + (\sigma_1^A \sigma_2^B \sigma_3^C) \sigma_1^B \sigma_2^C + (\sigma_1^A \sigma_2^C \sigma_3^C) \sigma_1^B \sigma_2^C - (\sigma_1^A \sigma_2^B \sigma_3^B) \sigma_1^B \sigma_2^C.$$  \hspace{1cm} (25)$$

In fact, if Eq.(24) holds true, then $\|B_3^2\| = 16$. By Eqs.(4) and (21) we immediately conclude Eq.(25). In the sequel, we show that a state $|\psi\rangle$ satisfying Eq.(24) must be of the form

$$|\psi\rangle = a|0\rangle_A|0\rangle_B|0\rangle_C + b|1\rangle_A|1\rangle_B|1\rangle_C,$$  \hspace{1cm} (26)$$

where $\{|0\rangle_A,|1\rangle_A\}$, $\{|0\rangle_B,|1\rangle_B\}$, and $\{|0\rangle_C,|1\rangle_C\}$ are orthogonal respectively on the first qubit, second one, and third one.

Let $A'' = A \times A'$, $B'' = B \times B'$, and $C'' = C \times C'$. Since Eq.(25) holds true, as shown above, $\{A, A', A''\}$, $\{B, B', B''\}$, and $\{C, C', C''\}$ all satisfy the algebraic identities Eqs.(7)-(10) that Pauli’s matrices satisfy. By choosing the $A''$-representation on the first qubit, $B''$-
representation on the second, and $C''$-representation on the third respectively, we have Eqs.(11)-(16) and
\[ C[0]C = e^{-i\gamma}|1\rangle_C, C[1]C = e^{i\gamma}|0\rangle_C, \]  
(27)
\[ C'[0]C = ie^{-i\gamma}|1\rangle_C, C'[1]C = -ie^{i\gamma}|0\rangle_C, \]  
(28)
\[ C''[0]C = |0\rangle_C, C''[1]C = -|1\rangle_C, \]  
(29)
for the $C''$-representation $\{|0\rangle_C, |1\rangle_C\} (0 \leq \gamma \leq 2\pi)$.

We write $|001\rangle_{ABC}$, etc., as shorthand for $|0\rangle_A \otimes |0\rangle_B \otimes |1\rangle_C$. Since $\{|e_A e_B e_C\}_{ABC} : e_A, e_B, e_C = 0, 1\}$ is an orthogonal basis of the three-qubit system, we can uniquely write
\[ |\psi\rangle = \sum_{e_A, e_B, e_C = 0, 1} \lambda_{e_A e_B e_C} |e_A e_B e_C\rangle_{ABC} \]  
with $\sum |\lambda_{e_1 e_2 e_3}|^2 = 1$. By using Eqs.(11), (16) and (29), we follow from Eq.(24) that
\[ \lambda_{001} = \lambda_{010} = \lambda_{100} = \lambda_{011} = \lambda_{101} = \lambda_{110} = 0. \]  
Thus $|\psi\rangle = \lambda_{000}|000\rangle_{ABC} + \lambda_{111}|111\rangle_{ABC}$ is of the form Eq.(26).

Now suppose that a state $|\psi\rangle$ satisfies Eq.(22). Since Eq.(22) is equivalent to that
\[ B_3(\psi) = 4|\psi\rangle, \]  
(30)
it concludes that $|\psi\rangle$ satisfies Eq.(24) and hence is of the form Eq.(26). Note that
\[ B_3 = B_2 \otimes \frac{1}{2} (C + C') + B'_2 \otimes \frac{1}{2} (C - C') \]  
where $B'_2 = A' B' + A' B + A B' - A B$ denote the same expression $B_2$ but with the $A$ and $A'$, $B$ and $B'$ exchanged. Then, by Eqs.(27) and (28) one has that
\[ B_3(\psi) = \frac{1}{2} ae^{-i\gamma} [(1 + i) B_2 + (1 - i) B'_2]|00\rangle_{AB}|1\rangle_C + \frac{1}{2} be^{i\gamma} [(1 - i) B_2 + (1 + i) B'_2]|11\rangle_{AB}|0\rangle_C. \]  
(31)
From Eq.(30) we conclude that
\[ \frac{1}{2} ae^{-i\gamma} [(1 + i) B_2 + (1 - i) B'_2]|00\rangle_{AB} = 4b|11\rangle_{AB}, \]  
(32)
and
\[ \frac{1}{2} be^{i\gamma} [(1 - i) B_2 + (1 + i) B'_2]|11\rangle_{AB} = 4a|00\rangle_{AB}. \]  
By Eq.(31) we have that
\[ 4|b| \leq \frac{1}{2} |a| (||B_2|| + ||-1 - i||B'_2||) \leq \frac{1}{2} |a| (\sqrt{2} \cdot 2\sqrt{2} + \sqrt{2} \cdot 2\sqrt{2}) = 4|a|, \]  
since $||B_2||, ||B'_2|| \leq 2\sqrt{2}$ as shown in the two-qubit case. This concludes that $|b| \leq |a|$. Similarly, by Eq.(32) we have that $|a| \leq |b|$. Therefore, we have that $a = \frac{1}{\sqrt{2}} e^{i\phi}, b = \frac{1}{\sqrt{2}} e^{i\theta}$ for some $0 \leq \phi, \theta \leq 2\pi$, that is,
\[ |\psi\rangle = \frac{1}{\sqrt{2}} (e^{i\phi}|000\rangle_{ABC} + e^{i\theta}|111\rangle_{ABC}). \]  
This immediately concludes that $|\psi\rangle$ can be obtained by a local unitary transformation of the GHZ state, precisely
\[ |\psi\rangle = (U_A U_B U_C) \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle), \]  
where
\[ U_A = U_1 \left( \begin{array}{cc} e^{i\phi} & 0 \\ 0 & 1 \end{array} \right), \quad U_B = U_2 \left( \begin{array}{cc} 1 & 0 \\ 0 & e^{i\theta} \end{array} \right), \]  
and $U_C = U_3$. Here, $U_1$ is the unitary transform from the original $\sigma_z^1$-representation to $A''$-representation on the first qubit, i.e., $U_1|0\rangle = |0\rangle_A$ and $U_1|1\rangle = |1\rangle_A$, and similarly, $U_2$ on the second qubit and $U_3$ on the third qubit, respectively.

To sum up, by using some subtle mathematical techniques we have shown that the Bell and GHZ states and the states obtained from them by local unitary transformations are the unique states that violate maximally the Bell-CHSH and Bell-Klyshko inequalities, respectively. This was conjectured by Gisin and Bechmann-Pasquinucci [8]. The key point of our argument involved here is by using the certain algebraic properties that Pauli’s matrices satisfy, which is based on the determination of local spin observables of the associated Bell operator. The method involved here is simpler (and more powerful) than one used in [9] and can be extended to the $n$-qubit case, which will be presented elsewhere. It is known that maximally entangled states should maximally violate the Bell inequality and all states obtained by local unitary transformations of a maximally entangled state are equally valid entangled states [12], we therefore obtain the characterizations of maximally entangled states in both two-qubit and three-qubit via the Bell-CHSH...
and Bell-Klyshko inequalities, respectively. Finally, we remark that the W state of three-qubit

$$|W\rangle = \frac{1}{3} (|001\rangle + |010\rangle + |100\rangle)$$

cannot be obtained from the GHZ state by a local unitary transformation and hence does not maximally violate the Bell-Klyshko inequality, although it is a “maximally entangled” state in the sense described in [16]. This also occurs in the GHZ theorem [5], that is, the W state does not provide an 100% contradiction between quantum mechanics and EPR’s local realism [17]. Since the Bell inequality and GHZ theorem are two main theme on the violation of EPR’s local realism, it concludes that from the point of view on the violation of EPR’s local realism, the W state cannot be regarded as a “maximally entangled” state and hence we need some new ideas for clarity of the W state [18].