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Genuinely high-dimensional nonlocality optimized by complementary measurements

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Abstract. Qubits exhibit extreme nonlocality when their state is maximally entangled and this is observed by mutually unbiased local measurements. This criterion does not hold for the Bell inequalities of high-dimensional systems (qudits), recently proposed by Collins–Gisin–Linden–Massar–Popescu and Son–Lee–Kim. Taking an alternative approach, called the quantum-to-classical approach, we derive a series of Bell inequalities for qudits that satisfy the criterion as for the qubits. In the derivation each d -dimensional subsystem is assumed to be measured by one of d possible measurements with d being a prime integer. By applying to two qubits ($d = 2$), we find that a derived inequality is reduced to the Clauser–Horne–Shimony–Holt inequality when the degree of nonlocality is optimized over all the possible states and local observables. Further applying to two and three qutrits ($d = 3$), we find Bell inequalities that are violated for the three-dimensionally entangled states but are not violated by any two-dimensionally entangled states. In other words, the inequalities discriminate three-dimensional (3D) entanglement from two-dimensional (2D) entanglement and in this sense they are genuinely 3D. In addition, for the two qutrits we give a quantitative description of the relations among the three degrees of complementarity, entanglement and nonlocality. It is shown that the degree of complementarity jumps abruptly to very close to its maximum as nonlocality starts appearing. These characteristics imply that complementarity plays a more significant role in the present inequality compared with the previously proposed inequality.

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1. Introduction

The complementarity principle lies at the heart of quantum mechanics. It contrasts the quantum phenomena with the reality of classical physics. Historically, complementarity is often identified with the wave–particle duality of matter. However, it is a more general notion. We say that two observables A and B are mutually complementary if precise knowledge of one of them implies that all possible outcomes of measuring the other one are equally probable [1]. In this sense the two observables are often said to be mutually unbiased. There have been experimental observations of complementarity such as in a quantum eraser that allow the investigation of complementarity in optical systems [2]. The complementarity principle implies that no matter how a system is prepared, there always exists a measurement whose outcome is utterly unpredictable [1]: it is not possible to obtain complete knowledge of the future in the sense of classical physics. Thus, complementarity is ‘simply an expression of the fact that in order to measure two mutually complementary quantities, we would have to use apparatuses which mutually exclude each other’ [3]. In classical theory, on the other hand, all observables are assumed compatible. That is, one observable can be measured without disturbing the others.

Nonlocality also discriminates between classical and quantum behavior, more precisely, their correlations [4]. The contrast of their correlations can be seen by using Bell inequalities, for instance, the Clauser–Horne–Shimony–Holt (CHSH) inequality for a bipartite two-dimensional (2D) system (two qubits) [5]. The CHSH inequality, a constraint of correlation that the two subsystems must obey due to local realism, is violated by quantum theory if they are in an entangled state. It is interesting to observe that in order to maximally violate CHSH inequality, it is necessary that local measurements are mutually complementary and the two subsystems are in a maximally entangled state [6]. This observation implies that nonlocality is revealed by an interplay of entanglement and complementary (or mutually unbiased) measurements, two fundamental notions in quantum theory. This claim looks reasonable as the bipartite system can be simulated by local hidden variable theory if the state is disentangled

or the measurements are compatible. A Bell inequality is said to satisfy the criterion of complementarity–entanglement–nonlocality (CEN) if it is maximally violated by mutually unbiased measurements and a maximally entangled state. The CEN criterion is also observed in the Clauser–Horne inequality of two qubits [7], the Greenberger–Horne–Zeilinger (GHZ) nonlocality of three qubits [8] and subsequently derived Bell inequalities of many qubits [9]. In particular, the role of complementarity in multi-qubit GHZ nonlocality was explicitly discussed in [10]. It is desired to know whether any Bell inequality for higher-dimensional systems (qudits) satisfies the CEN criterion. We discuss this problem in this paper.

To qudits rather than qubits, the Gisin–Peres approach can be applied where each of the local observables has a block-diagonal form in terms of two-valued observables [11]. This approach has been applied to arbitrary systems in showing their nonlocality. Due to its block-diagonal construction of local observables, on the other hand, it picks up only 2D nature by projecting high-dimensional entanglement. For instance, one may show the maximal violation of CHSH inequality for a mixed state, a statistical mixture of maximally entangled states in 2D *subspaces* [12]. In other words, the Gisin–Peres approach cannot contrast high-dimensional entanglement from 2D one. In this sense we say that the Gisin–Peres approach is genuinely 2D [13, 14]. On the other hand, we say that a Bell inequality is genuinely d -dimensional if d -dimensional entanglement attains the optimal degree of quantum violation and no sub-dimensional entanglement does. A similar notion, called a dimension witness, was proposed in [15]. Genuinely d -dimensional GHZ nonlocality has been shown for d or $(d + 1)$ qudits [14, 16] and an arbitrary odd number (≥ 3) of qudits [13], with d being an *even* integer.

There are also Bell inequalities that are known to be genuinely high dimensional: the Collins–Gisin–Linden–Massar–Popescu (CGLMP) inequality [17] and the Son–Lee–Kim (SLK) inequality [18]. However, unfortunately these do not satisfy the CEN criterion. The CGLMP inequality is maximally violated by a partially entangled state with mutually *biased* measurements, even though it is tight [19, 20]. The SLK inequality possesses a better characteristic such that it is maximally violated by a maximally entangled state but still with mutually biased measurements, satisfying the criterion only partially. Noting that two observables are allowed for each party in these inequalities, one might attribute these results to the restriction on the number of observables. It was conjectured in [19, 21, 22] that the ‘anomaly’ will disappear when more observables are allowed. However, it remains an open question, and we answer this partially in this paper.

In this paper, we derive a set of Bell inequalities for N qudits, each with d possible observables, that satisfy the CEN criterion. For this purpose, we take a quantum-to-classical approach, different from the conventional ones; we introduce a quantum identity, instead of a classical one, consisting of d mutually complementary observables so that we can derive a Bell operator by releasing the constraint of the observables. The form of the quantum identity varies in terms of a set of parameters so that we are to have a series of Bell operators. We prove that the maximum of the quantum Bell function remains invariant over the parameters. The series of Bell inequalities all satisfy the CEN criterion. To demonstrate the principal idea, we apply this approach to two qubits and show that the Bell inequality of the maximal ratio of the quantum maximum to the classical maximum (maximal QCR) over the parameter is reduced to the CHSH. By generalizing the quantum-to-classical approach to many qudits, we derive the general form of the Bell inequalities satisfying the CEN criterion. In particular, we investigate the two and three qutrit cases in detail. Among the derived Bell inequalities, the Bell inequality of the optimal QCR over the parameters discriminates three-dimensional (3D) entanglement

from 2D entanglement, i.e. it is violated for the three-dimensionally entangled states but is not violated by the two-dimensionally entangled states. In this sense the Bell inequality is genuinely 3D. These results hold for both the cases of two and three qutrits. In addition, for the two qutrits we give a quantitative description of the relations among the three degrees of complementarity, entanglement and nonlocality. It is shown that the degree of complementarity jumps abruptly to very close to its maximum as the nonlocality starts appearing. These characteristics imply that complementarity plays a more significant role in the present inequality compared with the CGLMP and SLK inequalities.

2. The quantum-to-classical approach

To derive a Bell inequality satisfying the CEN criterion, we take an alternative approach to the conventional method. The conventional approach has two essential steps: (C1) finding a classical identity of a constraint that classical observables must obey, and deriving a statistical inequality, called a Bell inequality, based on local hidden variable theory, and (C2) showing its violation by quantum observables on an entangled quantum state. We call it ‘the classical-to-quantum approach’. On the other hand, the present approach is reciprocal, i.e. the quantum-to-classical approach. Here, (Q1) we introduce a quantum-mechanical identity that complementary observables satisfy, so as to derive a Bell operator, and we find its maximal expectation over possible states and observables. Then, (Q2) we examine, for the corresponding classical Bell function, whether any local hidden variable theories reach the quantum maximum.

2.1. A set of Bell inequalities for two qubits

In order to clearly show our principal idea, we apply the quantum-to-classical approach to a two-qubit system as an example. Suppose that two qubits are distributed over a long distance and they are observed by two persons, say, Alice and Bob. They are permitted to independently choose one of two observables. Each local observable is assumed to be two-valued, taking a value of ± 1 . Quantum mechanically, two local observables for Alice are represented by Hermitian (or unitary) operators, \hat{a}_0 and \hat{a}_1 . Those for Bob are \hat{b}_0 and \hat{b}_1 . Every observable operator has eigenvalues of ± 1 .

A quantum identity to be introduced is composed of mutually complementary observables so that we temporarily assume the local observables to be mutually complementary: $\hat{a}_0 = \hat{b}_0 = \hat{\sigma}_x$ and $\hat{a}_1 = \hat{b}_1 = \hat{\sigma}_y$, where $\hat{\sigma}_x$ and $\hat{\sigma}_y$ are Pauli spin operators. Note that their eigenvectors form mutually unbiased bases:

$$|{}_x\langle i|j\rangle_y|^2 = \frac{1}{2}, \quad \forall i, j, \quad (1)$$

where $|i\rangle_x$ and $|j\rangle_y$ are eigenvectors of $\hat{\sigma}_x$ and $\hat{\sigma}_y$, respectively. Consider a linear sum of composite observables,

$$\hat{G} = \hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y. \quad (2)$$

This operator is called ‘generic’ as it is at the heart of the quantum identity. The quantum expectation of \hat{G} over all possible quantum states has a mathematical upper bound of 2, by using a triangle inequality and noting $|\langle \psi | \hat{\sigma}_{x,y} \otimes \hat{\sigma}_{x,y} | \psi \rangle| \leq 1, \forall |\psi\rangle$. The mathematical upper bound is reachable, that is, it is a quantum maximum for a maximally entangled state,

$$|2ES\rangle = \frac{1}{\sqrt{2}}(|0, 1\rangle + |1, 0\rangle), \quad (3)$$

where $|i, j\rangle = |i\rangle \otimes |j\rangle$ with a standard orthonormal basis $\{|0\rangle, |1\rangle\}$, the set of eigenvectors of $\hat{\sigma}_z$. The state $|2ES\rangle$ is a maximally entangled state of the two qubits and we say it is a 2D maximally entangled state when comparing with qutrit states. It is remarkable that the quantum maximum is reachable from a maximally entangled state. The generic operator has nothing to do with a nonlocality test: the classical function based on local hidden variable theories, corresponding to \hat{G} , also has a classical maximum equal to the quantum, implying no conflict between the local hidden variable theories and the quantum theory.

We shall derive a Bell operator by using a quantum identity, which is defined by the unitary transformation of the generic operator \hat{G} in equation (2). Choosing a local unitary operator \hat{U} in the form of

$$\hat{U} = |0\rangle\langle 0| + e^{i\pi H} |1\rangle\langle 1|, \quad (4)$$

where H is a parameter in the interval $[0, 2)$, the quantum identity is given by

$$\mathbb{1} \otimes \hat{U}^\dagger \hat{G} \mathbb{1} \otimes \hat{U} = \hat{\sigma}_x \otimes (\hat{\sigma}_x \cos \pi H - \hat{\sigma}_y \sin \pi H) + \hat{\sigma}_y \otimes (\hat{\sigma}_x \sin \pi H + \hat{\sigma}_y \cos \pi H), \quad (5)$$

where $\mathbb{1}$ is an identity operator. It is clear that the expectation of the transformed generic operator has the same maximum as the generic operator. The local observables have so far been assumed to be mutually complementary. This constraint is released such that the Pauli operators are replaced by arbitrary local observables \hat{a}_i (\hat{b}_j), each having eigenvalues ± 1 , for Alice (Bob). Then, we obtain a Bell operator

$$\begin{aligned} \hat{B}(\hat{a}_{k_1}, \hat{b}_{k_2}|H) &= \hat{a}_0 \otimes (\hat{b}_0 \cos \pi H - \hat{b}_1 \sin \pi H) + \hat{a}_1 \otimes (\hat{b}_0 \sin \pi H + \hat{b}_1 \cos \pi H) \\ &= \sum_{k_1, k_2=0}^1 R_{k_1 k_2}(H) \hat{a}_{k_1} \otimes \hat{b}_{k_2}, \end{aligned} \quad (6)$$

where $\mathbf{R}(H)$ is a rotation matrix by an angle πH . It is remarkable that the quantum identity determines the structure of the Bell operator and altering H leads to a variety of Bell operators.

As the local observables are arbitrary, it is nontrivial whether the Bell operator $\hat{B}(H)$ leads to the same maximum as the generic operator \hat{G} . We show that this is the case. For a given state $|\psi\rangle$, the expectation of the Bell operator \hat{B} is bounded from above as

$$\langle \psi | \hat{B} | \psi \rangle \leq \left| \sum_{k_1=0}^1 \langle \psi | \hat{a}_{k_1} \otimes \sum_{k_2=0}^1 R_{k_1 k_2} \hat{b}_{k_2} | \psi \rangle \right|, \quad (7)$$

where we omitted the arguments, \hat{a}_{k_1} , \hat{b}_{k_2} and H , of \hat{B} and \mathbf{R} for the sake of simplicity. The upper bound of equation (7) is given by the Schwarz inequality as

$$\begin{aligned} \langle \psi | \hat{B} | \psi \rangle &\leq \sqrt{2 \sum_{k_1=0}^1 \left| \langle \psi | \hat{a}_{k_1} \otimes \sum_{k_2=0}^1 R_{k_1 k_2} \hat{b}_{k_2} | \psi \rangle \right|^2} \\ &\leq \sqrt{2 \langle \psi | \sum_{k_1=0}^1 \hat{a}_{k_1} \hat{a}_{k_1}^\dagger \otimes \sum_{k_2, k_3=0}^1 R_{k_1 k_2} R_{k_1 k_3}^* \hat{b}_{k_2} \hat{b}_{k_3}^\dagger | \psi \rangle}. \end{aligned} \quad (8)$$

Noting that $\hat{a}_k \hat{a}_k^\dagger = \hat{b}_k \hat{b}_k^\dagger = \mathbb{1}$ and $\mathbf{R}^T \mathbf{R} = I$ with an identity matrix I , the inequality is rewritten as

$$\langle \psi | \hat{B} | \psi \rangle \leq \sqrt{2 \langle \psi | \mathbb{1} \otimes 2 \mathbb{1} | \psi \rangle} = 2. \quad (9)$$

Note that the upper bound is equal to the maximum of \hat{G} . This implies that the Bell operator leads to the same maximum as the transformed generic operator when the local observables are chosen to be mutually complementary ($\sigma_{x,y}$ for Alice and $\hat{U} \sigma_{x,y} \hat{U}^\dagger$ for Bob, respectively) and eventually as \hat{G} through the quantum identity in equation (5).

We now consider the classical upper bound of the Bell function B_{cl} corresponding to the Bell operator \hat{B} . For the purpose, we introduce a set of hidden variables λ and their probability distribution function $\rho(\lambda)$. By replacing the quantum local observables $\hat{a}_{0,1}$ ($\hat{b}_{0,1}$) of Alice (Bob) with the classical $\alpha_{0,1}(\lambda)$ ($\beta_{0,1}(\lambda)$), the classical Bell function is given as

$$B_{\text{cl}}(\alpha_{k_1}, \beta_{k_2} | H) = \int d\lambda \rho(\lambda) \boldsymbol{\alpha}^\dagger(\lambda) \mathbf{R}(H) \boldsymbol{\beta}(\lambda), \quad (10)$$

where $\boldsymbol{\alpha}(\lambda)$ and $\boldsymbol{\beta}(\lambda)$ are 2D vectors whose components are ± 1 depending on the hidden variables λ . The Bell inequality is given by

$$B_{\text{cl}}(\alpha_{k_1}, \beta_{k_2} | H) \leq C(H), \quad (11)$$

where $C(H)$ is the maximum of $B_{\text{cl}}(H)$ for each H , given by

$$C(H) = \sqrt{2} \left(\left| \cos \left(\frac{4H+1}{4} \pi \right) \right| + \left| \cos \left(\frac{4H-1}{4} \pi \right) \right| \right). \quad (12)$$

Figure 1 presents $C(H)$ with respect to the parameter H . It has a value in the interval $[\sqrt{2}, 2]$. If $C(H) < 2$ or the classical maximum is smaller than the quantum, the Bell inequality satisfies the CEN criterion for each H . The maximum of B_{cl} is always less than or equal to the quantum and $H = 1/4$ particularly maximizes the ratio of the quantum maximum to the classical, QCR, to be $\sqrt{2}$: $\text{QCR}(H) = 2/C(H)$. The Bell function B of $H = 1/4$ reduces to the CHSH function [5]. By adopting the quantum-to-classical approach, we demonstrated the derivation of the set of Bell inequalities satisfying the CEN criterion for the two qubits. This approach provides a systematic method for constructing a variety of Bell inequalities, among which we may choose the most nonlocal. We showed for the two qubits that the most nonlocal Bell function is equivalent to CHSH. In the following section we apply this approach to many qudits.

2.2. A set of Bell inequalities for many qudits

For a quantum system in d -dimensional Hilbert space, a maximal test has d distinct outcomes. Each value of the outcome is commonly assigned to the language of classical physics. For instance, if we measure two distinct outcomes in a Stern–Gerlach experiment for a given atomic beam, we interpret these outcomes $\pm\mu$ as the values that can be taken by a component of the magnetic moment μ of each atom. Since real numbers are usually related to these outcomes, a maximal test is represented by a Hermitian matrix [23]. This interpretation may provide useful information in connection with classical physics. Nevertheless, this trial is not always allowed such as in the case of spin and sometimes it might cause confusion or even unnecessary illusion. Furthermore, universal features in quantum physics should not depend on the details in correspondence to classical physics. For instance, two distinct outcomes result from a spin-1/2, a total angular momentum or two-level atom, and the interpretation of the

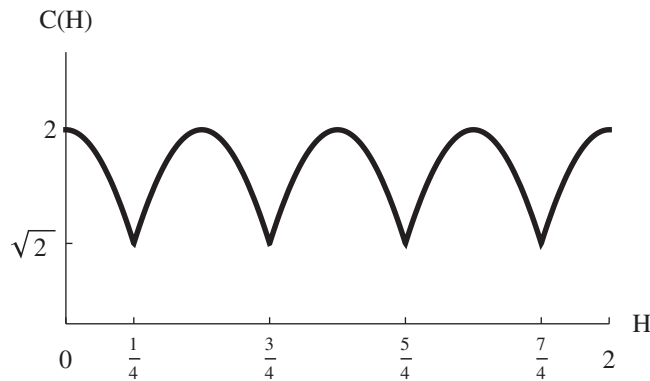


Figure 1. The maximum of the classical Bell function, $C(H)$, on varying the parameter H . In the quantum-to-classical approach, the quantum maximum of 2 remains invariant, independent of H . The classical maximum, $C(H)$, thus decides if the quantum theory violates the Bell inequality for a given H . Quantum violation is always observed as far as $C(H) \neq 2$. The ratio of the quantum and classical maxima is the largest when H is odd-integral quarters with $C(H) = \sqrt{2}$.

outcome values varies case by case, but the quantumness is universal. In this sense, as we are interested in the universality of quantum features, we may ascribe arbitrary numerical values to such outcomes. The arbitrariness may be regarded as a mathematical convenience. In particular, we may associate d complex numbers with d distinct outcomes of a given maximal test: each outcome takes an element in the set $S = \{1, \omega, \dots, \omega^{d-1} \mid \omega \equiv \exp(i\frac{2\pi}{d})\}$, a set of d th roots of unity over the complex field.

The number of mutually unbiased bases that one finds for a given d -dimensional Hilbert space is at most $(d + 1)$, and whenever d is a power of prime, exactly $(d + 1)$ mutually unbiased bases exist and can be constructed explicitly [24]. For an odd prime dimensional system, we associate each basis with an observable by assigning d th roots of unity to the eigenvalues. Besides the observable whose eigenvectors are the standard basis $\{|l\rangle\}$, the k th mutually complementary observable is written as

$$\hat{M}_k \equiv \sum_{l=0}^{d-1} \omega^{kl} |l\rangle \langle l+1|, \quad k = 0, 1, 2, \dots, d-1, \quad (13)$$

where the integer $l+1$ inside the ket or bra vector is meant to be the positive residue modulo d , i.e. $l+1 \bmod d$, and the convention of omitting ‘mod d ’ is used throughout this paper. These observables are said to be mutually complementary. Note that every observable is unitary. A set of the powers of mutually complementary observables forms a basis over the operator space.

In deriving Bell inequalities for d -dimensional systems, we focus on odd prime dimensions and assume that N qudits are spatially separated, and each qudit is observed by a person who is permitted to independently choose one of d observables whose set of eigenvalues is S . By adopting the quantum-to-classical approach, we introduce a set of generic operators in the form of

$$\hat{G}(n) = \frac{1}{2} \sum_{k_1, \dots, k_N=0}^{d-1} \delta_{K,0} \bigotimes_{p=1}^N \hat{M}_{k_p}^n + \text{h.c.}, \quad (14)$$

where $K \equiv \sum_{p=1}^N k_p$ for $n = 1, \dots, \frac{d-1}{2}$ that are integers. Here, $\delta_{K,0}$ is the Kronecker delta such that $\delta_{i,j} = 1$ if $i - j = 0 \pmod d$ and otherwise $\delta_{i,j} = 0$, $\bigotimes_{p=1}^N \hat{M}_{k_p}^n \equiv \hat{M}_{k_1}^n \otimes \dots \otimes \hat{M}_{k_N}^n$ and h.c. indicates the Hermitian conjugate of the previous term, which is introduced to take the real part of the average of the previous one. The upper bound of the quantum expectation of the generic operator $\langle \hat{G}(n) \rangle$ results in d^{N-1} by the triangle inequality and the unitarity of $\bigotimes_{p=1}^N \hat{M}_{k_p}^n$ for each n , as shown for the two-qubit case. The upper bound d^{N-1} is indeed the maximum attainable by the N -partite d -dimensional maximally entangled state,

$$|\text{MES}\rangle \equiv \frac{1}{\sqrt{d}} \sum_{l=0}^{d-1} |l, l, \dots, l\rangle. \quad (15)$$

The maximally entangled state $|\text{MES}\rangle$ is a common eigenvector of all the composite operators $\bigotimes_{p=1}^N \hat{M}_{k_p}^n$ in equation (14), i.e. for $\sum_{p=1}^N k_p = 0 \pmod d$ with the same eigenvalue 1. It is clear that the generic operator $\hat{G}(n)$ has the maximum of d^{N-1} if the state is $|\text{MES}\rangle$.

A set of quantum identities is introduced by applying a local unitary transformation on the generic operators. We choose such a local unitary operator \hat{U} in the form of

$$\hat{U} = \sum_{l=0}^{d-1} \omega^{H_l} |l\rangle\langle l|, \quad (16)$$

where $H_0 = 0$ and the other parameters H_i are in the interval $[0, d)$. By applying the local unitary operator to the generic operator $\hat{G}(n)$, we introduce a quantum identity that is given as

$$\hat{V}^\dagger \hat{G}(n) \hat{V} = \frac{1}{2} \sum_{k_1, \dots, k_N=0}^{d-1} F_{k_1 \dots k_N}(H_i, n) \bigotimes_{p=1}^N \hat{M}_{k_p}^n + \text{h.c.}, \quad (17)$$

where $\hat{V} \equiv \mathbb{1} \otimes \mathbb{1} \dots \otimes \hat{U}$ and the N th rank tensor $\mathbf{F}(H_i, n)$ is given as

$$F_{k_1 \dots k_N}(H_i, n) = \frac{1}{d} \sum_{l=0}^{d-1} \omega^{-(H_l - H_{l+n}) - n(l + (1/2)(n-1))K}. \quad (18)$$

We call the tensor $\mathbf{F}(H_i, n)$ a ‘form factor’ in the sense that it will determine the structure of the Bell operator. It is noteworthy that the expectation of the transformed generic operator has the same maximum of d^{N-1} as the generic operator. The complementary observables \hat{M}_{k_p} are now to be released to arbitrary local observables \hat{a}_{p,k_p} , whose eigenvalues belong to S , where the subscripts p and k_p denote the indices of the observers and their observables, respectively. By applying it, we propose a Bell operator, parameterized by H_i ,

$$\hat{B}(\hat{a}_{p,k_p} | H_i, n) = \frac{1}{2} \sum_{k_1, \dots, k_N=0}^{d-1} F_{k_1 \dots k_N}(H_i, n) \bigotimes_{p=1}^N \hat{a}_{p,k_p}^n + \text{h.c.} \quad (19)$$

In deriving the Bell operator in equation (19), we used the particular form of the local unitary operator $\mathbb{1} \otimes \mathbb{1} \dots \otimes \hat{U}$, which is rather concise. One may attempt to use a more general form such as $\hat{U}_1 \otimes \hat{U}_2 \dots \otimes \hat{U}_N$ with eigenvalues $\omega^{H_i^{(p)}}$ for each \hat{U}_p but one just obtains a Bell operator equivalent to equation (19) with a form factor replaced by $\mathbf{F}(\sum_{p=1}^N H_i^{(p)}, n)$.

We now show that the Bell operator $\hat{B}(\hat{a}_{p,k_p} | H_i, n)$ has the same maximum as the generic operator $\hat{G}(n)$ even though the local observables are arbitrary. The expectation of the Bell

operator $\langle \hat{B}(\hat{a}_{p,k_p} | H_i, n) \rangle$ is not greater than d^{N-1} over all possible states and local observables: for a given state $|\psi\rangle$, the upper bound of the expectation of the Bell operator is given as

$$\langle \psi | \hat{B}(n) | \psi \rangle \leq \left| \langle \psi | \sum_{k_1, \dots, k_N=0}^{d-1} F_{k_1 \dots k_N}(H_i, n) \bigotimes_{p=1}^N \hat{a}_{p,k_p}^n | \psi \rangle \right|, \quad (20)$$

$$\leq \sqrt{\sum_{k_2, l_2, \dots, k_N, l_N=0}^{d-1} d \delta_{\tilde{k}, \tilde{l}} \left| \langle \psi | \bigotimes_{p=2}^N \hat{a}_{p,k_p}^n (\hat{a}_{p,l_p}^n)^\dagger | \psi \rangle \right|}, \quad (21)$$

$$\leq d^{N-1}, \quad (22)$$

where $\tilde{k} \equiv \sum_{p=2}^N k_p$ ($\tilde{l} \equiv \sum_{p=2}^N l_p$) and we omitted the arguments of $\hat{B}(n)$ for simplicity. The first inequality is clear as the real part of a complex number is less than or equal to the absolute value. The second inequality results from the Schwarz inequality and the relations of $\hat{a}_{p,k_p}^n (\hat{a}_{p,k_p}^n)^\dagger = 1$ and $\sum_{k_1=0}^{d-1} F_{k_1, k_2, \dots, k_N}(H_i, n) F_{k_1, l_2, \dots, l_N}^*(H_i, n) = \delta_{\tilde{k}, \tilde{l}}$ (see equation (8)). The third inequality comes from the fact that the maximum of $|\langle \psi | \bigotimes_{p=2}^N \hat{a}_{p,k_p}^n (\hat{a}_{p,l_p}^n)^\dagger | \psi \rangle|$ is 1 and the number of elements in the summation is $d^{2(N-1)-1}$. The quantum upper bound is equal to the maximum of the transformed generic operator in equation (17), and it is attainable if the state is chosen to be maximally entangled (MES) and the local observables to be mutually complementary ($\hat{a}_{p,k_p} = \hat{M}_{k_p}$ for $p = 1, \dots, N-1$ and $\hat{a}_{N,k_N} = \hat{U} \hat{M}_{k_N} \hat{U}^\dagger$).

Let us consider a more general form of Bell operators such as

$$\hat{B}(\hat{a}_{p,k_p} | H_i) = \sum_{n=1}^{(d-1)/2} u_n \hat{B}(\hat{a}_{p,k_p} | H_i, n), \quad \sum_{n=1}^{(d-1)/2} u_n = 1, \quad u_n \geq 0 \quad \forall n, \quad (23)$$

which is a convex combination of the Bell operators $\hat{B}(\hat{a}_{p,k_p} | H_i, n)$. For a given H_i , every $\hat{B}(\hat{a}_{p,k_p} | H_i, n)$ has the same quantum maximum of d^{N-1} in the equal conditions of the state and the observables so that the maximum of $\hat{B}(\hat{a}_{p,k_p} | H_i)$ is also d^{N-1} , irrespective of the weight factors u_n . On the other hand, the classical maximum of the Bell function B_{cl} corresponding to $\hat{B}(\hat{a}_{p,k_p} | H_i)$ will depend on u_n as well as H_i and it has an opportunity to be decreased by varying u_n . When this is the case, one can find a certain convex combination that enhances the nonlocality degree.

We now consider local hidden variable theories for the classical Bell function B_{cl} . For the purpose, we introduce a set of hidden variables λ and their probability distribution function $\rho(\lambda)$. By replacing the quantum observables \hat{a}_{p,k_p} with the classical $\alpha_{p,k_p}(\lambda)$ for all p and k_p , the classical Bell function is given as

$$B_{cl}(\alpha_{p,k_p} | H_i) = \sum_{n=1}^{(d-1)/2} u_n B_{cl}(\alpha_{p,k_p} | H_i, n), \quad (24)$$

where $B_{cl}(\alpha_{p,k_p} | H_i, n)$ is given as

$$B_{cl}(\alpha_{p,k_p} | H_i, n) = \frac{1}{2} \int d\lambda \rho(\lambda) \sum_{k_1, \dots, k_N=0}^{d-1} F_{k_1 \dots k_N}(H_i, n) \prod_{p=1}^N \alpha_{p,k_p}^n(\lambda) + \text{c.c.} \quad (25)$$

Here c.c. stands for the complex conjugate of the previous term and $\alpha_{p,k_p}(\lambda) \in S$. The classical Bell function B_{cl} satisfies the inequality,

$$B_{\text{cl}}(\alpha_{p,k_p} | H_i) \leq C(H_i), \quad (26)$$

where $C(H_i)$ is the classical maximum. For each H_i , the classical maximum $C(H_i)$ is equal to the maximum of

$$\frac{1}{2} \sum_{n=1}^{(d-1)/2} \sum_{k_1, \dots, k_N=0}^{d-1} u_n F_{k_1 \dots k_N}(H_i, n) \prod_{p=1}^N \alpha_{p,k_p}^n + \text{c.c.}, \quad (27)$$

for all $\alpha_{p,k_p} \in S$. Note that the classical maximum $C(H_i)$ is a function of H_i , whereas the quantum maximum of d^{N-1} remains unchanged.

The quantum-to-classical approach has so far been applied to N qudits so as to derive the Bell functions satisfying the CEN criterion. In the following sections, we will employ such Bell functions for two and three qutrits and show that they are genuinely high dimensional. We will further show that the complementarity of the local observables is intimately related to the dimensional genuineness of the nonlocality.

3. A set of Bell inequalities for two qutrits

3.1. Bell inequalities in terms of correlation functions

For the Bell inequalities for two qutrits, we assume that each observer is allowed to independently choose one of three observables. Each local observable is assumed to take a value in the set $S = \{1, \omega, \omega^2 \mid \omega \equiv \exp(i\frac{2\pi}{3})\}$. The Bell operator in equation (23) is changed to, for the two qutrits,

$$\hat{B}(\hat{a}_{p,k_p} | H_i) = \frac{1}{2} \sum_{k_1, k_2=0}^2 F_{k_1 k_2}(H_i) \hat{a}_{1,k_1} \otimes \hat{a}_{2,k_2} + \text{h.c.}, \quad (28)$$

where we used $u_{n=1} = 1$ as there is a single case of $n = 1$. The form factor $\mathbf{F}(H_i)$ is given as

$$F_{k_1 k_2}(H_i) = \frac{1}{3}(\omega^{H_1} + \omega^{-H_1+H_2-K} + \omega^{-H_2-2K}), \quad (29)$$

where $K = k_1 + k_2$. The expectation of the Bell operator is not greater than 3 over all possible states and local observables. The upper bound 3 is indeed the maximum attainable by a maximally entangled state,

$$|3\text{ES}\rangle \equiv \frac{1}{\sqrt{3}} \sum_{l=0}^2 |l, l\rangle, \quad (30)$$

and mutually complementary observables. This state is called a 3D maximally entangled state, compared to a 2D maximally entangled state $(|0, 0\rangle + |1, 1\rangle)/\sqrt{2}$. The classical Bell function B_{cl} , corresponding to the quantum Bell operator $\hat{B}(\hat{a}_{p,k_p} | H_i)$, is given as

$$B_{\text{cl}}(\alpha_{p,k_p} | H_i) = \frac{1}{2} \int d\lambda \rho(\lambda) \alpha_1^\dagger(\lambda) \mathbf{F}(H_i) \alpha_2(\lambda) + \text{c.c.}, \quad (31)$$

and the Bell inequality as

$$B_{\text{cl}}(\alpha_{p,k_p} | H_i) \leq C(H_i), \quad (32)$$

where $\alpha_p(\lambda)$ is a 3D vector whose k_p th component is $\alpha_{p,k_p}(\lambda) \in S$ and $C(H_i)$ is the classical maximum. For each H_i , the classical maximum $C(H_i)$ is determined by the maximum of $(\alpha_1^\dagger \mathbf{F}(H_i) \alpha_2 + \text{c.c.})/2$ for all $\alpha_{p,k_p} \in S$. The classical maximum $C(H_i)$ is a function of H_i , whereas the quantum maximum of 3 remains unchanged. (We do not have to consider all the values of H_i due to the symmetries of the Bell functions under some transformations of H_i .)

We shall investigate symmetries for a set of Bell functions parameterized by H_i . Some of them are equivalent under certain transformations of H_i . We say that two Bell functions B_1 and B_2 are equivalent if the form factor \mathbf{F}_1 of one of them is transformed to the other's \mathbf{F}_2 when the former matrix elements are simply rearranged into the latter or when the former matrix is equal to the latter by a factor in S . First, the Bell functions $B(\alpha_{p,k_p}|H_i)$ are equivalent under the integral translations, $(H_1, H_2) \rightarrow (H_1 + Z_1, H_2 + Z_2)$, where Z_i are integers. A translated classical Bell function from equation (31) is given as

$$B'_{\text{cl}}(\alpha_{p,k_p}|H_i) = B_{\text{cl}}(\alpha_{p,k_p}|H_i + Z_i) \\ = \frac{1}{2} \int d\lambda \rho(\lambda) \sum_{k_1, k_2=0}^2 F_{k_1 - Z_1 - Z_2, k_2}(H_i) \omega^{Z_1} \alpha_{1, k_1}(\lambda) \alpha_{2, k_2}(\lambda) + \text{c.c.}, \quad (33)$$

where the subscript $k_1 - Z_1 - Z_2$ means the positive residue modulo 3 and $\omega^{Z_1} \in S$. This shows that B'_{cl} is equivalent to the original B_{cl} . Altering the order of the classical observables and/or their values leaves the given maximum invariant as the classical maximum is obtained over all possible values of the observables. Thus every pair of equivalent Bell functions has the same classical maximum. The translational symmetry is also valid for the quantum Bell functions. This implies the sufficiency of the confined region, $H_{1,2} \in [0, 1)$. Similarly, the Bell functions are also equivalent under the reflections along the different axes: $(H_1, H_2) \rightarrow (-H_2, -H_1)$, $(H_1, H_2) \rightarrow (H_2, H_1)$ and $(H_1, H_2) \rightarrow (H_1 - H_2, -H_2)$.

Using the quantum-to-classical approach, it has been shown that the quantum maximal expectation of every Bell operator $\hat{B}(\hat{a}_{p,k_p}|H_i)$ is 3, irrespective of the parameters H_i , over all the possible states and local observables, whereas the classical maximum of Bell function depends on H_i . We characterize the nonlocality by QCR, the ratio of the quantum maximum to the classical maximum: $\text{QCR}(H_i) = 3/C(H_i)$. Figure 2 presents $\text{QCR}(H_i)$ by varying the parameters (H_1, H_2) . The QCRs on the space H_1-H_2 are symmetric under the transformations of H_i discussed above. The largest QCR is located at a single point to which the seemingly six points are reduced by the symmetries. The largest QCR is about 1.12. This value is smaller than $(1 + \sqrt{11/3})/2 \approx 1.46$ (CGLMP) and $2/(0.25(3 \cot(\pi/12) - \cot(\pi/4)) - 1) \approx 1.29$ (SLK) for each qutrit with two observables [17, 18]. Nevertheless, the present Bell inequalities provide an important way to discriminate the dimensionality. In other words, they are not violated if the entangled state is of a lower dimension. In this sense, the present Bell inequalities are genuinely 3D (or a dimension witness in [15]). This characteristic is intimately related to the CEN criterion, particularly to the complementarity. We discuss this further in the following subsection.

3.2. Genuinely three-dimensional (3D) Bell inequality

To investigate the role of entanglement and complementarity in nonlocality, we have derived a set of Bell inequalities satisfying the CEN criterion. The inequalities are maximally violated by maximal entanglement and have no violation for separable states. Two interesting questions

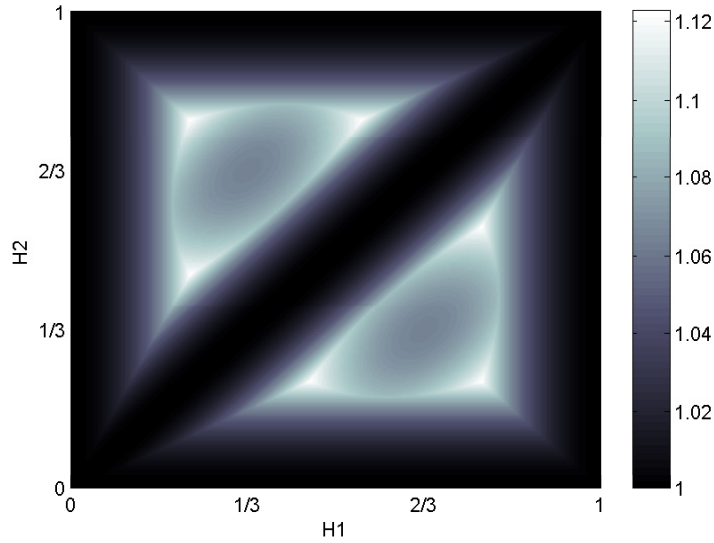


Figure 2. QCR, the ratio of the quantum maximum to the classical maximum, as a function of the parameters $H_{i=1,2}$ for two qutrits. Each pair (H_1, H_2) leads to a Bell inequality, and for a given Bell inequality the QCR is the value being optimized over all possible states and local observables. All the Bell inequalities satisfy the CEN criterion. The largest QCR is located at the seemingly six points that are reduced to a single point due to the symmetries (see the text). The largest QCR is about 1.12.

naturally arise: (i) What is the quantitative relation between entanglement and nonlocality? (ii) More importantly, for a given entanglement, how much complementarity is required to maximize nonlocality? To present the quantitative relation, we consider *all pure entangled states* in addition to the 3D maximally entangled state and we numerically optimize their QCRs, each over all possible local observables.

We quantify the degree of entanglement of a pure composite state $|\psi\rangle\langle\psi|$ by the von Neumann entropy $S(\hat{\rho}) = -\text{Tr}(\hat{\rho} \log_3 \hat{\rho})$, where $\hat{\rho}$ is the marginal state of $|\psi\rangle\langle\psi|$. We also quantify the degree of complementarity by employing the entropy of the transition probabilities between local observables. More explicitly, for two local observables \hat{a}_0 and \hat{a}_1 , the degree is defined by

$$C(\hat{a}_0, \hat{a}_1) = -\frac{1}{3} \sum_{i,j=0}^2 |{}_0\langle i|j\rangle_1|^2 \log_3 |{}_0\langle i|j\rangle_1|^2, \quad (34)$$

where $|i\rangle_k$ are the eigenstates of the observable \hat{a}_k . The degree satisfies $0 \leq C(\hat{a}_0, \hat{a}_1) \leq 1$. For three observables $\hat{a}_{0,1,2}$, the degree is inductively defined by

$$C(\hat{a}_0, \hat{a}_1, \hat{a}_2) = \frac{1}{3} \sum_{k_1 < k_2}^2 C(\hat{a}_{k_1}, \hat{a}_{k_2}). \quad (35)$$

In the nonlocality test, Alice uses the three local observables and her degree of complementarity is given by $C_A = C(\hat{a}_{1,0}, \hat{a}_{1,1}, \hat{a}_{1,2})$. Similarly, Bob's degree of complementarity is given by $C_B = C(\hat{a}_{2,0}, \hat{a}_{2,1}, \hat{a}_{2,2})$. The degree becomes the maximum, $C_{A(B)} = 1$, if and only if all the

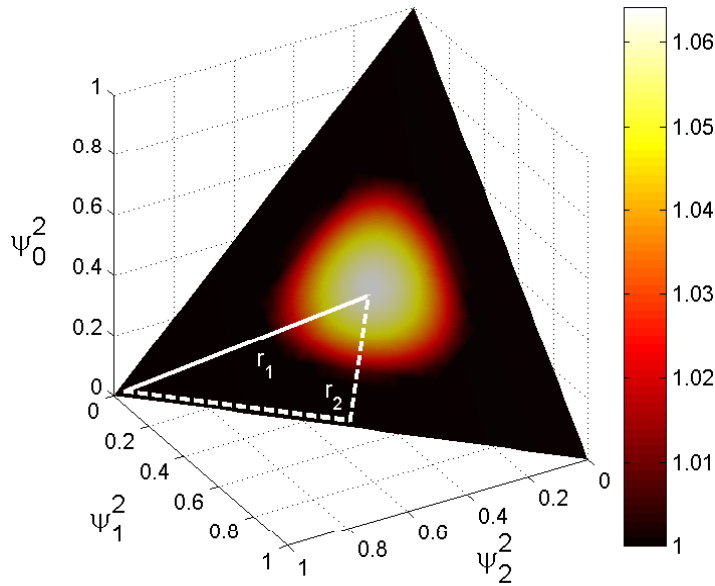


Figure 3. QCR of the Bell inequality with $(H_1, H_2) = (1/3, 2/3)$ in terms of pure qutrit states. The axes are the squares of Schmidt coefficients (see the text). Every pure state is a point on the triangle. The largest QCR is located at the center of the triangle that represents the 3D maximally entangled state. The inequality is not violated for any 2D entangled states located at the boundary of the triangle. These imply that the Bell inequality discriminates the 3D entanglement from the 2D and it is genuinely 3D.

observables of Alice (or Bob) are mutually complementary, whereas it vanishes, $C_{A(B)} = 0$, if they are all mutually compatible. We define a joint degree of complementarity by $C_{AB} = C_A C_B$, which is more relevant to the nonlocality in the sense that the nonlocality cannot be exhibited if either $C_A = 0$ or $C_B = 0$.

We now show that our Bell inequality of $(H_1, H_2) = (1/3, 2/3)$ is genuinely 3D⁴. For this purpose, consider a pure entangled state of two qutrits, which Schmidt decomposition changes to

$$|\psi\rangle = \psi_0|0, 0\rangle + \psi_1|1, 1\rangle + \psi_2|2, 2\rangle, \quad (36)$$

where ψ_i are non-negative real numbers satisfying $\sum_{i=0}^2 \psi_i^2 = 1$. In figure 3, the composite state is denoted by a point on the triangle defined by the plane of $\sum_{i=0}^2 \psi_i^2 = 1$ in the 3D space with the axes being Schmidt coefficients ψ_i^2 . Three vertices of the triangle represent product states, the points on the edges represent 2D entangled states that can be described by two qubits, and the interior points represent 3D entangled states. Figure 3 presents the QCR of the Bell function with $(H_1, H_2) = (1/3, 2/3)$ for each state. The QCR of a given state is numerically optimized by using the steepest descent method varying the ‘orientations’ of local observables [25]. It clearly shows that the largest QCR ($1/\cos \frac{\pi}{9} \approx 1.06$) is located at the center of the triangle that represents the 3D maximally entangled state with $\psi_i = \frac{1}{\sqrt{3}}$ for all i . The

⁴ The inequality of $(H_1, H_2) = (1/3, 2/3)$ is particularly chosen as it exhibits the largest violation if an additional phase is introduced in the form factor \mathbf{F} . Nevertheless, we do not pursue the details as they do not alter the main result but complicate the discussion.

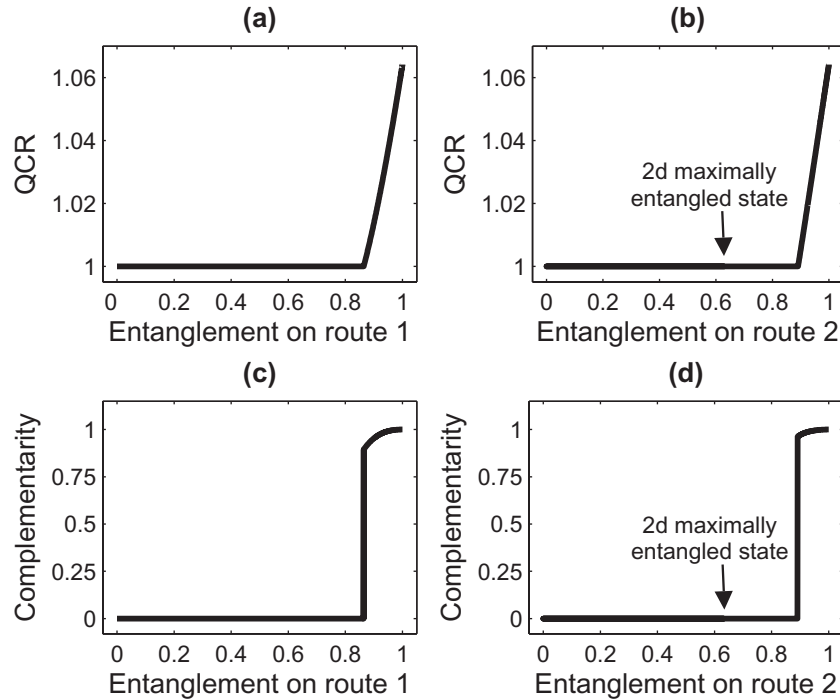


Figure 4. Quantitative relations among the three degrees of complementarity, entanglement and nonlocality for the Bell inequality with $(H_1, H_2) = (1/3, 2/3)$. We present QCR in terms of the states on the routes (a) r_1 and (b) r_2 in figure 3. No violation appears for the entanglement less than 0.86 (0.89) on the route r_1 (r_2). The QCR increases monotonically as the entanglement is increased further. The 2D entangled states are on the route r_2 and they do not violate the inequality. This implies that the inequality is genuinely 3D (or a dimension witness). In (c) and (d), we present the joint degree of complementarity of local observables by which the QCR is obtained for each given state. The joint degree abruptly *jumps* close to its maximum as the nonlocality starts appearing and reaches its maximum at the 3D maximally entangled state.

QCR of a quantum state decreases as one moves away from the center. This implies that the QCR increases as the entanglement increases. It is remarkable that no violation appears at the edges, i.e. no 2D entangled states violate the inequality. Therefore, the inequality is genuinely 3D as it discriminates 3D entanglement from 2D entanglement. We now present explicitly the quantitative relations among the complementarity, entanglement and nonlocality. Consider quantum states on two routes, shown in figure 3, from $|2, 2\rangle$ to $|3ES\rangle$ in equation (30). In route r_1 , the straight line includes entangled states with $\psi_0 = \psi_1$ and $\psi_2 \geq \psi_0$. In route r_2 , the dashed line includes 2D entangled states,

$$|\psi\rangle = \psi_1|1, 1\rangle + \psi_2|2, 2\rangle, \quad (37)$$

as well as 3D entangled states with $\psi_1 = \psi_2$ and $\psi_1 \geq \psi_0$. It is clearly seen from figures 4(a) and (b) that as the degree of entanglement is increased, the QCR increases monotonically to its maximum at the 3D maximally entangled state. In figure 4(b), it is shown that there is no violation for 2D entangled states. We start to see the violation only for 3D entangled states

whose entanglement degree is more than $\log_3 2 \approx 0.63$. This feature clearly shows that the present inequality is genuinely 3D (or a dimension witness), as discussed before. In figures 4(c) and (d), we present the joint degree of complementarity C_{AB} of the local observables by which the QCR is obtained for a given entangled state. It is clearly seen that C_{AB} abruptly jumps close to its maximum of unity when the nonlocality starts appearing and reaches its maximum at the 3D maximally entangled state. The sudden increase of the complementarity implies that the complementarity plays a more important role in the present inequality than in CGLMP and SLK that do not satisfy the CEN criterion. For states satisfying the inequality, the joint degree of complementarity, C_{AB} , vanishes and the local observables of Alice or Bob are compatible. The degree of entanglement of a state has a monotonic relation not only with the QCR of our Bell functions but also with the degree of complementarity of the local observables. These facts lead to another monotonic relation between the two degrees of QCR and complementarity. In other words, we show that not only does the Bell function of $(H_1, H_2) = (1/3, 2/3)$ satisfy the CEN criterion but also it induces monotonic relations among three degrees of quantities, i.e. the complementarity of the local observables, the entanglement of a state and the QCR of the Bell function. In the following section, we investigate Bell inequalities for three qutrits and show that the nonlocality is closely related to the entanglement.

4. A set of Bell inequalities for three qutrits

4.1. Bell inequalities in terms of correlation functions

Suppose that three qutrits are distributed to three observers, Alice, Bob and Charlie, and these are to be measured by them, respectively. Assuming that each observer is allowed to independently choose one of three observables that take an element in the set S as an outcome, the Bell operator in equation (23) is changed to

$$\hat{B}(\hat{a}_{p,k_p} | H_i) = \frac{1}{2} \sum_{k_1, k_2, k_3=0}^2 F_{k_1 k_2 k_3}(H_i) \hat{a}_{1, k_1} \otimes \hat{a}_{2, k_2} \otimes \hat{a}_{3, k_3} + \text{h.c.}, \quad (38)$$

where the form factor $\mathbf{F}(H_i)$ becomes

$$F_{k_1 k_2 k_3}(H_i) = \frac{1}{3} (\omega^{H_1} + \omega^{-H_1 + H_2 - K} + \omega^{-H_2 - 2K}), \quad (39)$$

where $K = k_1 + k_2 + k_3$. The upper bound of the quantum expectation of the Bell operator is 9, which is attainable by the 3D maximal GHZ state,

$$|3\text{GHZ}\rangle \equiv \frac{1}{\sqrt{3}} \sum_{l=0}^2 |l, l, l\rangle, \quad (40)$$

and mutually complementary observables. The classical upper bound of the Bell function B_{cl} is given as

$$B_{\text{cl}}(\alpha_{p,k_p} | H_i) = \frac{1}{2} \int d\lambda \rho(\lambda) \sum_{k_1, k_2, k_3=0}^2 F_{k_1 k_2 k_3}(H_i) \alpha_{1, k_1}(\lambda) \alpha_{2, k_2}(\lambda) \alpha_{3, k_3}(\lambda) + \text{c.c.}, \quad (41)$$

and the Bell inequality as

$$B_{\text{cl}}(\alpha_{p,k_p} | H_i) \leq C(H_i), \quad (42)$$

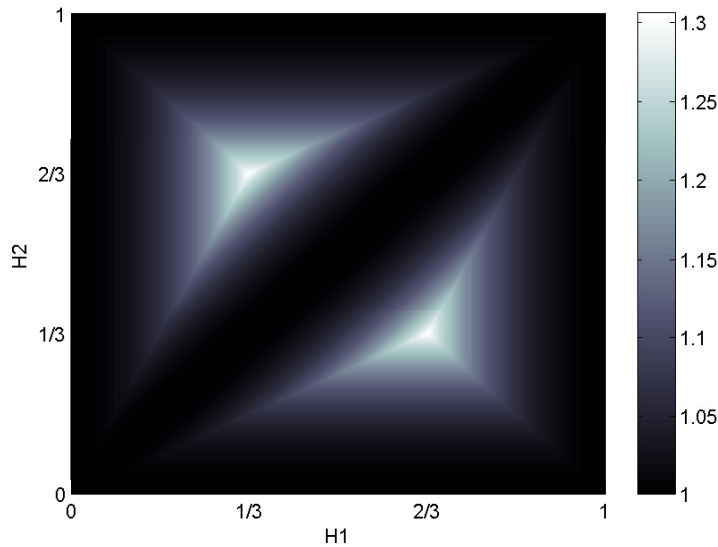


Figure 5. QCR of Bell inequalities for three qutrits, parameterized by $H_{i=1,2}$. Each point of (H_1, H_2) represents a Bell inequality. For a given Bell inequality, its QCR is the value being optimized over all possible states and local observables. All the Bell inequalities satisfy the CEN criterion. The largest QCR is located at a single point $(H_1, H_2) = (1/3, 2/3)$ to which the seemingly two points are reduced due to the symmetries. The largest QCR is $1/\cos \frac{2\pi}{9} \approx 1.31$.

where $\alpha_{1,k_1}(\lambda)$ ($\alpha_{2,k_2}(\lambda)$ and $\alpha_{3,k_3}(\lambda)$) $\in \mathcal{S}$ is the classical observable of Alice (Bob and Charlie) and $C(H_i)$ is the classical maximum for a given H_i . Note that the classical maximum $C(H_i)$ is a function of H_i , whereas the quantum maximum of 9 is constant over all H_i . Figure 5 presents QCR, the ratio of the quantum maximum to the classical maximum, by varying the parameters (H_1, H_2) : $\text{QCR}(H_i) = 9/C(H_i)$. The largest QCR is located at a single point $(H_1, H_2) = (1/3, 2/3)$ to which the seemingly two points are reduced by the symmetries, as in the case of the two qutrits. The largest QCR is $1/\cos \frac{2\pi}{9} \approx 1.31$.

4.2. The genuinely 3D and the genuinely tripartite Bell inequality

We have investigated a set of Bell inequalities satisfying the CEN criterion for the three qutrits: the inequalities are maximally violated by 3D maximal GHZ entanglement and mutually unbiased measurements. As in the case of the bipartite inequalities, we investigate whether the Bell inequality is genuinely 3D for $(H_1, H_2) = (1/3, 2/3)$. Consider a generalized GHZ state, simply called a GHZ state, which is in the form of

$$|\psi\rangle = \psi_0|0, 0, 0\rangle + \psi_1|1, 1, 1\rangle + \psi_2|2, 2, 2\rangle, \quad (43)$$

where ψ_i are non-negative real numbers satisfying $\sum_{i=0}^2 \psi_i^2 = 1$. In figure 6, the composite state is denoted by a point on the triangle, similarly to the case of the two qutrits. Three vertices of the triangle correspond to product states, the points on the edges correspond to 2D GHZ states, and the interior points correspond to 3D GHZ states. Figure 6 presents the QCR, for each possible state, of the Bell inequality with $(H_1, H_2) = (1/3, 2/3)$. The largest QCR is located at the center of the triangle, which represents the maximal 3D GHZ state. It is remarkable that no violations

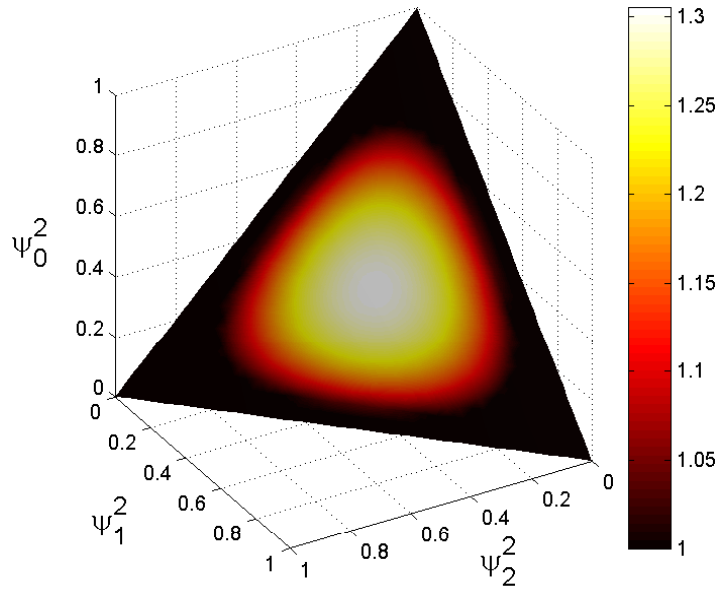


Figure 6. QCR of the Bell inequality with $(H_1, H_2) = (1/3, 2/3)$ for the three qutrits. Each point on the triangle stands for a generalized GHZ pure state in equation (43). The largest QCR is located at the center of the triangle, which represents the 3D maximal GHZ state, and the inequality is not violated for any 2D GHZ states located at the boundary of the triangle. This implies that the Bell inequality is genuinely 3D so as to discriminate the 3D GHZ entanglement from the 2D GHZ entanglement.

appear at the edges of the triangle, implying that the Bell inequality is not violated by 2D GHZ states,

$$|\psi\rangle = \psi_0|0, 0, 0\rangle + \psi_1|1, 1, 1\rangle. \quad (44)$$

Our numerical analysis results in no violation for any bi-separable (including separable) qutrit states and any qubit states. In this sense our Bell inequality of the three qutrits is genuinely tripartite as well as genuinely 3D.

5. Joint-probability representation

In this paper, we have presented Bell inequalities in terms of correlation functions. The inequalities can also be represented in terms of joint probabilities and one may prefer it. In the following, we formulate our inequalities in the joint-probability space for such convenience.

Lee *et al* [26] recently showed that a Bell function can be represented either in the correlation-function space or in the joint-probability space and the two representations are related by the discrete Fourier transformation. We just offer a brief description. For an N -partite d -dimensional system, a Bell operator including higher-order correlations can be written as

$$\hat{B}(\hat{a}_{p,k_p}) = \sum_{k_1, \dots, k_N=0}^{d-1} \sum_{n=0}^{d-1} \eta_{k_1 \dots k_N}(n) \bigotimes_{p=1}^N \hat{a}_{p,k_p}^n, \quad (45)$$

where \hat{a}_{p,k_p} are local observables whose eigenvalues are the d th roots of unity over the complex field. The form of the Bell operator in equation (45) does not lose any generality, noting that it contains the higher-order powers of observables. The n th order correlation function becomes

$$\left\langle \bigotimes_{p=1}^N \hat{a}_{p,k_p}^n \right\rangle = \sum_{\gamma=0}^{d-1} \omega^{n\gamma} P \left(\sum_{p=1}^N A_{p,k_p} = \gamma \right). \quad (46)$$

Here, letting $P(A_{1,k_1} = r_1, \dots, A_{N,k_N} = r_N)$ be the joint probability of the p th observer obtaining outcomes w^{r_p} on the measurement of \hat{a}_{p,k_p} , $P(\sum_{p=1}^N A_{p,k_p} = \gamma) = \sum_{r_1, \dots, r_N=0}^{d-1} P(A_{1,k_1} = r_1, \dots, A_{N,k_N} = r_N) \delta_{\tilde{r}, \gamma}$, where $\tilde{r} = \sum_{p=1}^N r_p$ and the Kronecker delta is defined below equation (14). Using equation (46), we can represent the Bell function of equation (45) in the joint-probability space:

$$\langle \hat{B}(\hat{a}_{p,k_p}) \rangle = \sum_{k_1, \dots, k_N=0}^{d-1} \sum_{\gamma=0}^{d-1} \xi_{k_1 \dots k_N}(\gamma) P \left(\sum_{p=1}^N A_{p,k_p} = \gamma \right), \quad (47)$$

where the coefficients $\xi_{k_1 \dots k_N}(\gamma)$ are the Fourier transformation of the coefficient $\eta_{k_1 \dots k_N}(n)$,

$$\xi_{k_1 \dots k_N}(\gamma) = \sum_{n=0}^{d-1} \eta_{k_1 \dots k_N}(n) \omega^{n\gamma}. \quad (48)$$

The present Bell function in equation (23) has been represented in the correlation-function space with the coefficients given by, for a given H_i ,

$$\begin{aligned} \eta_{k_1 \dots k_N}(0) &= 0, \\ \eta_{k_1 \dots k_N}(n) &= \frac{1}{2} u_n F_{k_1 \dots k_N}(H_i, n) \quad \text{for } n = 1, \dots, \frac{d-1}{2}, \\ \eta_{k_1 \dots k_N}(n) &= \frac{1}{2} u_{d-n} F_{k_1 \dots k_N}^*(H_i, d-n) \quad \text{for } n = \frac{d+1}{2}, \dots, d-1. \end{aligned} \quad (49)$$

By using the Fourier relation in equation (48), we can represent our Bell function in the joint-probability space with the coefficients

$$\xi_{k_1 \dots k_N}(\gamma) = \frac{1}{2} \sum_{n=1}^{(d-1)/2} u_n F_{k_1 \dots k_N}(H_i, n) \omega^{n\gamma} + \text{c.c.}, \quad (50)$$

for a given H_i .

6. Remarks

By taking the quantum-to-classical approach, we derived a series of Bell operators for multipartite odd prime dimensional systems, satisfying the CEN criterion, from the so-called quantum identity characterized by certain parameters H_i . We proved that the maximum of the quantum Bell function remains invariant over the parameters. To illustrate the present approach, we applied it to the two and three qutrits. Among the derived Bell inequalities, the Bell inequality of $(H_1, H_2) = (1/3, 2/3)$ leads to the optimal ratio of the quantum maximum to the classical maximum (QCR) over the parameters H_i . We found that it discriminates 3D entanglement from 2D entanglement, i.e. it is more violated for the three-dimensionally

entangled states. In fact, it is not violated by the two-dimensionally entangled states. In this sense the Bell inequality is genuinely 3D and it plays the role of a dimension witness. These results hold for both the cases of two and three qutrits. In addition, for the two qutrits we gave a quantitative description of the relations among the three degrees of complementarity, entanglement and non-locality. It was observed that the degree of complementarity jumps abruptly to very close to its maximum as the nonlocality starts appearing. These characteristics imply that complementarity plays a more important role in the present inequality compared with the conventional CGLMP and SLK inequalities that do not satisfy the CEN criterion.

It would be interesting to investigate whether there exists a Bell inequality that discriminates N -partite entanglement from entanglement of lesser subsystems. We will leave this question for further studies.

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