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

Zeqian Chen*
Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, P.O. Box 71010, 30 West District, Xiao-Hong Mountain, Wuhan 430071, China

(Received 2 February 2004; published 23 August 2004)

Maximally entangled states should maximally violate the Bell inequality. 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 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 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.

DOI: 10.1103/PhysRevA.70.024303 PACS number(s): 03.67.−a, 03.65.Ud

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-Clauser-Horne-Shimony-Holt (Bell-CHSH) inequality [4] for some choice of spin observables.

As is well known, maximally entangled states, such as Bell states and Greenberger-Horne-Zeilinger (GHZ) states [5], have become a key concept in quantum mechanics nowadays. On the other hand, from a practical point of view maximally entangled states have found numerous applications in quantum information [6]. A natural question is then how to characterize maximally entangled states. There are extensive earlier works on maximally entangled states [7]; however, this problem is far from being completely understood today. It is well known that maximally entangled states should maximally violate the Bell inequality [8]. Therefore, for characterizing maximally entangled states, it is suitable to study the states that maximally violate the Bell inequality. In the two-qubit case, Kar [9] has described all states that maximally violate the Bell-CHSH inequality. Kar mainly made use of an elegant technique, which was originally introduced in [10], based on the determination of the eigenvectors and eigenvalues of the associated Bell operator.

In this paper, it is proved that Bell states and the states obtained from them by local transformations are the unique states that violate maximally the Bell-CHSH inequality. The techniques involved here are based on the determination of local spin observables of the associated Bell operator. We show that a Bell operator presents a maximal violation on a state if and only if the associated local spin observables satisfy the certain algebraic identities that Pauli's matrices satisfy. Consequently, we can easily find those states that show maximal violation, which are the states obtained from Bell states by local transformations.

The method involved here is simpler (and more powerful) than one used in [9] and can be directly extended to the n-qubit case. We illustrate the three-qubit case and show that all states that violate the Bell-Klyshko inequality [11] are exactly GHZ states and the states obtained from them by local transformations. This was conjectured by Gisin and Bechmann-Pasquinucci [8]. Since all states obtained by local transformations of a maximally entangled state are equally valid entangled states [12], we thus give 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 labeled by 1 and 2. Let A,A' denote spin observables on the first qubit and B,B' on the second. For $A^{(\prime)}=\vec{a}^{(\prime)}\cdot\vec{\sigma}_1$ and $B^{(\prime)}=\vec{b}^{(\prime)}\cdot\vec{\sigma}_2$, 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 $\vec{a}^{(\prime)}$, $\vec{b}^{(\prime)}$ 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

$$\langle AB+AB'+A'B-A'B'\rangle \leqslant 2, \tag{1}$$

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

$$\mathcal{B}_2=AB+AB'+A'B-A'B'. \tag{2}$$

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

*Electronic address: zqchen@wipm.ac.cn

$$\mathcal{B}_2^2 = 4 - [A,A'][B,B'] = 4 + 4(A \times A')(B \times B'). \quad (3)$$

Since

$$\|A \times A'\|^2 = 1 - (A,A')^2, \|B \times B'\|^2 = 1 - (B,B')^2, \quad (4)$$

it is concluded that $\mathcal{B}_2^2 \leqslant 8$ and $\|\mathcal{B}_2^2\| = 8$ 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 exist a two-qubit state that maximally violates the Bell-CHSH inequality—i.e.,

$$\langle\psi|\mathcal{B}_2|\psi\rangle = 2\sqrt{2} \quad (6)$$

for some state ψ.

As follows, we show that every state ψ satisfying Eq. (6) can be obtained by a local transformation of the Bell states. Indeed, let $A''=A\times A'$ and $B''=B\times B'$. Since Eq. (5) holds true, it is concluded that both $(\vec{a},\vec{a}',\vec{a}'')$ and $(\vec{b},\vec{b}',\vec{b}'')$ 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 the 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

$$A|0\rangle_A = e^{-i\alpha}|1\rangle_A, A|1\rangle_A = e^{i\alpha}|0\rangle_A, \quad (12)$$

$$A'|0\rangle_A = ie^{-i\alpha}|1\rangle_A, A'|1\rangle_A = -ie^{i\alpha}|0\rangle_A \quad (13)$$

$(0\leqslant\alpha\leqslant 2\pi)$. Similarly, we have that

$$B|0\rangle_B = e^{-i\beta}|1\rangle_B, B|1\rangle_B = e^{i\beta}|0\rangle_B, \quad (14)$$

$$B'|0\rangle_B = ie^{-i\beta}|1\rangle_B, B'|1\rangle_B = -ie^{i\beta}|0\rangle_B, \quad (15)$$

$$B''|0\rangle_B = |0\rangle_B, B''|1\rangle_B = -|1\rangle_B, \quad (16)$$

for the B'' representation $\{|0\rangle_B,|1\rangle_B\}$ $(0\leqslant\beta\leqslant 2\pi)$.

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 ψ maximizes $\mathcal{B}_2$, it also maximize $\mathcal{B}_2^2=4+4A''B''$ 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

$$be^{i(\alpha+\beta)}(1-i) = \sqrt{2}a, \ \ ae^{-i(\alpha+\beta)}(1+i) = \sqrt{2}b,$$

and so

$$a = \frac{1}{\sqrt{2}}e^{i(\alpha+\beta+\theta-\pi/4)}, \ \ b = \frac{1}{\sqrt{2}}e^{i\theta},$$

where $0\leqslant\theta\leqslant 2\pi$. Thus,

$$|\psi\rangle = e^{i\theta}\frac{1}{\sqrt{2}}(e^{i(\alpha+\beta-\pi/4)}|00\rangle_{AB} + |11\rangle_{AB}).$$

Let U_1 be the unitary transform from the original σ_z^1 representation to the 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

$$U_A = e^{i\theta}U_1, \ U_B = U_2\begin{pmatrix} e^{i(\alpha+\beta-\pi/4)} & 0 \\ 0 & 1 \end{pmatrix}.$$

Then U_A and U_B are unitary operators on the first and second qubits, 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 transformation of the Bell state $(1/\sqrt{2})(|00\rangle+|11\rangle)$.

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

$$\langle A'B'C + A'BC' + AB'C' - ABC\rangle \leqslant 2, \quad (19)$$

which holds true when assuming EPR's local realism [2].

We define the three-qubit Bell operator [15]

$$\mathcal{B}_3 = A'B'C + A'BC' + AB'C' - ABC. \quad (20)$$

A simple computation yields

$$\begin{aligned}\mathcal{B}_3^2 = 4 - [A,A'][B,B'] - [A,A'][C,C'] - [B,B'][C,C'] = 4 \\ + 4[(A\times A')(B\times B') + (A\times A')(C\times C') \\ + (B\times B')(C\times C')]. \quad (21)\end{aligned}$$

Accordingly, by Eq. (4) we have $\|\mathcal{B}_3^2\|\leqslant 16$ and so $\|\mathcal{B}_3\|\leqslant 4$. As follows, we will prove that a state $|\psi\rangle$ maximally violates the Bell-Klyshko inequality, Eq. (19), i.e.,

$$\langle\psi|\mathcal{B}_3|\psi\rangle = 4, \tag{22}$$

if and only if it is of the form

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

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

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

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

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

$$A = U_A^* \sigma_x^A U_A,\ A' = U_A^* \sigma_y^A U_A,$$

$$B = U_B^* \sigma_x^B U_B,\ B' = U_B^* \sigma_y^B U_B,$$

and

$$C = U_C^* \sigma_x^C U_C,\ C' = U_C^* \sigma_y^C U_C.$$

This is so, because $|\mathrm{GHZ}\rangle$ satisfies Eq. (22) for the Bell operator:

$$\mathcal{B}_3 = \sigma_y^A\sigma_y^B\sigma_x^C + \sigma_y^A\sigma_x^B\sigma_y^C + \sigma_x^A\sigma_y^B\sigma_y^C - \sigma_x^A\sigma_x^B\sigma_x^C.$$

Here $\vec{\sigma}_1 = (\sigma_x^A, \sigma_y^A, \sigma_z^A)$, $\vec{\sigma}_2 = (\sigma_x^B, \sigma_y^B, \sigma_z^B)$, and $\vec{\sigma}_3 = (\sigma_x^C, \sigma_y^C, \sigma_z^C)$ are the Pauli matrices for qubits 1, 2, and 3, respectively.

The key point of the proof is that the converse holds true; i.e., the maximal violation of the Bell-Klyshko inequality of three qubit occurs only for the GHZ state and the states obtained from it by local transformations, as similar as the two-qubit case. We begin with the fact that if there exists a state $|\psi\rangle$ satisfying

$$\mathcal{B}_3^2|\psi\rangle = 16|\psi\rangle, \tag{24}$$

then

$$(A,A') = (B,B') = (C,C') = 0. \tag{25}$$

In fact, if Eq. (24) holds true, then $\|\mathcal{B}_3^2\| = 16$. 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

$$|\psi\rangle = a|000\rangle + b|111\rangle, \tag{26}$$

where $|a|^2 + |b|^2 = 1$.

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

$$C|0\rangle_C = e^{-i\gamma}|1\rangle_C,\ C|1\rangle_C = e^{i\gamma}|0\rangle_C, \tag{27}$$

$$C'|0\rangle_C = ie^{-i\gamma}|1\rangle_C,\ C'|1\rangle_C = -ie^{i\gamma}|0\rangle_C, \tag{28}$$

$$C''|0\rangle_C = |0\rangle_C,\ C''|1\rangle_C = -|1\rangle_C, \tag{29}$$

for the C'' representation $\{|0\rangle_C, |1\rangle_C\}$ $(0 \leqslant \gamma \leqslant 2\pi)$.

We write $|001\rangle_{ABC}$, etc., as shorthand for $|0\rangle_A \otimes |0\rangle_B \otimes |1\rangle_C$. Since $\{|\epsilon_A\epsilon_B\epsilon_C\rangle_{ABC} : \epsilon_A, \epsilon_B, \epsilon_C = 0, 1\}$ is an orthogonal basis of the three-qubit system, we can uniquely write

$$|\psi\rangle = \sum_{\epsilon_A,\epsilon_B,\epsilon_C=0,1} \lambda_{\epsilon_A\epsilon_B\epsilon_C}|\epsilon_A\epsilon_B\epsilon_C\rangle_{ABC},$$

with $\Sigma|\lambda_{\varepsilon_1\varepsilon_2\varepsilon_3}|^2 = 1$. By using Eqs. (11), (16), and (29), it follows 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 of Eq. (26).

Now suppose that a state $|\psi\rangle$ satisfies Eq. (22). Since Eq. (22) is equivalent to

$$\mathcal{B}_3|\psi\rangle = 4|\psi\rangle, \tag{30}$$

it is concluded that $|\psi\rangle$ satisfies Eq. (24) and hence is of the form of Eq. (26). Note that

$$\mathcal{B}_3 = \mathcal{B}_2 \otimes \frac{1}{2}(C + C') + \mathcal{B}_2' \otimes \frac{1}{2}(C - C'),$$

where $\mathcal{B}_2' = A'B' + A'B + AB' - AB$ denote the same expression $\mathcal{B}_2$ but with the A and A', B, and B' exchanged. Then, by Eqs. (27) and (28) one has

$$\mathcal{B}_3|\psi\rangle = \frac{1}{2}ae^{-i\gamma}[(1+i)\mathcal{B}_2 + (1-i)\mathcal{B}_2']|00\rangle_{AB}|1\rangle_C + \frac{1}{2}be^{i\gamma}[(1-i)\mathcal{B}_2 + (1+i)\mathcal{B}_2']|11\rangle_{AB}|0\rangle_C.$$

From Eq. (30) we conclude that

$$\frac{1}{2}ae^{-i\gamma}[(1+i)\mathcal{B}_2 + (1-i)\mathcal{B}_2']|00\rangle_{AB} = 4b|11\rangle_{AB} \tag{31}$$

and

$$\frac{1}{2}be^{i\gamma}[(1-i)\mathcal{B}_2 + (1+i)\mathcal{B}_2']|11\rangle_{AB} = 4a|00\rangle_{AB}. \tag{32}$$

By Eq. (31) we have that

$$4|b| \leqslant \frac{1}{2}|a|(|1+i|\|\mathcal{B}_2\| + |1-i|\|\mathcal{B}_2'\|) \leqslant \frac{1}{2}|a|(\sqrt{2}\times 2\sqrt{2} + \sqrt{2}\times 2\sqrt{2}) = 4|a|,$$

since $\|\mathcal{B}_2\|$, $\|\mathcal{B}_2'\| \leqslant 2\sqrt{2}$ as shown in the two-qubit case. This concludes that $|b| \leqslant |a|$. Similarly, by Eq. (32) we have that $|a| \leqslant |b|$ and so $|a| = |b|$. Therefore, we have that $a = (1/\sqrt{2})e^{i\phi}$, $b = (1/\sqrt{2})e^{i\theta}$ for some $0 \leqslant \phi$, $\Theta \leqslant 2\pi$—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 transformation of the GHZ state, because

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

where

$$U_A = U_1\begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix}, \quad U_B = U_2\begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix},$$

and $U_C = U_3$. Here, U_1 is the unitary transform from the original σ_z^1 representation to the 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 transformations are 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 transformations of a maximally entangled state are equally valid entangled states [12]; we therefore obtain the characterizations of both two-qubit and three-qubit maximally entangled states via the Bell-CHSH and Bell-Klyshko inequalities, respectively. Finally, we remark that the three-qubit W state

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

cannot be obtained from the GHZ state by a local transformation [16] 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 Greenberger-Horne-Zeilinger theorem [5]; that is, the W state does not provide a 100% contradiction between quantum mechanics and Einstein, Podolsky, and Rosen's local realism [17]. Since the Bell inequality and GHZ theorem are two main themes on the violation of EPR's local realism, it is concluded that from the point of view of 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].

[1] J. S. Bell, Physics (Long Island City, N.Y.) **1**, 195 (1964).
[2] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935).
[3] N. Gisin, Phys. Lett. A **154**, 201 (1991).
[4] J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt, Phys. Rev. Lett. **23**, 880 (1969).
[5] D. M. Greenberger, M. A. Horne, and A. Zeilinger, in *Bell's Theorem, Quantum Theory, and Conceptions of the Universe*, edited by M. Kafatos (Kluwer, Dordrecht, 1989), p. 69; N. D. Mermin, Phys. Today **43**(6), 9 (1990); N. D. Mermin, Am. J. Phys. **58**, 731 (1990).
[6] N. Gisin, G. Ribordy, W. Tittle, and H. Zbinden, Rev. Mod. Phys. **74**, 145 (2002); M. Nielsen and I. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
[7] A search for "maximally entangled states" in tittle on www.arxiv.org/quant-ph yields 35 results.
[8] N. Gisin and H. Bechmann-Pasquinucci, Phys. Lett. A **246**, 1 (1998).
[9] G. Kar, Phys. Lett. A **204**, 99 (1995); J. L. Cereceda, *ibid.* **212**, 123 (1996).
[10] S. L. Braunstein, A. Mann, and M. Revzen, Phys. Rev. Lett. **68**, 3259 (1992).
[11] D. N. Klyshko, Phys. Lett. A **172**, 399 (1993); A. V. Belinskii and D. N. Klyshko, Phys. Usp. **36**, 653 (1993).
[12] N. Linden and S. Popescu, Fortschr. Phys. **46**, 567 (1998).
[13] B. S. Cirel'son, Lett. Math. Phys. **4**, 93 (1980).
[14] W. Pauli, Z. Phys. **43**, 601 (1927).
[15] L. Hardy, Phys. Lett. A **160**, 1 (1991).
[16] W. Dür, G. Vidal, and J. I. Cirac, Phys. Rev. A **62**, 062314 (2000).
[17] A. Cabello, Phys. Rev. A **63**, 022104 (2001).
[18] A. Sen(De), U. Sen, M. Wieśniak, D. Kaszlikowski, and M. Żukowski, Phys. Rev. A **68**, 062306 (2003).