Quantum Nonlocality of Arbitrary Dimensional Bipartite States

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We study the nonlocality of arbitrary dimensional bipartite quantum states. By computing the maximal violation of a set of multi-setting Bell inequalities, an analytical and computable lower bound has been derived for general two-qubit states. This bound gives the necessary condition that a two-qubit state admits no local hidden variable models. The lower bound is shown to be better than that from the CHSH inequality in judging the nonlocality of some quantum states. The results are generalized to the case of high dimensional quantum states, and a sufficient condition for detecting the non-locality has been presented.

Quantum mechanics is inherently nonlocal, as revealed by the violation of Bell inequality\(^1\). A bipartite quantum state may violate some Bell inequalities such that the local measurement outcomes can not be modeled by classical random distributions over probability spaces. Namely, the state admits no local hidden variable (LHV) model.

The nonlocality and quantum entanglement play important roles in our fundamental understandings of physical world as well as in various novel quantum informational tasks\(^2,3\). A quantum state without entanglement must admit LHV models\(^4,9\). However, not all the entangled quantum states are of nonlocality\(^10–12,14\). To show that a quantum state admits a LHV model, it is sufficient to construct such LHV model explicitly\(^10,12\). To show that a quantum state admits no LHV models, it is sufficient to show that it violates a Bell inequality\(^15,16\). Quantum states that violate Bell inequalities are also useful in building quantum protocols to decrease communication complexity\(^17\) and provide secure quantum communication\(^18,19\). Moreover, since the nonlocality is detected by the violation of Bell inequalities, quantum nonlocality could be quantified in terms of the maximal violation value for all Bell inequalities. However, it is a formidable task either to show that a state admits an LHV model, or to show that a state violates a Bell inequality.

Let \( A_i, B_j, i = 1, 2, \ldots, n \), be observables with respect to the two subsystems of a bipartite state, with eigenvalues \( \pm 1 \). Let \( M \) be a real matrix with entries \( M_{ij} \) such that \( \sum_{i,j} M_{ij} = 1 \). Denote \( I = \sum_{i,j} M_{ij} A_i \otimes B_j \) the corresponding Bell operator. Define

\[
Q = \sup_{\rho} \left( \sum_{i,j} M_{ij} A_i \otimes B_j \right) \left( \rho \right)
\]

where \( \langle I \rangle = tr(\rho I) \) stands for the mean value of the Bell operator associated to state \( \rho \). Obviously a quantum state \( \rho \) can never be described by a LHV model if and only if \( Q \) is strictly larger than 1.

In\(^10–14\), the authors have investigated the nonlocality of Werner states. For two-qubit Werner state

\[
\rho_w = x | \psi^- \rangle \langle \psi^- | + (1 - x) | \psi^+ \rangle \langle \psi^+ | = \frac{1}{2}( | 01 \rangle - | 10 \rangle ) \sqrt{2},
\]

the quantity \( Q \) is proved to be \( \frac{4}{3} K_0(3) \) in\(^12\), where \( K_0(3) \) is the Grothendieck's constant of order three. However, since up to now one does not know the exact value of the Grothendieck's constant \( K_0(3) \), \( Q \) is still not known. The upper and lower bounds of the threshold value of this parameter \( Q \) have been refined by constructing better LHV models\(^10–12\) or by finding better Bell inequalities\(^3,14\).

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In the paper we study the nonlocality of arbitrary two-qubit states and present an analytical and computable lower bound of the quantity \( Q \) by computing the maximal violation of a set of multi-setting Bell inequalities. The lower bound is shown to be better than that derived in terms of the CHSH inequality for some quantum states. We also present a sufficient condition that a high dimensional quantum state admits LHV models.

**Results**

**Lower bound of \( Q \) for two-qubit quantum states.** A two-qubit quantum state \( \rho \) can be always expressed in terms of Pauli matrices \( \sigma_i \), \( i = 1, 2, 3 \),

\[
\rho = \frac{1}{4} I \otimes I + \sum_{i=1}^{3} r_i \sigma_i \otimes I + \sum_{j=1}^{3} s_j I \otimes \sigma_j + \sum_{i,j=1}^{3} t_{ij} \sigma_i \otimes \sigma_j,
\]

(2)

where \( r_i = \frac{1}{4} \text{Tr}(\rho \sigma_i \otimes I) \), \( s_j = \frac{1}{4} \text{Tr}(\rho I \otimes \sigma_j) \) and \( t_{ij} = \frac{1}{4} \text{Tr}(\rho \sigma_i \otimes \sigma_j) \). We denote \( T \) the matrix with entries \( t_{ij} \).

The key point in computing \( Q \) is to find \( \max_{a,b \in \{0,1\}} \{I\} \) over all \( M \) under the condition \( \max_{a,b \in \{0,1\}} \{M_{ab}\} = 1 \). In \( n^4 \) a Bell operator has been introduced,

\[
I = \frac{1}{n^2} \sum_{i,j=1}^{n} \left[ A_i \otimes B_j + \sum_{1 \leq i < j \leq n} C_{ij} \otimes (B_i - B_j) + \sum_{1 \leq i < j \leq n} (A_i - A_j) \otimes D_{ij} \right],
\]

(3)

where \( A_i, B_j, C_{ij} \) and \( D_{ij} \) are observables of the form \( \sum_{i=1}^{3} x_i \sigma_i \) with \( x = (x_1, x_2, x_3) \) the unit vectors.

To find an analytical lower bound of \( Q \), we consider infinite many measurements settings, \( n \rightarrow \infty \). Then the discrete summation in (3) is transformed into an integral of the spherical coordinate over the sphere \( S^2 \subset R^3 \). We denote the spherical coordinate of \( S^2 \) by \( (\phi, \theta) \) with \( \theta = (\theta_1, \theta_2, \theta_3) \) can parameterized by \( x_i = \sin \phi_i \sin \phi_2, x_2 = \sin \phi_1 \cos \phi_2, x_3 = \cos \phi_1 \). For any \( 0 \leq a < b \leq \frac{\pi}{2} \), we denote \( \Omega_{ab} = \{ x \in S^2 : a < \phi(x) < b \} \).

**Theorem 1:** For arbitrary two-qubit quantum state \( \rho \) given by (2), we have

\[
Q \geq \max \left[ 4 \frac{s_{ab} s_{cd}}{s_{ab}^2} \int_{\Omega_a} \int_{\Omega_b} \langle \vec{x}, T \vec{y} \rangle \, d\mu(\vec{x}) \, d\mu(\vec{y}) + 2 \frac{s_{ab}^2}{s_{ab}^4} \int_{\Omega_a} \int_{\Omega_b} |T(\vec{x} - \vec{y})| \, d\mu(\vec{x}) \, d\mu(\vec{y}) \right].
\]

(4)

where \( T^* \) stands for the transposition of \( T \) and \( s_{ab} = \int_{\Omega_a} d\mu(\vec{x}) \). The maximum on the right side of the inequality goes over all the integral area \( \Omega_a \times \Omega_b \) with \( 0 \leq a < b \leq \frac{\pi}{2} \) and \( 0 \leq c < d \leq \frac{\pi}{2} \).

See Methods for the proof of theorem 1.

The bound (4) can be calculated by parameterizing the integral in terms of the sphere coordinates. Once a two-qubit is given, the corresponding matrix \( T \) is given. And the bound is solely determined by \( T \). This is similar to the CHSH inequality, where the maximal violation is given by the two larger singular values of \( T \).

As an example, consider \( T = \text{diag}(p_1, p_2, p_3) \), we have

\[
s_{ab} = \int_0^{2\pi} \int_0^b \sin \phi \, d\phi \, d\phi.,
\]

(5)

\( s_{cd} \) in (4) are similarly given. The first two terms in \( s_{ab} \) (4) are given by

\[
\int_{\Omega_a} \int_{\Omega_b} \langle \vec{x}, T \vec{y} \rangle \, d\mu(\vec{x}) \, d\mu(\vec{y}) = \int_a^b \int_c^d \int_0^{2\pi} \int_0^{2\pi} f(\sin \phi_1 \sin \phi_2 d\phi_1 d\phi_2 d\phi_3 d\phi_4),
\]

(6)

\[
\int_{\Omega_a} \int_{\Omega_b} |T(\vec{x} - \vec{y})| \, d\mu(\vec{x}) \, d\mu(\vec{y}) = \int_a^b \int_c^d \int_0^{2\pi} \int_0^{2\pi} g(\sin \phi_1 \sin \phi_2 d\phi_1 d\phi_2 d\phi_3 d\phi_4),
\]

(7)

where

\[
f = p_1 \sin \phi_1 \sin \phi_2 \sin \phi_3 \sin \phi_4 + p_2 \sin \phi_1 \cos \phi_1 \sin \phi_2 \cos \phi_2 + p_3 \cos \phi_1 \sin \phi_1, \\
g = \left[ p_1^2 (\sin \phi_1 \sin \phi_2 \sin \phi_3)^2 + p_2^2 (\sin \phi_1 \cos \phi_1 \sin \phi_2)^2 \right] \frac{1}{2}.
\]
The last term in (4) is similarly to the second term, with $T$ being replaced by $T^t$.

Thus for any given two-qubit quantum state, by substituting $T$ into the integral, we have the lower bound of $Q$. The maximum taken over $\Omega_a \times \Omega_b$ can be searched by varying the integral ranges. The Werner state considered in 10–14 is a special case that $p_1 = p_2 = p_3 = p$. From our Theorem 1, we have that for $0.7054 < x \leq 1$, the lower bound of $Q$ is always larger than that is derived from the maximal violation of the CHSH inequality, see Fig. 1.

Let us now consider the generalized Bell diagonal two-qubit states in detail,

$$\rho = \frac{1}{4} \left( I \otimes I - p_1 \sigma_1 \otimes \sigma_1 - p_2 \sigma_2 \otimes \sigma_2 - p_3 \sigma_3 \otimes \sigma_3 \right).$$

(8)

The positivity property requires that the parameters $\{p_1, p_2, p_3\}$ must be inside a regular tetrahedron with vertexes $\{-1, -1, 1\}, \{1, -1, -1\}, \{1, 1, 1\}, \{-1, 1, -1\}$. By computing the lower bound of $Q$ according to Theorem 1, we detect the regions where the quantum states can never be described by LHV models, see Fig. 2.

By setting $p_1 = 0.9, p_2 = 0.9$ and $p_3 = 0.9$, one has the the cross-sectional view, see Fig. 3.

**High dimensional case.** Generalizing our approach to high dimensional case, now we study the nonlocality of general $d \times d$ bipartite quantum states. To detect the nonlocality of a quantum state, the important thing is to find a 'good' Bell operator. For even $d$, we set $\Gamma_1, \Gamma_2$ and $\Gamma_3$ to be block-diagonal matrices, with each block an ordinary Pauli matrix, $\sigma_1, \sigma_2$ and $\sigma_3$ respectively, as described in Eq for $\Gamma_1$ and $\Gamma_3$. When $d$ is odd, we set the elements of the $k$th row and the $k$th column in $\Gamma_1, \Gamma_2$ and $\Gamma_3$ to be zero, with the rest elements of $\Gamma_1, \Gamma_2$ and $\Gamma_3$ being the block-diagonal matrices like the case of even $d$. Let $\Gamma_0$ be a $d \times d$ matrix whose only nonvanishing entry is $(\Gamma_0)_{mm} = 1$ for $m \in 1, 2, \ldots, d$, for odd $d$ and be a null matrix for even $d$. We define observables $A = \tilde{a} \cdot \Gamma$ and $B = \tilde{b} \cdot \Gamma$, where $\Gamma = (\Gamma_0, \Gamma_1, \Gamma_2, \Gamma_3)$, $\tilde{a} = (1, a_1, a_2, a_3)$ and $\tilde{b} = (1, b_1, b_2, b_3)$ are vectors with norm $\sqrt{2}$. It is easy to check that the eigenvalues of the observables $A$ and $B$ are either 1 or $-1$.

We define the Bell operator to be

$$I_d = \frac{1}{n^2} \left| \sum_{i,j=1}^n A_i \otimes B_j + \sum_{1 \leq i < j \leq n} C_{ij} \otimes (B_i - B_j) + \sum_{1 \leq i < j \leq n} (A_i - A_j) \otimes D_{ij} \right|,$$

(9)

where $A, B, C$ and $D$ are observables of the form $\tilde{a}_i \cdot \Gamma, \tilde{b}_j \cdot \Gamma, \tilde{c}_i \cdot \Gamma$ and $\tilde{d}_j \cdot \Gamma$ respectively; $\tilde{a}_i, \tilde{b}_j, \tilde{c}_i$ and $\tilde{d}_j$ are vectors with norm $\sqrt{2}$. 

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**Figure 1.** The lower bounds (denoted by $f(x)$) of $Q$ in Theorem 1 (solid line) and that obtained from the CHSH inequality (dashed line).
The Bell operator (9) has the same structure as that in (3), but fits for \(d \times d\) quantum system. For a \(d \times d\) quantum state \(\rho\), we set \(\gamma\) to be a matrix with elements \(\gamma_{ij} = \text{tr}(\rho \Gamma_i \otimes \Gamma_j)\), \(i, j = 0, 1, 2, 3\). A lower bound of \(Q\) defined in (1) for \(d \times d\) quantum system can be readily obtained as the follows.

**Theorem 2**: For any quantum state \(\rho\) in \(d \times d\) quantum system \(\mathcal{H}_{AB}\), we have that

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Figure 2. The quantum states \(\rho_w\) that admits no LHV models are listed by the points parameterized by \((p_1, p_2, p_3)\).

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Figure 3. The same cross-sectional view of Fig. 2 for all \(p_1 = 0.9, p_2 = 0.9\) and \(p_3 = 0.9\).
where $\gamma'$ stands for the transposition of $\gamma$, and $s_{\alpha\beta} = \int_{\Omega_{a}^{b} \times \Omega_{b}^{a}} d\mu (\bar{x})$. The maximum on the right side of the inequality is taken over all the selection of integral area $\Omega_{a}^{b} \times \Omega_{b}^{a}$ with $0 \leq a < b \leq \frac{\pi}{2}$ and $0 \leq c < d \leq \frac{\pi}{2}$.

See Methods for the proof of theorem 2.

According to the definition of $Q$ in (1), we have that if the lower bound for $Q$ in theorem 2 is larger than one, then a quantum state in $d \times d$ bipartite quantum system can never be described by an LHV model. The bound can readily calculated, similar to the two-qubit case, once the matrix $\gamma$ for state is given.

Let us consider the isotropic state $\rho_{I}^{20,21}$, a mixture of the singlet state $\rho = \sum_{i=1}^{3} \alpha_{i} \beta_{i}^{*} |i\rangle \langle i| + 1-x |1\rangle \langle 1| + x |2\rangle \langle 2|$, $0 \leq x \leq 1$. $\rho_{I}$ is entangled for $x > \frac{1}{2} \left(1 + \frac{\sqrt{3}}{4}\right)$. For $d=3$, $\rho_{I}$ is entangled for $x > \frac{1}{4}$. From Theorem 2, $\rho_{I}$ is nonlocal for $x > 0.7653$.

As another example we consider the state $\rho$ from mixing the singlet state $\rho = \sum_{i=1}^{3} \alpha_{i} \beta_{i}^{*} |i\rangle \langle i| + 1-x |1\rangle \langle 1| + x |2\rangle \langle 2|$, $0 \leq x \leq 1$. $\rho_{I}$ is entangled for $x > \frac{1}{2} \left(1 + \frac{\sqrt{3}}{4}\right)$. For $d=3$, $\rho_{I}$ is entangled for $x > \frac{1}{4}$. From Theorem 2, $\rho_{I}$ is nonlocal for $x > 0.7653$.

Discussions

Nowadays, quantum nonlocality is a fundamental subject in quantum information theory such as quantum cryptography, complexity theory, communication complexity, estimates for the dimension of the underlying Hilbert space, entangled games, etc. Thus it is a basic question to check and to qualify the nonlocality of a quantum state. We have derived an analytical and computable lower bound of the quantum violation by using a Bell inequality with infinitely many measurement settings. The bound is shown to be better than that is obtained from the CHSH inequality and the discrete models. Sufficient conditions for the LHV description of high dimensional quantum states have also derived. Apart from the computation of maximal violations for bipartite Bell inequalities, our methods can also contribute to the analysis of the nonlocality of multipartite quantum systems.

Methods

Proof of Theorem 1. For any two-qubit quantum state $\rho$ given in (2), we have

$$Q \geq \max \left| \left( \frac{1}{n^{2}} \sum_{i=1}^{n} \text{tr} \left( A_{i} \otimes B_{j} \rho \right) \right) + \sum_{1 \leq i < j \leq n} \text{tr} \left( C_{y} \otimes \left( B_{i} - B_{j} \right) \rho \right) + \sum_{1 \leq i < j \leq n} \text{tr} \left( \left( A_{i} - A_{j} \right) \otimes D_{y} \rho \right) \right|,$$

Figure 4. Quantum states $\rho$ parameterized by $(\alpha, \beta)$ that admit no LHV model (blue regions).
\[
\begin{align*}
&= \max_{n} \frac{4}{n^2} \left| \sum_{i,j=1}^{n} \sum_{k,l=1}^{3} \alpha_{ik} b_{ij} b_{kl} + \sum_{1 \leq i < j \leq n} \sum_{k,l=1}^{3} \beta_{ik} \beta_{jl} + \sum_{1 \leq i < j \leq n} \sum_{k,l=1}^{3} (\alpha_{ik} - \alpha_{jl}) d_{ij} d_{kl} \right| \\
&= \max_{n} \frac{4}{n^2} \left| \sum_{i,j=1}^{n} \langle \tilde{a}_i, T \tilde{b}_j \rangle + \sum_{1 \leq i < j \leq n} \langle \tilde{c}_i, T (\tilde{b}_i - \tilde{b}_j) \rangle + \sum_{1 \leq i < j \leq n} \langle T' (\tilde{a}_i - \tilde{a}_j), \tilde{a}_j \rangle \right| \\
&= \max_{n} \frac{4}{n^2} \left| \sum_{i,j=1}^{n} \langle \tilde{a}_i, T \tilde{b}_j \rangle + \sum_{1 \leq i < j \leq n} \left| T (\tilde{b}_i - \tilde{b}_j) \right| + \sum_{1 \leq i < j \leq n} \left| T' (\tilde{a}_i - \tilde{a}_j) \right| \right|
\end{align*}
\]

Under the limit \( n \to \infty \), we have

\[
Q \geq \max_{n} \left| \frac{4}{s_{ab} s_{cd}} \int_{O_0^d \times O_0^d} (\tilde{x}, T \tilde{y}) \, d\mu (\tilde{x}) \, d\mu (\tilde{y}) \right| + \frac{2}{s_{cd}^2} \int_{O_0^d \times O_0^d} T (\tilde{x} - \tilde{y}) \, d\mu (\tilde{x}) \, d\mu (\tilde{y})
\]

which proves (4).

**Proof of Theorem 2.** With the special selected observables of the form \( \tilde{a} \cdot \Gamma \) for \( d \times d \) quantum systems, we have that

\[
Q \geq \max |\{I_d\}| = \max \left| \frac{1}{n^2} \left| \sum_{i,j=1}^{n} \operatorname{tr} (A_i \otimes B_j \rho) + \sum_{1 \leq i < j \leq n} \operatorname{tr} (C_{ij} \otimes (B_i - B_j) \rho) \right|^2 \right|
\]

\[
= \frac{1}{n^2} \max \left| \sum_{i,j=1}^{n} \sum_{k,l=0}^{3} \alpha_{ik} b_{ij} \gamma_{kl} + \sum_{1 \leq i < j \leq n} \sum_{k,l=0}^{3} (\gamma_{ij} b_{ij} - \gamma_{kl} b_{ij} + (\alpha_{ik} - \alpha_{jl}) d_{ij} \gamma_{kl}) \right|
\]

\[
= \frac{1}{n^2} \max \left| \sum_{i,j=1}^{n} \langle \tilde{a}_i, \gamma \tilde{b}_j \rangle + \sum_{1 \leq i < j \leq n} \left| (\gamma (\tilde{b}_i - \tilde{b}_j) + (\gamma (\tilde{a}_i - \tilde{a}_j) \right| \right|
\]

\[
\geq \max \left| \frac{1}{s_{ab} s_{cd}} \int_{O_0^d \times O_0^d} (\tilde{x}, \gamma \tilde{y}) \, d\mu (\tilde{x}) \, d\mu (\tilde{y}) \right| + \frac{1}{2 s_{cd}^2} \int_{O_0^d \times O_0^d} \gamma (\tilde{x} - \tilde{y}) \, d\mu (\tilde{x}) \, d\mu (\tilde{y})
\]

where in the last step, we have taken the limit \( n \to \infty \).

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Author Contributions
M. Li and S.-M. Fei wrote the main manuscript text. T. Zhang, B. Hua, and X.Q. Li-Jost computed the examples. All authors reviewed the manuscript.

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