Necessary and sufficient criterion for extremal quantum correlations in the simplest Bell scenario

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In the study of quantum nonlocality, one obstacle is that the analytical criterion for identifying the boundaries between quantum and postquantum correlations has not yet been given, even in the simplest Bell scenario. We propose a plausible, analytical, necessary and sufficient condition ensuring that a nonlocal quantum correlation in the simplest scenario is an extremal boundary point. Our extremality condition amounts to certifying an information-theoretical quantity; the probability of guessing a measurement outcome of a distant party optimized using any quantum instrument. We show that this quantity can be upper and lower bounded from any correlation in a device-independent way, and we use numerical calculations to confirm that coincidence of the upper and lower bounds appears to be necessary and sufficient for the extremality.

In this paper, we propose a plausible, analytical, necessary and sufficient condition ensuring that a nonlocal quantum correlation is extremal. To this end, we focus on the optimal probability of guessing a measurement outcome of a distant party, which was shown to play a crucial role in constraining quantum correlations \[19\]. We show that the guessing probability can be upper and lower bounded from any correlation in a device-independent way, and as a result when the upper and lower bounds coincide, the guessing probability can be certified (i.e., uniquely determined irrespective of details when realizing a correlation). We use numerical calculations to confirm that this certifiability condition appears to be necessary and sufficient for the extremality.

To begin with, let us briefly summarize preliminaries. For details, see \[3\] and the references therein. In the simplest Bell scenario, Alice performs a measurement on a shared quantum state \(\psi\). Tsirelson showed that the Bell inequality of the Clauser-Horne-Shimony-Holt (CHSH) type \(9\) is violated up to \(2\sqrt{2}\) by quantum correlations \(3\). The correlation attaining the Tsirelson bound is an extremal point of the convex set of quantum correlations. Since Einstein, Podolsky and Rosen proposed a paradox \[1\] in 1935, quantum nonlocality has been a central topic in fundamental science. In 1964, Bell showed that the nonlocal correlations predicted by quantum mechanics are inconsistent with local realism \(2\). The nonlocal correlations do not contradict the no-signaling principle, but it was later found that the strength of quantum correlations is more restricted than that allowed by the no-signaling principle \(3, 4\). Since then, many efforts have been made to determine the fundamental principles limiting quantum nonlocality \(5, 6\). In these studies, however, one serious obstacle is that the analytical criterion for identifying the boundaries between quantum and postquantum correlations has not yet been given, even in the simplest Bell scenario.

In the simplest Bell scenario, where two remote parties, Alice and Bob, each perform two binary measurements on a shared quantum state, Tsirelson showed that the Bell inequality of the Clauser-Horne-Shimony-Holt (CHSH) type \(9\) is violated up to \(2\sqrt{2}\) by quantum correlations \(3\). The correlation attaining the Tsirelson bound is an extremal point of the convex set of quantum correlations. When marginal probabilities of obtaining the measurement outcomes are unbiased, the boundaries are identified using the Tsirelson-Landau-Masanes (TLM) analytical criterion \(10, 12\). In a general case where marginals may be biased, several methods work for identifying the boundaries, such as the Navascués-Pironio-Acín (NPA) hierarchy \(13, 14\), the see-saw iteration algorithm \(15, 16\), and the quantifier elimination algorithm \(17\), but obtaining the analytical criterion is a long-standing open problem. Recently, it was shown that the geometry of the quantum set has rich and counterintuitive features \(18\); specifically, contrary to the case of unbiased marginals, flat (i.e., non-extremal) boundaries made from nonlocal correlations exist (other than the edges of the probability space), which indeed tells us the difficulty of the problem. Therefore, it is reasonable and worthwhile to determine the analytical criterion for identifying extremal points, instead of full boundaries, as the quantum set is a convex hull of extremal points.

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exceeds 2 if and only if the correlation is nonlocal, where the maximization is taken over the four positions of the minus sign in the CHSH expression. A local correlation is an extremal point of the quantum set if and only if it is a deterministic correlation. In this paper, therefore, we exclusively consider extremal correlations made from a nonlocal quantum correlation.

Let us then recall the bound on nonlocality in terms of the guessing probability \([19]\), i.e.,

\[
\sum_{x y} s_x u_{x y} (1 - x y) \langle A_x B_y \rangle \leq \left[ \sum_{x} s_x^2 (D_x^B)^2 \right]^{1/2}.
\]  

Any quantum realization must satisfy this inequality for any real \(s_x\) and \(u_{x y}\) such that \(u_{00} u_{01} = u_{10} u_{11}\) and \(\sum_{x y} u_{x y}^2 = 1\). The quantity \(D_x^B\) describes the guessing probability; Bob's optimal probability of guessing Alice's outcome \(a\) is \((1 + D_x^B)^2 / 2\) (when Bob's conditional states are pure). The precise definition is given by Eq. (6) below.

The necessary and sufficient condition for the fulfillment of Eq. (3) and of the complement inequality in terms of Alice's guessing probability \(\forall s_x, u_{x y}\) is

\[
|C_{00} C_{01} - C_{10} C_{11}| \leq (1 - C_{00}^2)^{1/2} (1 - C_{01}^2)^{1/2} + (1 - C_{10}^2)^{1/2} (1 - C_{11}^2)^{1/2}
\]

for both \(C_{x y} = \langle A_x B_y \rangle / D_x^B\) and \(\tilde{C}_{x y} = \langle A_x B_y \rangle / D_y^A\). When \(C_{x y} = \langle A_x B_y \rangle\), Eq. (4) reproduces the TLM inequality, and the saturation is necessary and sufficient for the extremality of nonlocal quantum correlations in the case of unbiased marginals \(\langle A_x \rangle = \langle B_y \rangle = 0\) \([18, 20]\).

Therefore, Eq. (4) is said to be the scaled TLM inequality, as the correlation function \(\langle A_x B_y \rangle\) is scaled by \(D_x^B\) and \(D_y^A\). As preliminarily mentioned in [19], every extremal correlation including the case of biased marginals appears to saturate the scaled TLM inequality, whose numerical evidence is explicitly shown later. However, it was also shown that the saturation alone is insufficient for identifying the extremality.

To search for a complete set of conditions, let us focus on the fact that, for a given \(\{ \langle A_x B_y \rangle, \langle A_x \rangle, \langle B_y \rangle \}\), the upper bounds of \(D_x^B\) and \(D_y^A\) can also be determined irrespective of the details of the realizations. This can be done by using the method based on the NPA hierarchy \([13, 14]\) as follows: Let us consider the states of \(\{ |\psi\rangle, |A_x \rangle, |B_y \rangle, |X\rangle \}\) has the form

\[
\Gamma = \begin{pmatrix}
1 & \langle A_0 \rangle & \langle A_1 \rangle & \langle B_0 \rangle & \langle B_1 \rangle & 1 & 2_{36} \\
1 & 2_{23} & 1 & \langle A_0 B_0 \rangle & \langle A_0 B_1 \rangle & \langle A_1 B_0 \rangle & \langle A_1 B_1 \rangle \\
1 & \gamma_{45} & 1 & \gamma_{45} & 1 & 2_{56} \\
1 & \gamma_{56} & 1 & \gamma_{56} & 1 & 1
\end{pmatrix}
\]

where only the upper triangular part is shown. Since

\[
D_x^B = \max_{\langle \psi | X^2 \rangle = 1} \langle \psi | A_x X | \psi \rangle = \max_{\langle X | X \rangle = 1} \langle A_x | X \rangle,
\]

the upper bound of \(D_x^B\) \((D_y^B)\) is obtained by maximizing \(\gamma_{26} (\gamma_{36})\) under the constraint that the real symmetric matrix \(\Gamma\) is positive semidefinite. Here, the maximization of \(\gamma_{26}\) and \(\gamma_{36}\) are done separately. However, this method, corresponding to the lowest level of the NPA hierarchy, does not work well, as \(|X\rangle = |A_x\rangle\) is always a solution and the maximum cannot be less than 1. Let us then move on to the next \(1 + AB\) level of the NPA hierarchy. Namely, let us further introduce \(A_x B_y \langle \psi \rangle\) and \(A_x X \langle \psi \rangle\), and construct the \(12 \times 12\) Gram matrix (with constraints between the matrix elements). Then, the bounds less than 1 can be obtained (mainly numerically, though). The upper bounds of \(D_y^A\) are obtained in the same way. Throughout this paper, these bounds are called device-independent upper bounds.

Now, consider a realization such that \(D_x^B\) and \(D_y^A\) coincide with the device-independent upper bounds, and further saturates Eq. (3) for an appropriate choice of \(s_x\) and \(u_{x y}\), hence saturating Eq. (4). Such a correlation has a significant property: \(D_x^B\) and \(D_y^A\) are unique irrespective of the realizations, as they are tightly bounded from above and below. Namely, they can be certifiably determined by \(\{ \langle A_x B_y \rangle, \langle A_x \rangle, \langle B_y \rangle \}\), as of the certification of, e.g., randomness \([21]\).

Note that, even in this time, \(B_y\) itself generally does not coincide with an optimal operator for guessing the outcome of \(A_x\), and vice versa (see Appendix C in \([19]\)). This certifiability of \(D_x^B\) and \(D_y^A\), despite that they depend on the state and the measurements, may implicitly imply that the realization is unique up to local isometry, i.e., the realization can be self-tested \([22]\), as in the case of unbiased marginals where every nonlocal boundary correlation self-tests the maximally entangled state \([23]\). Therefore, such a correlation is a good candidate of an extremal correlation, as a correlation must be extremal if it is self-testable \([18]\). Moreover, if this insight is true, the certifiability of \(D_x^B\) and \(D_y^A\) ensures that the device-independent bounds are attained by a two-qubit realization, as every extremal correlation in the simplest Bell scenario has a two-qubit realization \([3, 23]\).

In two-qubit realizations, where projective measurements of rank 1 are performed on a two-qubit entangled pure state \(|\psi\rangle = \cos \chi |00\rangle + \sin \chi |11\rangle\), since the guessing probability is given by \(D_x^B = \text{tr} |\rho_{0|x}^B - \rho_{1|x}^B|^2\) \([24]\), with \(\rho_{a|x}\) being Bob's local state conditioned on \(a\), and similarly for \(D_y^A\), we have (see Appendix A for details)

\[
(D_x^B)^2 = \langle A_x \rangle^2 + \sin^2 2 \chi, \quad (D_y^A)^2 = \langle B_y \rangle^2 + \sin^2 2 \chi
\]

It is then found that, for a given \(\{ \langle A_x B_y \rangle, \langle A_x \rangle, \langle B_y \rangle \}\), the entanglement of \(|\psi\rangle\) specified by \(\sin^2 2 \chi\) is determined as a consistent solution of four quadratic equations to be

\[
S_{xy}^+ \equiv \frac{1}{2} \left[ J_{xy} \pm \sqrt{J_{xy}^2 - 4 K_{xy}^2} \right],
\]

\[
J_{xy} \equiv \langle A_x B_y \rangle^2 - \langle A_x \rangle^2 - \langle B_y \rangle^2 + 1,
\]

\[
K_{xy} \equiv \langle A_x B_y \rangle - \langle A_x \rangle \langle B_y \rangle + \langle A_x \rangle (\langle B_y \rangle - 1).
\]
\[ K_{xy} = \langle A_x B_y \rangle - \langle A_z \rangle \langle B_y \rangle. \] (8)

For each \( x \) and \( y \), one of the two solutions \( S_{xy}^\pm \) agrees with \( \sin^2 2\chi \). Since \( D^B_x \) and \( D^A_y \) are increasing functions of \( \sin^2 2\chi \) as in Eq. (7), we immediately obtain the following analytical upper bounds in two-qubit realizations:

\[ (D^B_x)^2 \leq (A_x)^2 + S_{xy}^+ \quad \text{and} \quad (D^A_y)^2 \leq (B_y)^2 + S_{xy}^+. \] (9)

These hold for every \( x \) and \( y \). Note that the simultaneous saturation of these eight inequalities requires that \( \sin^2 2\chi = S_{xy}^+ \) for every \( x \) and \( y \), while cases such as \( \sin^2 2\chi = S_{00}^+ = S_{01}^+ = S_{11}^+ \) frequently occur in general two-qubit realizations. We have compared Eq. (9) with the corresponding device-independent bound obtained numerically (by the random tests as used in Fig. 2 below). The results indicate that, for two-qubit realizations saturating both Eqs. (7) and (4), the two bounds agree with each other within numerical accuracy, as expected. Moreover, it is found that any correlation, whose (non-two-qubit) realization saturates both Eqs. (4) and (9), and fulfills one more condition

\[ \prod_{xy} [(1 - S_{xy}^+)(A_x B_y) - \langle A_x \rangle \langle B_y \rangle] \geq 0, \] (10)

always has a two-qubit realization (see Appendix A). Note that Eq. (10) is merely redundant, when two-qubit realizations only are considered.

Therefore, the necessary and sufficient condition we propose for the extremality is the simultaneous saturation of the two inequalities given by Eq. (4) and the eight inequalities given by Eq. (9), and fulfillment of Eq. (10).

To check the validity, it suffices to investigate two-qubit realizations, because of the existence of a two-qubit realization due to Eq. (8) and Eq. (10), and the certifiability of \( D^B_x \) and \( D^A_y \) already confirmed numerically. We have performed numerical calculations to check the necessity of the proposed extremal condition as follows: For a randomly constructed Bell expression Eq. (4), where without loss of generality all coefficients are randomly selected from \([-1, 1]\), a two-qubit realization that maximizes the expression is obtained via the seesaw iteration algorithm \[12, 13\] using the semidefinite programming package \[23\]. A correlation picked up in this way using a random Bell expression (a random hyperplane in the probability space) could be a point on a non-extremal boundary, if the hyperplane were precisely parallel to the boundary. However, such a coincidence is quite rare in the random tests; hence a point picked up is in practice always an extremal point. For the same reason, the random tests cannot pick up a given extremal point unless it has infinite supporting hyperplanes. However, an implicit continuity assumption for the continuous distribution of the other extremal points justifies this methodology (see, e.g., Fig. 1 in [18]).

For such realizations obtained randomly, Fig. 1 shows the relation between the left-hand side (LHS) and the right-hand side (RHS) of Eq. (4). When the correlation functions are not scaled by either \( D^A_x \) or \( D^B_y \), the LHS is less than or equal to the RHS, as shown by the black dots, which is an expected behavior of the (non-scaled) TLM inequality. However, as shown by the red dots, the equality holds when the correlation functions are scaled by \( D^A_x \) or \( D^B_y \), hence suggesting that the saturation of Eq. (4) is indeed necessary for the extremality. Note that the saturation is equivalent to the fulfillment of (see Appendix A)

\[ \prod_{xy} \sin(\phi^B_x - \theta^B_y) \leq 0 \quad \text{and} \quad \prod_{xy} \sin(\phi^A_y - \theta^A_y) \leq 0, \] (11)

which is numerically more feasible for verifying the saturation of Eq. (4) than checking Eq. (4) itself. Here, \( \phi^B_x \) is the angle of the Bloch vector of \( \rho^B_x \), \( \theta^B_y \) is the angle of the measurement basis of \( B_y \), and similarly for Alice. The inset in Fig. 1 shows the distributions of \( C_{\text{CHSH}}, \prod_{xy} \sin(\phi^B_x - \theta^B_y), \) and \( \prod_{xy} \sin(\phi^A_y - \theta^A_y) \) for realizations chosen randomly. The results indicate that Eq. (11) is satisfied for all extremal correlations, which strengthens the results of the main body of Fig. 1.

We have also performed similar numerical calculations and confirmed that \( (D^B_x)^2 - (A_x)^2 \) and \( (D^A_y)^2 - (B_y)^2 \) are closer to \( S_{xy}^+ \) than \( S_{xy}^- \) for every \( x \) and \( y \) and for all extremal correlations chosen randomly. Namely, the numerical results suggest that the saturation of Eq. (4) is also necessary for the extremality.

Let us then investigate the sufficiency. We present the
numerical evidence that a correlation generated by a two-qubit realization, which saturates both Eqs. (4) and (9), is always located at a quantum boundary. In the calculations, we randomly construct a realization by selecting $\theta_x^A, \theta_y^B,$ and $\chi$ uniformly. The realization is discarded if it does not satisfy Eq. (11). Otherwise, it is kept, and

$$\Delta = \max_{xy} \{ \langle A_x \rangle^2 + S_{xy}^+ - (D_x^B)^2, \langle B_y \rangle^2 + S_{xy}^+ - (D_y^A)^2 \}$$

is calculated. The realization constructed in this way saturates both Eqs. (4) and (9) only when $\Delta = 0$. Letting $p$ be the correlation generated by the realization, we then investigate the quantum realizability of $q = \lambda p + (1 - \lambda)I$, where $I$ is the completely random correlation given by $\langle A_x B_y \rangle = \langle A_x \rangle = \langle B_y \rangle = 0$. Concretely, we obtain the maximum possible value of $\lambda$, denoted by $\lambda_{\text{max}}$, using the $1 + AB$ level of the NPA hierarchy method for each of the realizations constructed randomly (including the case of $\Delta \neq 0$). Since $\lambda_{\text{max}}$ obtained via the NPA method is an upper bound such that $q$ is quantum realizable but $p$ is known to be quantum realizable, $\lambda_{\text{max}} = 1$ means that $p$ is located at a quantum boundary (see the schematic picture in Fig. 2). Figure 2 shows the results of the calculations, which indicate that $\lambda_{\text{max}} = 1$ always holds when $\Delta = 0$. We have also confirmed that all data points with $\lambda_{\text{max}} = 1$ for $\Delta > 0$ correspond to the edge of the probability space $\min p(ab|xy) = 0$. Note that the device-indepen- dent upper bounds of $D_x^B$ and $D_y^A$ are typically monotonically decreasing in $\lambda$, while the lower bounds in Eq. (3) are monotonically increasing [19]. These monotonicitics also suggest that $p$, where the two bounds meet, must be located at a quantum boundary.

Unfortunately, however, the above calculations cannot exclude the possibility that $p$ is located at a non-extremal boundary. In the first place, does there exist any two-qubit realization that can generate such a non-extremal (and nonlocal) boundary correlation? This alone is an intriguing but difficult problem as discussed in [26, 27]. In the case of a correlation whose two-qubit realization satisfies both Eqs. (4) and (9), however, the certifiability of $D = (D_x^B, D_y^A, D_x^L, D_y^L)$ (confirmed numerically) strongly constrains the possibility of being a non-extremal boundary correlation. For a correlation written by two extremal correlations as $\lambda p + (1 - \lambda)p_1$, a realization with $\sqrt{\Delta D^2(p_0) + (1 - \lambda)D^2(p_1)}$ necessarily exists [19], but it must coincide with $D(\lambda p_0 + (1 - \lambda)p_1)$ so that $D$ is unique. This coincidence is quite unlikely due to the nonlinear characteristics of the bounds Eq. (9), unless the bounds are constant over the entirety of the boundary. For example, Fig. 3 plots the bounds along the non-extremal boundary illustrated in the figure, where the nonlinearity indeed prevents the coincidence. Figure 3 also indicates that the disagreement between the realizations combined with the numerical results (and the initial insight regarding self-testing) motivate us to make the following conjecture:

**Conjecture 1.** In nonlocal quantum correlations, a correlation is extremal if and only if it fulfills Eq. (11) and the realization saturates Eqs. (4) and (9).

Note that, in the case of unbiased marginals, the saturation of Eq. (9) implies $D_x^B = D_y^A = 1$, and Eq. (4) is reduced to the TLM inequality, as it should be. Our
conjectured criterion also correctly identifies the analytical examples of extremal correlations in [28, 29], and even the non-exposed extremal correlation of the Hardy point [18, 30]. Moreover, in the case of local correlations, the inset of Fig. 2 suggests that the criterion ensures the boundary condition (C\text{\text{CHSH}}=2), but not necessarily extremality due to the correlation of, e.g., Eq. (12). Note further that Fig. 2 also suggests the following.

Conjecture 2. The 1+AB level of the NPA hierarchy (i.e., almost quantumness [31]) is sufficiently strong to tightly bound every extremal correlation.

It is immediately noticed that we can eliminate \( D^A \) and \( D^B \) by combining Eqs. (4) and (9). The resultant set of inequalities must suffice for identifying the extremality by virtue of the certifiability of \( D^B \) and \( D^A \). However, separating the extremal condition into Eqs. (4) and (9) will be advantageous in searching for fundamental principles that limit nonlocal correlations, as the principles leading to Eqs. (4) and (9) will be independent of each other. For example, the information causality (IC) principle [32] successfully explains the Tsirelson bound and even some curved quantum boundaries [33], and it was expected that the IC principle could explain every quantum boundary. As not in [19] (see also Appendix A), however, the IC principle cannot explain extremal boundaries generated from a partially entangled state, as it cannot explain the saturation of Eq. (4) unless \( D^B = D^A = 1 \), where Eq. (9) plays no role, i.e., the IC principle is unrelated to Eq. (9). On the other hand, the cryptographic principle possibly explains the saturation of Eq. (4) when \( D^B, D^A < 1 \) [20], but it cannot explain Eq. (9).

What is the fundamental principle that leads to Eq. (9)? This is an important open problem, but the physical meaning of Eq. (7), on which Eq. (9) is based, is relatively obvious: the entanglement bound for the guessing probability in an uncertainty game [34, 35].

When Alice and Bob share a maximally entangled state (\( \sin^2 2\chi = 1 \)), Bob can perfectly guess Alice’s outcome for both \( x = 0, 1 \) as \( D^B = 1 \), and the unentanglement between \( A_0 \) and \( A_1 \) vanishes [1]. The guessing probability decreases as the entanglement decreases, and for an unentangled state (\( \sin^2 2\chi = 0 \)), the guessing probability is solely determined by the uncertainty \( \Delta A_x = \sqrt{1 - \langle A_x^2 \rangle} \) as \( D^B = \langle A_x^2 \rangle \) (see [24, 26, 37] for a slightly different link between nonlocality and uncertainty). Since correlations with biased marginals are generated from a partially entangled state, it is natural that the amount of entanglement is involved in the extremality condition. Hence, a fundamental principle that leads to Eq. (9) must be the one that more or less explains the entanglement bound in an information-theoretical way.

The plausible analytical condition that limits the strength of extremal quantum correlations in the simplest Bell scenario was determined. We hope that this analytical condition will result in a new fundamental principle behind quantum mechanics to be found.

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Appendix A: Two-qubit realization

Here, the details of two-qubit realizations, where projective measurements of rank 1 are performed on a two-qubit entangled state \( |\psi \rangle \), are described. By applying appropriate local unitary transformations, Alice’s and Bob’s observables are written as

\[
A_x = \cos \theta^A_x \sigma_1 + \sin \theta^A_x \sigma_3, \quad B_y = \cos \theta^B_y \sigma_1 + \sin \theta^B_y \sigma_3, \tag{A1}
\]

where \( \sigma_1, \sigma_2, \sigma_3 \) are the Pauli matrices. Since any Bell expression is then maximized when \( \rho = |\psi \rangle \langle \psi | \) is real symmetric, \( |\psi \rangle \) can be expressed by further rotating the local bases as

\[
|\psi \rangle = \cos \chi |00 \rangle + \sin \chi |11 \rangle \quad (0 < \chi \leq \pi/4). \tag{A2}
\]

Under this parameterization, we have

\[
\langle A_x B_y \rangle = \sin \theta^A_x \sin \theta^B_y + \cos \theta^A_x \cos \theta^B_y \sin 2\chi, \tag{A3}
\]

\[
\langle A_x \rangle = \sin \theta^A_x \cos 2\chi, \tag{A4}
\]

\[
\langle B_y \rangle = \sin \theta^B_y \cos 2\chi. \tag{A5}
\]

Moreover, define the angles \( \phi^A_x \) and \( \phi^A_y \) as

\[
\text{tr}_A A_x |\psi \rangle = \frac{\langle A_x \rangle}{2} I + \frac{D^B_x}{2} (\cos \phi^B_x \sigma_1 + \sin \phi^B_x \sigma_3),
\]

\[
\text{tr}_B B_y |\psi \rangle = \frac{\langle B_y \rangle}{2} I + \frac{D^A_y}{2} (\cos \phi^A_y \sigma_1 + \sin \phi^A_y \sigma_3). \tag{A6}
\]

It is found that

\[
D^B_x = \sqrt{\sin^2 \theta^B_x + \cos^2 \theta^B_x \sin^2 2\chi} = \text{tr} |\psi \rangle \langle \psi | - \rho^B_{11}, \tag{A7}
\]

\[
D^B_y = \sqrt{\sin^2 \theta^B_y + \cos^2 \theta^B_y \sin^2 2\chi} = \text{tr} |\psi \rangle \langle \psi | - \rho^B_{00}, \tag{A8}
\]

where \( \rho^B_{00} = \text{tr} |\psi \rangle \langle \psi | - \rho^B_{11}, \rho^B_{11} = \text{tr} |\psi \rangle \langle \psi | - \rho^B_{00} \).

Let us then determine the entanglement specified by \( \sin^2 2\chi \) for a given \( \{ \langle A_x B_y \rangle, \langle A_x \rangle, \langle B_y \rangle \} \). Eliminating \( \theta^A_x \) and \( \theta^B_y \) from Eqs. (A3)–(A7), we have

\[
\langle A_x B_y \rangle = \frac{\langle A_x \rangle \langle B_y \rangle \pm \sin 2\chi \sqrt{1 - \langle A_x^2 \rangle^2 \cos^2 2\chi} \sqrt{1 - \langle B_y^2 \rangle^2 \cos^2 2\chi}}{\cos^2 2\chi},
\]

and thus we have the quadratic equation for \( \cos^2 2\chi \), i.e.,

\[
\cos^2 2\chi + (J_{xy} - 2) \cos^2 2\chi + K_{xy}^2 - J_{xy} + 1 = 0. \tag{A8}
\]

Since this must hold for every \( x \) and \( y \), there are four quadratic equations in total. Two solutions of each quadratic equation are given by \( \sin^2 2\chi = S_{xy}^\pm \).

Let us see that, when a (non two-qubit) realization of a correlation simultaneously saturates the scaled TLM inequalities, \( (D^B_x)^2 \leq \langle A_x \rangle^2 + S_{xy}^+, (D^B_y)^2 \leq \langle B_y \rangle^2 + S_{xy}^- \),
and further fulfills $\prod_{xy}[(1 - S_{xy})^2 - (A_x B_y) - \langle A_x \rangle (B_y)] \geq 0$, the correlation also has a two-qubit realization. When $S_{xy}^+ = 1$, since $D_A^B - D_A^B \leq 1$, it is found that $D_A^B = D_A^B = 1$ in the original realization, and the existence of a two-qubit realization is obvious from the TLM criterion. When $0 < S_{xy}^+ < 1$, a two-qubit realization can be constructed as follows: first determine $x$ from $\sin^2 2x = S_{xy}^+$, and next determine $\theta_A^B$ and $\theta_B^B$ from Eq. (A1) and Eq. (A5), respectively. This two-qubit realization can reproduce $\langle A_x B_y \rangle$ of the original realization by adjusting the signs of $\cos \theta_B^y$ and $\cos \theta_B^y$ as $S_{xy}^+$ is a solution of Eq. (A8), and $\prod_{xy}[(A_x B_y) - \langle A_x \rangle (B_y)] \geq 0$. Moreover, since $D_A^B$ and $D_A^B$ of the two-qubit realization are the same as those of the original realization, the two-qubit realization saturates the scaled TLM inequality, if the original realization does.

Note that

$$\sin \theta_A^x = D_A^B \sin \phi_A^B, \quad \cos \theta_A^y = D_A^B \cos \phi_A^B / \sin 2x,$$

$$\sin \theta_B^y = D_A^y \sin \phi_B^y, \quad \cos \theta_B^y = D_A^y \cos \phi_B^y / \sin 2x(A9)$$

hence,

$$\frac{\langle A_x B_y \rangle}{D_A^B} = \cos(\phi_A^B - \phi_B^y), \quad \frac{\langle A_x B_y \rangle}{D_A^y} = \cos(\phi_A^y - \theta_A^x).$$

When $\tilde{C}_{xy} = \cos(\phi_A^x - \theta_B^y) \equiv \cos \delta_{xy} = 0$, by noticing that

$$\tilde{C}_{00} \tilde{C}_{11} - 2 \tilde{C}_{01} \tilde{C}_{11} = \cos \delta_{00} \cos \delta_{01} - \cos \delta_{10} \cos \delta_{11} \quad \text{and} \quad \cos \delta_{00} = \cos \delta_{01} - \cos \delta_{10} = - \sin \delta_{01} \sin \delta_{10} + \sin \delta_{11} = - \sin \delta_{01} \sin \theta_{01} + \sin \delta_{10} \sin \delta_{11},$$

it is not difficult to see that the necessary and sufficient condition for the saturation of the scaled TLM inequality is given by $\sin \delta_{00} \sin \delta_{01} \sin \delta_{10} \sin \delta_{11} \leq 0$.

**Appendix B: Insufficiency of IC principle**

We briefly noted in [19] that the information causality (IC) principle is insufficient for the full identification of the quantum boundaries for bipartite settings, no matter what protocol is considered. However, the paper was criticized because the explanation was considered unclear or the point was completely misunderstood. Here, we explain the point in more detail.

Let us recall the derivation of the IC principle. In the general setting of communication, where Alice is given a bit string $\tilde{x} = (x_1, x_2, \cdots)$ and sends $\tilde{m}$ to Bob as a message, the information about $\tilde{x}$ obtainable by Bob is characterized by the mutual information $I(\tilde{x} : \tilde{m} | \rho_B)$, where $\rho_B$ is the state of Bob’s half of the no-signaling resources. Using the no-signaling condition and the information-theoretical relations respected by quantum mechanics, it was shown in [22] that

$$I(\tilde{x} : \tilde{m} | \rho_B) \leq H(\tilde{m}) - H(\tilde{m} | \tilde{x} | \rho_B) \leq H(\tilde{m}). \quad (B1)$$

Since the entropy $H(\tilde{m})$ cannot exceed the number of bits in $\tilde{m}$, the IC principle is derived. Here, we consider the case where the number of message bits is finite such that $H(\tilde{m})$ is finite.

The point is that the term $H(\tilde{m} | \tilde{x} | \rho_B)$ in Eq. (B1) is inevitably nonzero in some cases; hence, the satisfaction of Eq. (B1) is impossible. Namely, the IC principle has omitted the nonnegligible term in its derivation.

Suppose that Alice and Bob share $n$ identical “quantum boxes”, each of which accepts inputs $(u, v)$ and produces outputs $(a, b)$ according to the conditional probabilities $p(ab|uv)$, where the simplest Bell scenario is considered (see Fig. 4). A protocol may connect the inputs and outputs of the $n$ boxes in a complicated way, but let us denote Alice’s outcomes as $\tilde{a} = (a_1, a_2, \cdots, a_n)$, where $a_i$ is the outcome of the $i$-th quantum box. Now, consider a correlation located at an extremal boundary and showing $D_A^B < 1$. This means that Bob’s local states (of a single box) for different values of $a$ become nonorthogonal; thus, he cannot completely determine $a$. Since $D_A^B$ is generally upper bounded in a device-independent way, his ambiguity about $a$ is inevitable, irrespective of the details of the realization of the quantum box. In this way, each $a_i$ has ambiguity for Bob. This ambiguity is so strong that he cannot determine $\tilde{a}$ even if he knows $\tilde{x}$ (and even if he knows all of Alice’s inputs $\tilde{u}$ to the boxes), i.e., $H(\tilde{a} | \tilde{x} | \rho_B) > 0$. Since $\tilde{m}$ is constructed from $\tilde{x}$ and $\tilde{a}$, it is clear from Eq. (B1) that any protocol whose $\tilde{m}$ contains the information of $\tilde{a}$ and $H(\tilde{m} | \tilde{x} | \rho_B) > 0$ cannot achieve $I(\tilde{x} : \tilde{m} | \rho_B) = H(\tilde{m})$.

Note that no redundant coding technique can reduce Bob’s ambiguity about $\tilde{a}$, as the ambiguity originates from $\rho_B$, which is not under Alice’s control. For example, $\tilde{a} \tilde{a} \tilde{a}$ has exactly the same ambiguity as $\tilde{a}$ for Bob.
If Alice postselects the boxes with the same output \( a \) to multiply Bob’s local state such as \( \rho_{01u}^B \otimes \rho_{01u}^B \otimes \rho_{01u}^B \otimes \cdots \), she can reduce Bob’s ambiguity, but such postselection is not allowed. Although Alice can control the value of \( a \) via the input \( u \) to some degree, \( a \) is nevertheless determined in a probabilistic way by \( p(a|u) \), and it is impossible to completely eliminate Bob’s ambiguity about \( a \).

More concretely, let us consider the quantum box that is realized by a pure partially entangled state and showing \( D_0^B, D_1^B < 1 \). Namely, the outcome \( a \) is ambiguous for both \( u = 0 \) and \( 1 \), and all \( a \)'s are always ambiguous for Bob. The only way for \( H(\tilde{m}|\tilde{x}\rho_B) = 0 \) is that \( \tilde{m} \) does not contain any information of \( \tilde{a} \) at all. This is because, since \( \tilde{m} \) is constructed from \( \tilde{a} \) and \( \tilde{x} \), and thus \( H(\tilde{m}|\tilde{a}\tilde{x}\rho_B) = 0 \), we have \( H(\tilde{m}|\tilde{x}\rho_B) = H(\tilde{m}|\tilde{x}\rho_B) - H(\tilde{m}|\tilde{a}\tilde{x}\rho_B) = I(\tilde{a}:\tilde{m}|\tilde{x}\rho_B) \). Namely, \( H(\tilde{m}|\tilde{x}\rho_B) = 0 \) implies \( I(\tilde{a}:\tilde{m}|\tilde{x}\rho_B) = 0 \); any information about \( \tilde{a} \) must not be obtained via \( \tilde{m} \). In this case, the achievement of \( I(\tilde{x}:\tilde{m}\rho_B) = H(\tilde{m}) \) may be possible (the IC inequality can be saturated even in a purely classical case [38]), but the protocol does not utilize the quantum correlation at all. This protocol, of course, cannot explain the outperformance of the pure entangled state at all (recall that every pure entangled state violates some Bell inequality [39], and hence cannot explain the corresponding extremal boundary).

This is the case of the quantum box showing \( D_0^B < 1 \) but \( D_1^B = 1 \). Namely, the outcome \( a \) is ambiguous only when \( u = 0 \). To achieve \( H(\tilde{m}|\tilde{x}\rho_B) = 0 \), the protocol can only utilize the unambiguous outcomes when \( u = 1 \). In this case, however, without changing the performance of the protocol, we can replace all \( a_i \)'s corresponding to \( u_i = 0 \) with a fixed value, e.g., 1 (because these are not used), and the correlation produced by the quantum boxes is replaced with the classical one. This implies that the behavior of the protocol can be simulated exactly using classical correlations; hence, this protocol cannot explain the outperformance of the pure entangled state again.

In the other remaining case where \( D_0^B = D_1^B = 1 \), if the quantum box is realized by a pure partially entangled state, the produced correlation is classical, because Alice’s measurement bases for \( u = 0 \) and 1 both agree with the Schmidt basis of the pure state.

From the above, it is concluded that the nonlocal extremal boundaries that can be tightly explained by the IC principle are those realized by a maximally entangled state, where \( D_0^B = D_1^B = D_1^D = D_1^I = 1 \).

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