Geometrical self-testing of partially entangled two-qubit states

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Keywords: quantum nonlocality, Bell inequality, self-testing, device-independent quantum information processing

Abstract

Quantum nonlocality has recently been intensively studied in connection to device-independent quantum information processing, where the extremal points of the set of quantum correlations play a crucial role through self-testing. In most protocols, the proofs for self-testing rely on the maximal violation of the Bell inequalities, but there is another known proof based on the geometry of state vectors to self-test a maximally entangled state. We present a geometrical proof in the case of partially entangled states. We show that, when a set of correlators in the simplest Bell scenario satisfies a condition, the geometry of the state vectors is uniquely determined. The realization becomes self-testable when another unitary observable exists on the geometry. Applying this proven fact, we propose self-testing protocols by intentionally adding one more measurement. This geometrical scheme for self-testing is superior in that, by using this as a building block and repeatedly adding measurements, a realization with an arbitrary number of measurements can be self-tested. Besides the application, we also attempt to describe nonlocal correlations by guessing probabilities of distant measurement outcomes. In this description, the quantum set is also convex, and a large class of extremal points is identified by the uniqueness of the geometry.

1. Introduction

It was shown by Bell that the nonlocal correlations predicted by quantum mechanics are inconsistent with local realism [1]. Bell nonlocality, or quantum nonlocality, has attracted many research interests over the years (see [2] for a review). Recently, it has been intensively studied in connection to device-independent quantum information processing (see [3, 4] for reviews), where the extremal points of the convex set of quantum correlations plays a crucial role through self-testing.

The correlation that attains the maximal quantum violation of $2\sqrt{2}$ [5] in the Clauser–Horne–Shimony–Holt inequality [6] is an extremal point of the quantum set, for which the quantum realization (state and measurements) is unique up to unavoidable local isometry. This implies that attaining the value of $2\sqrt{2}$ can self-test the state and the measurements in the Bell experiment [7]. When a realization is a unique maximizer of a Bell inequality, the realized correlation is a self-testable extremal point. Although there exist non-exposed extremal points that cannot be a unique maximizer of any Bell inequality, a correlation is extremal when the realization is self-testable [8]. In this way, self-testability and extremality are intimately connected. In most protocols, the proofs for self-testing rely on the maximal violation of the Bell inequalities. However, even in the simplest Bell scenario (two parties and two binary measurements on each party), the maximal violation by a partially entangled state is known for only a few Bell inequalities [9–13], and not many protocols are proposed for self-testing partially entangled states [14–18].

On the other hand, the proof for self-testing in [19] is fascinating, because no Bell inequality is used directly. In the simplest Bell scenario, when marginal probabilities of outcomes are unbiased, the boundaries of the quantum set are identified by the Tsirelson–Landau–Masanes (TLM) criterion [20–22]. The proof in [19] relies on the fact that the geometry of the state vectors is uniquely determined when the TLM criterion is satisfied (and the anti-commutation relation between observables is proven on the geometry). However, this geometrical
proof is restricted to the case of a maximally entangled state by the restriction of the TLM criterion. In a general case, where an extremal correlation may be realized by a partially entangled state, the criterion for the identification has been only conjectured, based on the probabilities of guessing outcomes of a distant party (referred as ‘guessing probability’ hereafter) [23].

In this paper, we present a geometrical proof in the case of partially entangled states. We show that, when a set of correlators in the simplest Bell scenario satisfies a condition, the geometry of state vectors is uniquely determined. The realization becomes self-testable when another unitary observable exists on the geometry to prove anti-commutation relation. Applying this proven fact, we propose self-testing protocols by intentionally adding one more measurement to prove the anti-commutation relation. This geometrical scheme for self-testing is superior in that, by using this as a building block and repeatedly adding measurements, a realization with an arbitrary number of measurements can be self-tested.

Beside applications, efforts have been made to describe the quantum set having a complicated structure [24–26, 8, 27] in a more tractable way; some descriptions exist such as covariance [28] and entropy [29]. For this purpose, we attempt to describe nonlocal correlations by guessing probabilities. We show that the quantum realizable set is also convex in this description, and a large class of extremal points is identified by the uniqueness of the geometry of state vectors. Moreover, with the help of this extremality, we show that the sufficiency of the extremal criterion conjectured in [23] can be reduced to certifiability of guessing probabilities.

This paper is organized as follows: in section 2, we briefly summarize the preliminaries. For details, see [2–4] and the references therein. For clarity, we first introduce the description of correlations by guessing probabilities in section 3, and discuss the properties of the quantum set, such as the extremality and self-testability. In section 4, we investigate the geometrical properties of realizations in the standard description of correlations. Finally, as an application, we propose self-testing protocols for partially entangled states in section 5, whose self-testability is geometrically proven, regardless of the validity of the conjectured extremal criterion. A summary is given in section 6.

2. Preliminaries

In the simplest Bell scenario, Alice (Bob) performs one of two binary measurements on a shared state depending on a given random bit x (y), and obtains an outcome a = ±1 (b = ±1). The properties of a nonlocal correlation are described by a set of conditional probabilities \( \{ p(ab|xy) \} \) referred as a ‘behavior’, which specifies a point in the probability space. As \( p(ab|xy) = \frac{1}{2} [1 + \alpha C_A + \beta C_B + \gamma C_{xy}] \) for no-signaling correlations, with \( C_A \) and \( C_B \) being a bias of the marginal \( p(a|x) \) and \( p(b|y) \), any no-signaling correlation can be described by a behavior \( \{ C_A, C_B, C_{xy} \} \). Such a behavior specifies a point in the 8-dimensional no-signaling space, which we denote by the C-space.

A behavior \( \{ C_A, C_B, C_{xy} \} \) is realized by quantum mechanics, if and only if there exist a shared quantum state \( |\psi\rangle \) and the observables \( A_x (B_y) \) of Alice (Bob), such that \( A_x^2 = B_y^2 = I \), \( C_A = \langle \psi | A_x | \psi \rangle \), \( C_B = \langle \psi | B_y | \psi \rangle \), and \( C_{xy} = \langle \psi | A_x B_y | \psi \rangle \). We use \( \langle \cdots \rangle \) as the abbreviation of \( \langle \psi | \cdots | \psi \rangle \). Any state vector has a real-vector representation [20, 30, 31]. For example, when \( |\psi\rangle \) is represented by components as \( |\psi\rangle = (c_0, c_1, \cdots) \) with \( c_i \in \mathbb{C} \), \( \tilde{\psi} = (\text{Re} c_0, \text{Im} c_0, \text{Re} c_1, \text{Im} c_1, \cdots) \) is a real-vector representation.

The realizable behaviors constitute a convex set in the C-space, denoted by \( \mathcal{Q}_C \). In the unbiased case where \( C_A = C_B = 0 \), a behavior belongs to \( \mathcal{Q}_C \), if and only if the TLM inequality [20–22]

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

is satisfied for \( C_{xy} = C_{yx} \) (together with \( p(ab|xy) \geq 0 \)).

Using the correlators of a behavior \( \{ C_A, C_B, C_{xy} \} \), let us introduce the quantities \( S_{xy} \) given by

\[
S_{xy} = \frac{1}{2} |J_{xy}| \pm \sqrt{\frac{1}{4} J_{xy}^2 - 4 K_{xy}},
\]

\[
J_{xy} = C_{xy} - (C_A^2 - (C_B^2) + 1, \quad K_{xy} = C_{xy} - C_A C_B.
\]

Suppose that the following holds for a set \( \{ p_{xy} \} \)

\[
S_{00} = S_{01} = S_{10} = S_{11}, \quad H = \Pi_{xy} [1 - S_{xy}^p] C_{xy} - C_A C_B \geq 0,
\]

(3)
where $p_{xy}$ is either ‘+’ or ‘−’. Letting the value of $S_{xy}^B$ be equal to $\sin^2 2\chi$, the following is also introduced:

$$d^B_\chi \equiv (C^A_\chi)^2 + \sin^2 2\chi, \quad d^A_\chi \equiv (C^B_\chi)^2 + \sin^2 2\chi.$$  \hfill (4)

Then, to identify the nonlocal extremal points of $Q_C$, the following criterion has been conjectured in [23].

**Conjecture 1.** A nonlocal behavior $\{C^A_\chi, C^B_\chi, C_{xy}\}$ is an extremal point of $Q_C$, if and only if equation (3) holds as $S_{00}^B = S_{01}^B = S_{00}^A = S_{11}^A$, and inequality (1) is saturated for both scaled correlators $C_{xy} = C_{xy}/\sqrt{d^B_\chi}$ and $C_{xy} = C_{xy}/\sqrt{d^A_\chi}$.

Note that the fulfillment of equation (3) for some $\{p_{xy}\}$ (not necessarily as $S_{00}^B = S_{01}^B = S_{00}^A = S_{11}^A$) is necessary (and even sufficient in the case of $\sin^2 2\chi < 1$) for the existence of a two-qubit realization in the form of

$$A_x = \sin \theta^A_x \sigma_1 + \cos \theta^A_x \sigma_3, \quad B_y = \sin \theta^B_y \sigma_1 + \cos \theta^B_y \sigma_3,$$

$$|\psi\rangle = \cos \chi |00\rangle + \sin \chi |11\rangle,$$  \hfill (5)

where $(\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices (but there is no $\sigma_2$ term), and hence also necessary for the extremality of $Q_C$ (see the supplemental material of [23]). Note further that the definition of $\theta^A_\chi$ and $\theta^B_\chi$ are changed from [32, 33, 23] for convenience $\theta^A_\chi \rightarrow \pi/2 - \theta^A_\chi$ and $\theta^B_\chi \rightarrow \pi/2 - \theta^B_\chi$.

Moreover, for a given $\{C^A_\chi, C^B_\chi, C_{xy}\}$, the quantity $D^B_\chi$ and $D^A_\chi$ (explained later) has a device-independent upper bound, which can be obtained by the Navascués–Pironio–Acín (NPA) hierarchy [35, 36], and the following is also implicitly conjectured in [23].

**Conjecture 2.** When a nonlocal behavior $\{C^A_\chi, C^B_\chi, C_{xy}\}$ satisfies the same condition as Conjecture 1, $d^B_\chi$ and $d^A_\chi$ coincides with the device-independent upper bound of $(D^B_\chi)^2$ and $(D^A_\chi)^2$, respectively.

### 3. Quantum set in D-space

As mentioned, $C^A_\chi$ is the bias of $p(a|x)$, but it is also the bias of Bob’s optimal probability of guessing Alice’s outcome $a$, without the use of any side information. In the nonlocality scenario, however, Bob has a half of a shared state; the local state $\rho_{0|x}$ (conditioned on Alice’s outcome $a$), and by the use of it the guessing probability is generally increased. Therefore, it seems another natural way of describing nonlocal correlations to use the guessing probabilities optimized under $\rho_{0|x}$. For this purpose, we focus on the quantities introduced in [32, 33]

$$D^B_\chi \equiv \max_{(X_a) = 1} \langle A_x X_b \rangle, \quad D^A_\chi \equiv \max_{(X^A_i) = 1} \langle X_{a_i} B_y \rangle,$$  \hfill (6)

where the maximization is taken over any Hermite operator $X_b(X_a)$ on Bob’s (Alice’s) side. Indeed, when $\rho_{0|a|x}$ and $\rho_{1|a|x}$ are both pure states, the maximum in the definition of $D^B_\chi$ is attained when $X_b = I$ [32]; hence $D^B_\chi$ becomes equal to $\text{tr}(|\psi_a\rangle\langle\psi_a| - \rho_{0|a|x})$, coinciding with the bias of Bob’s optimal guessing probability [34].

Let us then describe a correlation by a behavior $\{\delta^B_\chi, \delta^A_\chi, C_{xy}\}$, such that it is realized by quantum mechanics if and only if there exist $|\psi\rangle$, $A_{\chi}^2 = B_{\chi}^2 = I$, $\delta^B_\chi = (D^B_\chi)^2$, $\delta^A_\chi = (D^A_\chi)^2$, and $C_{xy} = \langle \psi | A_x B_y | \psi \rangle$. The reason for taking the square of $D^B_\chi$ and $D^A_\chi$ will become clear soon. Such a behavior specifies a point in an 8-dimensional space, which we denote by the $D$-space. Note that the behaviors in the $C$-space and the $D$-space have no one-to-one correspondence. For example, the completely random correlation is uniquely represented by $\{C^A_\chi = 0, C^B_\chi = 0, C_{xy} = 0\}$ in the $C$-space but represented in the $D$-space by $\{\delta^B_\chi = 0, \delta^A_\chi = 0, C_{xy} = 0\}$ and $\{\delta^B_\chi = 1, \delta^A_\chi = 1, C_{xy} = 0\}$. The former is realized by $A_x = B_y = \sigma_1|00\rangle + \sigma_3|11\rangle$ and the latter is realized by $A_x = \sigma_1, B_y = \sigma_3$.

Now, let us investigate the properties of the behaviors in the $D$-space. When the behaviors $p_{xy}$ are realized by quantum mechanics, there always exists a realization of the behavior $p_{xy} = \sum_i \lambda_i |\psi_i\rangle$ for any $\lambda_i > 0$ such that $\sum_i \lambda_i = 1$. This is because, as shown in appendix A, although $(D^B_\chi)^2$ and $(D^A_\chi)^2$ are convex in general such that

$$[D^B_\chi(p_{xy})]^2 \leq \sum_i \lambda_i [D^B_\chi(\psi_i)]^2,$$  \hfill (7)

the equality holds, at least when each local state of the realization of $p_{xy}$ has orthogonal support, and hence,

**Lemma 1.** The behaviors $\{\delta^B_\chi, \delta^A_\chi, C_{xy}\}$, which are realized by quantum mechanics, constitute a convex set.

This set, denoted by $Q_D$, is then at least enclosed by the hyperplanes in the $D$-space defined from the following inequalities:
\[
B^A = -\sum_{x} V^x_x \delta^x_x + \sum_{x \neq y} V^x_y \delta^x_y \leq \frac{1}{4d^a}, 
\]
\[
B^B = -\sum_{x} V^x_x \delta^x_x + \sum_{x \neq y} V^x_y \delta^x_y \leq \frac{1}{4d^b}, 
\]
where the coefficients satisfy \( V^x_x \geq 0, \Pi V^x_y \leq 0, \) and \( V^x_y \leq -V^y_x V^0_0 V^1_1 \) for both \( c = A, B \). Note that \( V^0_0 \) is the coefficient of \( C^a \), while \( V^0_1 \) is the coefficient of \( C^b \). The quantum bound of the inequalities is given by
\[
q^c = \frac{V^c_c}{(s^c_c)^2}, \quad s^c_c = \frac{X}{\sqrt{V^0_0 V^1_1}}, \quad s^c_i = \frac{-X}{\sqrt{V^0_1 V^1_0}}, 
\]
\[
X = V^0_0 V^1_1 + (V^0_0)^2 - V^0_0 V^1_0 (V^1_0)^2 + (V^1_1)^2. 
\]
This is due to the proposed quantum bound shown in [32]. Indeed, \( u^b_{xy} = (-1)^V_{ab} s^b_{xy}/s^a_{xy} \) fulfills \( \sum_{xy} (u^b_{xy})^2 = 1 \) and \( u^b_{xy} u^a_{xy} = u^a_{xy} u^a_{xy} \); hence any realization obeys
\[
B^B = -q^b \sum_{x} s^b_{xy} \delta^a_{xy}^2 + \sum_{x \neq y} s^b_{xy} u^a_{xy} (-1)^V_{ab} \langle A_x B_y \rangle 
\]
\[
\leq -q^b \sum_{x} s^b_{xy} \delta^a_{xy}^2 + \sum_{x \neq y} (s^b_{xy} \delta^a_{xy})^2 \leq \frac{1}{4d^a}. 
\]
The same holds for \( B^A \) by using \( u^a_{xy} = (-1)^V_{ab} s^a_{xy}/s^b_{xy} \). The inequalities (8) and (9) are respected by any quantum realization, which we denote by quantum Bell inequalities in analogy to the Bell inequalities.

It is convenient to introduce another classical set, which is enclosed by inequalities (10). It is known that each extremal point of \( Q_D \) has a two-qubit realization [5, 37]. This is due to the fact that \( A_0 \) and \( A_1 \) (\( B_0 \) and \( B_1 \) as well) are simultaneously block-diagonalized by appropriate local bases with the block size of at most 2 [37]. However, this cannot be applied to the case of \( Q_D \) due to the convexity of \( (D^a)^2 \) and \( (D^b)^2 \) as inequality (7). Fortunately, however, we have the following:

**Lemma 2.** A behavior in \( Q_D \), which simultaneously saturates the quantum Bell inequalities (8) and (9), has a two-qubit realization.

**Proof.** As the maximization in \( D^B \) is rewritten by using the Lagrange multiplier \( l \) as
\[
D^B = \max_{x \in \mathbb{R}^2} \{ \langle \psi | A_x | \psi \rangle - l (\langle \psi | X_0^a | \psi \rangle - 1) \}, 
\]
any realization must satisfy
\[
\text{tr}_A A^\dagger_x | \psi \rangle \langle \psi | = \frac{D^B}{2} \text{tr}_A (F^A | \psi \rangle \langle \psi | F^A \rangle), 
\]
where \( F^A \) is an optimal operator attaining the maximum. Let \( \hat{\psi}, \hat{A}_x, \hat{B}_y, \) and \( \hat{F}^A \) be the real-vector representation for \( | \psi \rangle, \langle \psi | \), \( A_x | \psi \rangle \), and \( F^A | \psi \rangle \), respectively, which are all unit vectors. Then, equation (12) implies
\[
\hat{A}_x \cdot \hat{F}^A = D^B, \quad \hat{A}_x \cdot \hat{B}_y = D^B \hat{F}^A \cdot \hat{B}_y, \quad \hat{A}_x \cdot \hat{\psi} = D^B \hat{F}^A \cdot \hat{\psi}. 
\]
On the other hand, the saturation of inequality (8) implies that inequality (1) is saturated for \( \hat{C}_{xy} = \hat{A}_x \cdot \hat{B}_y / D^B = \hat{F}^A \cdot \hat{B}_y \), which ensures that four real vectors \( \hat{B}_y \), \( \hat{B}_y \), \( \hat{F}^A \), and \( \hat{F}^A \) lie in the same \( B \)-plane [19] as shown in figure 1. Similarly, the saturation of inequality (9) implies that four real vectors \( \hat{A}_1, \hat{B}_1, \hat{E}_y, \) and \( \hat{E}_y \) lie in the same \( A \)-plane, where \( \hat{E}_y \) is the real vector optimizing \( D^B \). However, as a high-dimensional vector space is considered, the relationship between the two planes has not been determined yet.

Suppose that \( \hat{A}_0 = \pm \hat{A}_1 \) and \( \hat{B}_0 = \pm \hat{B}_1 \). Let the projection of \( \hat{\psi} \) to the \( A \)-plane (\( B \)-plane) be \( \hat{\psi}_A (\hat{\psi}_B) \). Moreover, let the projection of \( | \psi \rangle \) to the \( A \)-plane be \( | \psi \rangle \). From the laws of sines and cosines, \( | \psi \rangle \) is given by
\[
\frac{(\hat{A}_0 \cdot \hat{\psi}_B)^2 + (\hat{A}_1 \cdot \hat{\psi}_B)^2 - 2(\hat{A}_0 \cdot \hat{\psi}_B)(\hat{A}_1 \cdot \hat{\psi}_B) \cos \Delta}{\sin^2 \Delta}, 
\]
where \( \Delta \) is the angle between \( \hat{A}_0 \) and \( \hat{A}_1 \). From equation (13),
\[
\hat{A}_x \cdot \hat{\psi}_B = D^B \hat{F}^A \cdot \hat{\psi}_B = D^B \hat{F}^A \cdot \hat{\psi} = \hat{A}_x \cdot \hat{\psi} = \hat{A}_x \cdot \hat{\psi}_A, 
\]
and consequently we have \( | \psi \rangle = | \psi \rangle \). Similarly, we have \( | \psi \rangle = | \psi \rangle \). This implies that the two planes intersect with \( \hat{\psi} = \hat{\psi}_A = \hat{\psi}_B \) being a common vector as shown in figure 1. The two-qubit realization of equation (5) can realize the same geometry of real vectors.
When $\tilde{A}_0 = \pm \tilde{A}_1, \tilde{A}_c$ and $\tilde{B}_0$ lie in a 3-dimensional subspace. Moreover, the saturation of inequality (1) for scaled correlators occurs only when $\tilde{A}_0$ coincides with $\pm \tilde{E}_0$ or $\pm \tilde{E}_1$, and $\tilde{F}_0$ coincides with $\pm \tilde{B}_0$ or $\pm \tilde{B}_1$. The behavior in the $D$-space realized by such a simple geometry can be realized by equation (5). Similarly, when $\tilde{B}_0 = \pm \tilde{B}_1$. 

As such a behavior saturates inequality (1) for scaled correlators, it is located at a boundary of $Q_{\text{crypt}}$. Conversely, a boundary behavior of $Q_{\text{crypt}}$ generally does not have a realization with the geometry of figure 1 and cannot be realized by quantum mechanics; hence,

**Lemma 3.** $Q_D$ is a strict subset of $Q_{\text{crypt}}$.

Hereafter, to describe the geometry of figure 1, we also use the shortcut notations of

$$\Delta_{ij}^c \equiv \phi_i^c - \phi_j^c, \quad \Delta \theta^c \equiv \theta_0^c - \theta_1^c, \quad \Delta \phi^c \equiv \phi_0^c - \phi_1^c,$$

for both $c = A, B$. See figure 1 for the definition of $\phi_0^c$ and $\phi_1^c$. Note that, as inequality (1) is saturated for scaled correlators, the geometry of figure 1 satisfies

$$\prod_{xy} \sin \Delta_{xy}^B \leq 0 \quad \text{and} \quad \prod_{xy} \sin \Delta_{xy}^A \leq 0. \quad (17)$$

When such a geometry is given, we can easily construct the quantum Bell inequalities (8) and (9) that are simultaneously saturated by the geometry, as shown in appendix B. Conversely, let us investigate the realizations to maximize such a given pair of the quantum Bell inequalities. Note that there exists unavoidable ambiguity of the realizations, which is referred as obvious symmetries hereafter, as the four geometries with the parameters \{ $\theta_0^A, \theta_1^A; \chi$, $\pi - \theta_0^A, \pi - \theta_1^A; \chi$, $\pi + \theta_0^B, \pi + \theta_1^B; \chi$ \} realize the same behavior in the $D$-space. In general, the realization that saturates either inequality (8) or (9) is not unique; hence belonging to a flat surface of $Q_D$. The realization is characterized by $\Delta \theta^B$ and $\Delta \theta^A$, respectively, such that $\Delta_{xy}^B$ and $\Delta_{xy}^A$ are determined for a given $\Delta \theta^B$ and $\Delta \theta^A$, respectively. However, $\langle A_x B_y \rangle = D_x^B \cos \Delta_{xy}^B = D_x^A \cos \Delta_{xy}^A$ must hold in figure 1. As a result, to saturates both inequalities (8) and (9), $\Delta \theta^B$ and $\Delta \theta^A$ are constrained to satisfy

Figure 1. Geometry of real vectors, where $\tilde{F}_0, \tilde{F}_1, \tilde{F}_c$, and $\tilde{B}_0, \tilde{B}_1, \tilde{E}_0, \tilde{E}_1$, and $\tilde{A}_1$ lie in the $B$-plane ($A$-plane), respectively. The two planes intersect at the angle of $\pi/2 - 2\chi$, with $\tilde{E}_c$ being a common vector. The angle between $\tilde{E}_c$ and $\tilde{A}_c$ is denoted by $\theta_c^A$ (or $\theta_c^B$), and that between $\tilde{E}_c$ and $\tilde{B}_c$ is denoted by $\theta_c^B$ (or $\theta_c^A$). As inequality (1) is saturated by scaled correlators, inequality (17) holds in this geometry. We assume, without loss of generality, $0 \leq \chi \leq \pi/4$ throughout this paper.
where the parameters of the original geometry used for constructing a given pair of the Bell inequalities are indicated by an overline such as $\overline{\Delta \theta}$. The parameters $\alpha$ and $\beta$ are given by $-\sin \overline{\Delta_{10}}/ \sin \overline{\Delta_{01}}$ and $\sin \overline{\Delta_{1i}}/ \sin \overline{\Delta_{0i}}$, respectively. As details are given in appendix B, when equation (18) only has a trivial solution of $\cos \Delta \theta^c = \cos \overline{\Delta \theta}$ for both $c = A, B$, the realizations become unique up to obvious symmetries, and we have

**Lemma 4.** The geometry of a realization, which simultaneously saturates the quantum Bell inequalities (8) and (9), is unique up to obvious symmetries when equation (18) only has a trivial solution; hence such a behavior is an extremal point of $Q_D$.

For a given pair of quantum Bell inequalities, no pair of $\alpha^c$ and $\beta^c$ is identical in general and equation (18) only has a trivial solution. This implies that the behaviors realized by two-qubit realizations equation (5) with the parameters satisfying inequality (17) are generally extremal for $Q_D$, constituting a large class of extremal points. Note that the uniqueness of the realization is not necessarily required for the extremality, and hence lemma 4 does not exclude the possibility that the behaviors realized by equation (5) with inequality (17) are all extremal.

In any case, for an extremal behavior of $Q_D$ proven by lemma 4, the geometry of real vectors is unique up to the obvious symmetry. Is such a behavior self-testable? The answer is negative by two reasons (apart from the problem of how $D^B$ and $D^A$ is determined by experiments). The first is that $|\tilde{\psi}'|$ in figure 1 is undetermined; $|\tilde{\psi}'|$ can be determined through $\langle A_x \rangle = |\tilde{\psi}'| \cos \theta^A_x$ or $\langle B_y \rangle = |\tilde{\psi}'| \cos \theta^B_y$, but these are unspecified in the $D$-space. The second relates to the convexity of $(D^B)^2$ and $(D^A)^2$. As shown in appendix C, there exists an example in which the correlation $p$, despite being an extremal point of $Q_D$, may have two different realizations due to the strict convexity. However, in some cases, we can exclude the possibility of such strict convexity, that is, the certifiability of $D^B$ and $D^A$.

Suppose that Conjecture 2 holds true. As inequality (1) is saturated for scaled correlators, $(D^B)^2$ and $(D^A)^2$ are also lower bounded by $d^B$ and $d^A$ [23]; hence those are certifiable, and we have $(D^B)^2 = d^B$ and $(D^A)^2 = d^A$. This correlation, denoted by $p$, is then found to be an extremal point of $Q_D$ by lemma 4. When a realization of $p$ is decomposed into two-qubit realizations of $p$, based on the block-diagonalization [37], $(D^B)^2$ and $(D^A)^2$ must not be strictly convex; otherwise we would construct a realization whose $D^B$ or $D^A$ exceeds the device-independent upper bound by using orthogonal bases. Moreover, because the correlation $p$ is an extremal point of $Q_D$, all $p$ must exhibit the same behavior $(d^B, d^A, C_B)$ in the $D$-space. Then, the geometry of the two-qubit realizations is uniquely determined up to the obvious symmetry by lemma 4. The symmetry leaves the ambiguity between $(C_A, C_B)$ and $(-C_A, -C_B)$, but the latter is clearly inappropriate. In this way, the extremality of $Q_D$, combined with the certifiability of $D^B$ and $D^A$, makes the realization unique; hence, lemma 5.

**Lemma 5.** If Conjecture 2 holds true, the extremal behaviors of $Q_D$ by lemma 4 are self-testable extremal points of $Q_C$.

This lemma implies that the sufficiency of Conjecture 1 relies on the validity of Conjecture 2. Note that, under the truth of Conjecture 2, the self-testable extremal points of $Q_C$, by lemma 5 are such that inequality (3) is satisfied as $S_{a0} = S_{01} = S_{10}^+ = S_{11}^+$, inequality (1) is saturated by both $\tilde{C}_{xy} = C_{xy} / \sqrt{d^B}$ and $\tilde{C}_{xy} = C_{xy} / \sqrt{d^A}$, and equation (18) only has a trivial solution. As mentioned above, the information of $(C_A, C_B)$ is necessary for self-testing to specify $|\psi'|$, and it is indeed used in lemma 5 through equation (3).
4. Quantum set in $C$-space

From now on, let us show some geometrical properties of the realizations for the behaviors in the standard $C$-space. Note that these hold true regardless of the validity of Conjectures 1 and 2. To begin with, we show that the geometry of the realization of a behavior in the $C$-space is uniquely determined when the correlators satisfy a condition:

**Lemma 6.** For a nonlocal behavior \( \{ C_x^A, C_y^B, C_y^C \} \) which satisfies inequality (3) for some \( \{ P_y \} \) (not necessarily as \( S_{00} = S_{01} = S_{10} = S_{11} \) and saturates inequality (1) for both \( C_{xy} = C_{xy} \sqrt{d_x^A} \) and \( \bar{C}_{xy} = C_{xy} \sqrt{d_x^A} \), the geometry of the realization is unique up to obvious symmetries.

The unique geometry is the same as figure 1, but the obvious symmetry now refers the ambiguity between \( \{ \theta_x^A, \theta_y^B, \chi \} \) and \( \{ -\theta_x^A, -\theta_y^B, \chi \} \). Moreover, \( |\psi| \) is determined to \( \cos 2\chi \) as in the two-qubit realizations of equation (5). The proof is given in appendix D. The difference from the proof of lemma 2 is that \( d_x^B \) and \( d_y^A \) by equation (4) are not ensured to coincide with \( (D_y^A)^2 \) and \( (D_y^A)^2 \), and we cannot use equation (12). For the same reason, \( \bar{E}_x \) and \( \bar{E}_y \), in figure 1, are now not ensured to attain \( D_y^B \) and \( D_y^A \), \( \sqrt{d_x^B} \bar{E}_x \) is merely the projection of \( \bar{A}_x \) to the $B$-plane.

In this way, the geometry is uniquely determined for not necessarily \( S_{00} = S_{01} = S_{10} = S_{11} \). However, this uniqueness does not ensure the extremality of \( Q_C \). This is in contrast to lemma 4, where quantum Bell inequalities are maximized by a unique geometry, and the extremality of \( Q_D \) is ensured. Indeed, the nonlocal correlation \( P \) in appendix C, where \( S_{00} = S_{01} = S_{10} = S_{11} \), is an explicit counter example for extremality. Interestingly, \( P \) is located in the strict interior of the quantum set, according to the $1 + AB$ level of the NPA hierarchy [38]. This also implies that, even though \( |\psi| \) is located to be the same as the two-qubit realizations, the uniqueness is still insufficient for self-testing. The condition \( S_{00} = S_{01} = S_{10} = S_{11} \) is crucial, apart from the unique determination of the geometry, for making the realization self-testable through the certification of \( D_y^B \) and \( D_y^A \), as shown by lemma 5.

However, other than the unproved certification condition, a more general condition that makes the unique geometry self-testable is found as follows:

**Lemma 7.** For a nonlocal behavior \( \{ C_x^A, C_y^B, C_y^C \} \), which has a unique geometry by lemma 6, the realization is self-testable, if and only if a real vector representation \( \tilde{G} \) of \( G(\psi) \), with \( G \) being a local unitary observable, exists in either $A$-plane or $B$-plane (other than $\pm \bar{A}_x$ and $\pm \bar{B}_y$).

**Proof.** As the geometry is uniquely determined as figure 1 by lemma 6, the ‘only if’ part is obvious: when the realization is self-testable, it is a two-qubit realization of equation (5), where any one of \( \bar{E}_x \) and \( \bar{E}_y \) can be regarded as \( \tilde{G} \) because \( F_x \) and \( E_y \) are local and unitary \( (F_x^2 = E_y^2 = I) \). Let us prove the ‘if’ part. We again use the notation of equation (16). For the operator \( Z_y \) defined by

\[
Z_y = \sin \frac{\theta_y^B}{\Delta \theta^B} B_y - \sin \theta_y^B B_y,
\]

we have \( \langle \psi | Z_y^2 | \psi \rangle = 1 \) as \( \tilde{B}_0 \cdot \tilde{B}_1 = \cos \Delta \theta^B \), and similarly for \( Z_A \). As the unit vectors \( Z_{0y} | \psi \rangle \) and \( Z_{1y} | \psi \rangle \) are both directed along \( \tilde{G} \), we have \( Z_{0y} | \psi \rangle = \frac{1}{\cos \theta_y^B} | \psi \rangle = Z_{1y} | \psi \rangle \). Suppose now that \( \tilde{G} \) lies in the $B$-plane with \( G \) being Bob’s unitary observable \( (G^2 = I) \). Letting the angle between \( \tilde{G} \) and \( \tilde{G} \) be \( \eta \), it is written as

\[
G | \psi \rangle = \frac{\sin \eta \theta_y^B | \psi \rangle - \sin (\eta \theta^B - \theta_y^B) Z_{0y} | \psi \rangle}{\sin \theta_y^B},
\]

for \( y = 0, 1 \). Moreover, as \( G \) commutes with \( Z_A \) and \( G^2 = I \), we have \( \langle \psi | GZ_A Z_A G | \psi \rangle = \langle \psi | Z_{1y}^2 | \psi \rangle = 1 \) and

\[
\sin^2 \theta_y^B = \sin^2 \eta \theta^B + \sin^2 (\eta \theta^B - \theta_y^B) \langle \psi | Z_{0y}^2 | \psi \rangle
- 2 \sin \eta \theta^B \sin (\eta \theta^B - \theta_y^B) \langle \psi | Z_{1y} Z_{0y} | \psi \rangle.
\]

From this and equation (19), we have \( \langle \psi | Z_{1y}^2 | \psi \rangle = 1 \); hence \( Z_{1y} | \psi \rangle \) is a unit vector. As \( \langle \psi | Z_{0y}^2 | \psi \rangle = 1 \), we have \( Z_{0y} | \psi \rangle = | \psi \rangle \), which proves the anti-commutation relation of

\[
(\bar{B}_y B_y + B_y \bar{B}_y) | \psi \rangle = 2 \cos \Delta \theta^B | \psi \rangle.
\]
As $Z_B^2 |\psi\rangle = Z_B^2 |\psi\rangle = |\psi\rangle$, the anti-commutation relation between $A_0$ and $A_1$ is also proven. Let us define $X_B$ by

$$X_B = \frac{\cos \theta_B^B B_1 - \cos \theta_B^B B_0}{\sin \Delta \theta^B}$$

(23)

and similarly $X_A$. With the anti-commutation relations of $B_A$ and $A_A$, we can confirm

$$(X_B)^2 |\psi\rangle = (X_A)^2 |\psi\rangle = |\psi\rangle$$

and

$$(X_B Z_B + Z_B X_B) |\psi\rangle = (X_A Z_A + Z_A X_A) |\psi\rangle = 0.$$  However, $|\psi\rangle$ has not been determined yet. From equation (D4), we have

$$\langle \psi | Z_A X_A X_B Z_B |\psi\rangle = -\langle \psi | X_A X_B Z_A Z_B |\psi\rangle = -\sin 2 \chi,$$

$$\langle \psi | X_A X_B Z_A |\psi\rangle = \langle \psi | X_B X_A Z_B |\psi\rangle = \cos 2 \chi.$$  (24)

This implies that the four state vectors (not in the real-vector representation) of $X_A Z_A |\psi\rangle$, $X_A |\psi\rangle$, $X_B |\psi\rangle$, and $X_B Z_B |\psi\rangle$ lie in the same plane in a complex vector space, as shown in figure 2. Moreover, this figure shows that $(X_A X_B |\psi\rangle = 0$; hence $Z_A |\psi\rangle$ and $X_A X_B |\psi\rangle$ are orthogonal to each other. As the components of $|\psi\rangle$ to these orthogonal vectors are given by $\langle Z_A |\psi\rangle = \cos 2 \chi$ and $\langle X_B |\psi\rangle = \sin 2 \chi$, we can conclude

$$|\psi\rangle = \sin 2 \chi X_A X_B |\psi\rangle + \cos 2 \chi Z_A |\psi\rangle.$$  (25)

By operating $X_A X_B$ on both sides, we have

$$\sin 2 \chi X_A X_B Z_A |\psi\rangle = \frac{\sin 2 \chi X_A X_B |\psi\rangle - \sin^2 2 \chi |\psi\rangle}{\cos 2 \chi} = \cos 2 \chi |\psi\rangle - Z_A |\psi\rangle,$$

(26)

and $\cos \chi X_A X_B (I - Z_A) |\psi\rangle = \sin \chi (I + Z_A) |\psi\rangle$. Then, the local unitary transformation $\Phi \equiv \Phi_A \otimes \Phi_B$ commonly used for self-testing [3] shown in figure 3 results in

$$\Psi |\psi\rangle |00\rangle = \frac{1}{4} \{ (I + Z_A)(I + Z_B) |\psi\rangle |00\rangle + X_B (I + Z_A)(I - Z_B) |\psi\rangle |01\rangle + X_A (I - Z_A)(I + Z_B) |\psi\rangle |10\rangle + X_A X_B (I - Z_A)(I - Z_B) |\psi\rangle |11\rangle \}$$

$$= \frac{(I + Z_A) |\psi\rangle}{2 \cos \chi} (\cos \chi |00\rangle + \sin \chi |11\rangle),$$  (27)

Figure 2. Four state vectors lie in the same plane, and $X_0 |\psi\rangle$ and $X_A Z_A |\psi\rangle$ are orthogonal, which also implies that $Z_0 |\psi\rangle$ and $X_A X_0 |\psi\rangle$ are orthogonal because $\langle X_0 Z_0 |\psi\rangle = 0$.
and consequently $|\psi\rangle$ is locally equivalent to $\cos \chi |00\rangle + \sin \chi |11\rangle$. Similarly, we also have

$$\Phi X_A X_B |\psi\rangle \langle 00\rangle = |\text{junk}\rangle (\cos \chi |11\rangle + \sin \chi |00\rangle),$$

and so on, and measurements are self-tested.

For self-testability, the proof of the anti-commutation relation between $B_0$ and $B_1$ (equation (22)) is crucial.

To prove it, lemma 7 implies that the third unitary observable $G$, whose real vector lies in the same $B$-plane, is necessary. In the unbiased case where $\chi = \pi/4$, the four vectors $\vec{A}_0, \vec{A}_1, \vec{B}_0, \vec{B}_1$ all lie in the same plane, and $A_x$ can be used as the third unitary observable [19]. However, in the other general case of $0 < \chi < \pi/4$, $\vec{A}_x$ and $\vec{A}_1$ lie in a different $A$-plane, and $A_x$ cannot be used anymore. It is not limited, but the optimal operator $F_x$ for $D_x$ is a good candidate for $G$. Interestingly, in the special case that $\vec{F}_0 = \vec{B}_0$ and $\vec{F}_1 = \vec{B}_1$, the candidate for $G$ is missing in the $B$-plane, but the correlation in this case is always local.

5. Scheme for self-testing partially entangled state

As shown in section 3, under the conjectured certifiability of $D^B_x$ and $D^A_x$, the realizations are automatically self-testable by lemma 5; however, Conjecture 2 has not been proven. Fortunately, however, lemma 7 tells us how to self-test such realizations irrespective of the validity of the conjecture; it suffices to intentionally introduce a unitary observable by adding one more binary measurement.

The simplest protocol may be to add the measurement of $Z_B$. Let us add a binary measurement to the Bell scenario, such as the Bell (2, 3, 2)-scenario but on Bob’s side only, whose observable is $B_2$ ($B_2^2 = 1$). Suppose that the correlators by the original set $\{A_0, A_1, B_0, B_1\}$ satisfy the condition in lemma 6, and the geometry of real vectors is determined as figure 1, where $\sin 2\chi$ is also determined. When the additional correlators satisfy

$$\langle A_x B_2 \rangle = \cos \theta_2^A = \langle A_x \rangle / \cos 2\chi, \quad \langle B_2 \rangle = \cos 2\chi,$$

for both $x = 0, 1$, $\vec{B}_2$ is ensured to lie in the $A$-plane and is directed along $\vec{v}'$. Then, in this protocol, $B_2 |\psi\rangle = Z_0 |\psi\rangle = Z_4 |\psi\rangle$ can be directly used for proving the anti-commutation relation of $B_2$ ($A_x$ also) as in the proof of lemma 7.

The additional measurement is not restricted to $Z_B$. In the second protocol, suppose that the correlators by $\{A_0, A_1, B_0, B_1\}$ also satisfy the condition in lemma 6, in addition to the original $\{A_0, A_4, B_0, B_1\}$. Then, as $\vec{v}'$, $\vec{B}_0, \vec{B}_1$ lie in the same plane, $\vec{B}_2$ is ensured to lie in the $B$-plane, and again, $B_2$ can be used as the third observable for proving the anti-commutation relation between $B_0$ and $B_1$; the proof of lemma 7 runs similarly, and the realization is self-tested.

Note that $B_2$ is also self-tested at the end of both protocols. Obviously, the scheme of the second protocol can be repeated to add more measurements on both sides of Alice and Bob. In this way, by using the geometry of figure 1 as a building block, the two-qubit realizations in the form of equation (5) with arbitrary number of measurements (whose basis lies in the $X$-$Z$ plane) can be self-tested.

6. Summary

In this paper, we studied the self-testability and extremality from the viewpoint of the geometry of the state vectors of the realizations for quantum correlations, and showed a condition that determines the geometry
uniquely. Interestingly, in the case of the realizations using partially entangled states, the condition for the unique determination of the geometry is strictly looser than that for the self-testability.

We first showed that the saturation of the TLM inequality for scaled correlators, together with the existence of a two-qubit realization in the form of equation (5), uniquely determines the geometry of state vectors in both cases of the D-space and the C-space (lemma 4 and 6). The uniqueness of the geometry generally ensures the extremality of $Q_D$, because it is a unique simultaneous maximizer of two quantum Bell inequalities in the D-space. In the case of the C-space, however, such quantum Bell inequalities are lacking, and the uniqueness of the geometry is insufficient for the extremality of $Q_C$. Indeed, there exists a two-qubit realization such that, despite being an extremal point of $Q_D$, it is not an extremal point of $Q_C$ due to the convexity of guessing probabilities. This suggests that the structure of $Q_D$ is simpler than $Q_C$. The complete characterization of the extremal points of $Q_D$ is an intriguing open problem.

We next showed that, when the conjectured certifiability of the guessing probabilities holds true, the self-testability in the C-space (hence the extremality of $Q_C$) comes to be ensured by the extremality of $Q_D$ (lemma 5). Namely, the sufficiency of the extremality criterion conjectured in [23] was shown to rely on the certifiability of guessing probabilities. The proof of the certifiability (i.e. the proof of the device-independent upper bound of guessing probabilities) seems quite challenging but attractive, because it would also lead to the discovery of the information principles [2, 39] behind quantum mechanics, and 'almost quantumness' [40] as well.

Moreover, the realization with a unique geometry becomes self-testable if and only if another unitary observable exists on the geometry (lemma 7). Applying this proven fact, we proposed self-testing protocols for partially entangled two-qubit states, where one more measurement is intentionally added to prove the anti-commutation relation between observables. This geometrical scheme provides a building block used for a more complicated geometry. Indeed, repeatedly adding measurements by this scheme, a realization with an arbitrary number of measurements can be self-tested. It is an open problem of how robust this scheme is.

As all the known nonlocal extremal points in the simplest Bell scenario are self-testable, it is natural to expect that the true extremal criterion must be the one that determines the geometry of state vectors as well as the TLM criterion. The conjectured criterion in [23] fulfills this expectation. Interestingly, although the validity of the conjecture has not been proven, the property of determining the geometry proves the self-testability of the realizations in the Bell scenario with more measurement settings as in the above self-testing protocols.

Acknowledgments

This work was supported by JSPS KAKENHI Grant No. 17K05579.

Appendix A. Convexity of $D^B_x$

Let $\rho_{|k|}$ be Bob’s subnormalized conditional state. For any convex decomposition $\rho_{|k|} = \sum_i \lambda_i \rho^{(i)}_{|k|}$, we have

$$D^B_x = \max_{x_a} \text{tr}(\rho_{|1|} - \rho_{-1|}) X_B$$

$$= \max_{x_a} \sum_{i} \lambda_i \text{tr}(\rho^{(i)}_{|1|} - \rho^{(i)}_{-1|}) X_B$$

$$= \max_{x_a} \sum_{i} \lambda_i \text{tr}[(\rho^{(i)}_{|1|} - \rho^{(i)}_{-1|}) \otimes (i) (i)](X_B \otimes I_y)$$

$$\leq \max_{x_a} \sum_{i} \lambda_i \text{tr}[(\rho^{(i)}_{|1|} - \rho^{(i)}_{-1|}) \otimes (i)](X_{B_a})$$

$$= \left[ \sum_{i} \lambda_i \left( \max_{x_a} \text{tr}(\rho^{(i)}_{|1|} - \rho^{(i)}_{-1|}) X_B^{(i)}) \right)^2 \right]^{1/2},$$

where $a$ denotes the ancilla. At the last equality, we used the formula $(D^B_x)^2 = \sum_{kk'} |a_{kk'}|^2 / (m_k + m_{k'})$, where $a_{kk'} = \langle k| (\rho_{|1|} - \rho_{-1|}) |k'\rangle$ are the matrix elements with respect to the eigenstates of $\rho_{|1|} + \rho_{-1|}$ with $m_k$ and $m_{k'}$ being the eigenvalues, as shown in appendix A of [32]. See also [33].

Appendix B. Uniqueness of geometry I

First, we explicitly show how to construct a pair of the quantum Bell inequalities (8) and (9) that is simultaneously saturated by a given geometry of figure 1 (i.e. a given set of the geometrical parameters $\{\theta_x^A, \theta_x^B, \chi\}$). The saturation condition for the first inequality in inequality (11) is that, for $X_e \equiv \sum_{y} u_y^B (-1)^y B_y$, 
\[ X_\kappa \propto F_\kappa = \frac{(\sin \Delta_0^\kappa B_0 - \sin \Delta_1^\kappa B_1)}{\sin \Delta^\kappa}, \]
\[ (s_0^\kappa D_0^\kappa)^2(X_0^\kappa) = (s_1^\kappa D_1^\kappa)^2(X_0^\kappa), \] (B1)

and the coefficients of the quantum Bell inequalities must satisfy
\[ u_{00}^\kappa \sin \Delta_{00}^\kappa = -u_{01}^\kappa \sin \Delta_{01}^\kappa, \quad u_{10}^\kappa \sin \Delta_{10}^\kappa = u_{11}^\kappa \sin \Delta_{11}^\kappa, \]
\[ (s_0^\kappa D_0^\kappa)^2 \sin \Delta_{01}^\kappa \sin \Delta_{10}^\kappa = (s_1^\kappa D_1^\kappa)^2 \sin \Delta_{11}^\kappa \sin \Delta_{01}^\kappa, \]
\[ (s_0^\kappa D_0^\kappa)^2 + (s_1^\kappa D_1^\kappa)^2 = \frac{1}{4(q')^2}, \] (B2)

where the last equation is the saturation condition for the second inequality of inequality (11). It is then sufficient to choose for both \( \epsilon = A, B \) as follows:
\[ u_{00}^\epsilon = a \sin \Delta_{00}^\epsilon, \quad u_{01}^\epsilon = -a \sin \Delta_{01}^\epsilon, \]
\[ u_{10}^\epsilon = b \sin \Delta_{10}^\epsilon, \quad u_{11}^\epsilon = b \sin \Delta_{11}^\epsilon, \]
\[ s_0^\epsilon = D_0^\epsilon a, \quad s_1^\epsilon = D_0^\epsilon b, \quad 1/f' = 2\sqrt{(s_0^\epsilon D_0^\epsilon)^2 + (s_1^\epsilon D_1^\epsilon)^2}, \]
\[ a = \frac{1}{\sin \Delta_{10}^\epsilon} \sqrt{\frac{\sin \Delta_{11}^\epsilon \sin \Delta_{00}^\epsilon - \sin \Delta_{01}^\epsilon \sin \Delta_{00}^\epsilon}{\sin \Delta_{11}^\epsilon \sin \Delta_{10}^\epsilon - \sin \Delta_{01}^\epsilon \sin \Delta_{10}^\epsilon}}, \]
\[ b = \frac{1}{\sin \Delta_{10}^\epsilon} \sqrt{\frac{\sin \Delta_{11}^\epsilon \sin \Delta_{00}^\epsilon - \sin \Delta_{01}^\epsilon \sin \Delta_{00}^\epsilon}{\sin \Delta_{11}^\epsilon \sin \Delta_{10}^\epsilon - \sin \Delta_{01}^\epsilon \sin \Delta_{10}^\epsilon}}. \] (B3)

Next, let us show conversely that, for a given set of such coefficients of quantum Bell inequalities, the geometrical parameters satisfying equation (B2) are unique (up to obvious symmetries). Let \( \alpha^\epsilon \equiv u_{00}^\epsilon / u_{01}^\epsilon \) and \( \beta^\epsilon \equiv u_{10}^\epsilon / u_{11}^\epsilon \). Once we choose \( \Delta^\epsilon \), \( \tan \Delta_{00}^\epsilon \) is determined from equation (B2) as
\[ \tan \Delta_{00}^\epsilon = \frac{-\alpha^\epsilon \sin \Delta^\epsilon}{1 + \alpha^\epsilon \cos \Delta^\epsilon}, \quad \tan \Delta_{01}^\epsilon = \frac{\sin \Delta^\epsilon}{\cos \Delta^\epsilon + \alpha^\epsilon}, \]
\[ \tan \Delta_{10}^\epsilon = \frac{1/f'}{1 - \frac{1}{f'} \cos \Delta^\epsilon}, \quad \tan \Delta_{11}^\epsilon = \frac{\sin \Delta^\epsilon}{\cos \Delta^\epsilon - \frac{1}{f'}}, \]
and as a result, \( D_0^\epsilon \) and \( D_1^\epsilon \) is also determined by \( \Delta^\epsilon \) as
\[ (D_0^\epsilon)^2 = \frac{1}{4(s_0^\epsilon q')^2} \left( \alpha^\epsilon + \frac{1}{\alpha^\epsilon} + 2 \cos \Delta^\epsilon \right), \]
\[ (D_1^\epsilon)^2 = \frac{1}{4(s_1^\epsilon q')^2} \left( \beta^\epsilon + \frac{1}{\beta^\epsilon} + 2 \cos \Delta^\epsilon \right). \] (B4)

For these solutions to represent the same realization, \( (A_0^\epsilon B_0^\epsilon)^2 = (D_0^\epsilon \cos \Delta_0^\epsilon)^2 = (D_1^\epsilon \cos \Delta_1^\epsilon)^2 \) must hold for every \( \epsilon \) and \( \gamma \); hence equation (18) must hold, where the original geometrical parameters appears in equation (B2) are indicated by an overline. When equation (18) only has a trivial solution of \( \cos \Delta^\epsilon = \cos \Delta^\epsilon \), we observe \( D_0^\epsilon = D_0^\epsilon \) and \( D_1^\epsilon = D_1^\epsilon \) from equation (B4). Moreover, from \( D_0^\epsilon D_0^\epsilon \sin \Delta^\epsilon = \sin 2\chi \sin \Delta^\epsilon \) and \( 0 \leq \chi \leq \pi/4 \), we have \( \chi = \chi \) as \( \tan \Delta^\epsilon = \tan(\Delta_{00}^\epsilon - \Delta_{10}^\epsilon) = \pm \tan \Delta^\epsilon \). From \( (D_0^\epsilon)^2 = \cos^2 2\chi \cos^2 \Delta^\epsilon + \sin^2 2\chi \), we have \( \cos^2 \Delta^\epsilon = \cos^2 \Delta^\epsilon \), and similarly \( \cos^2 \Delta^\epsilon = \cos^2 \Delta^\epsilon \). Considering the possible combination of signs carefully, it is found that the allowed solutions of equation (B2) are only \( \{ \delta^A, \delta_B, \chi \}, \{ -\delta^A, -\delta_B, \chi \}, \{ \pi - \delta^A, \pi - \delta_B, \chi \} \), and \( \{ \pi + \delta^A, \pi + \delta_B, \chi \} \).

**Appendix C. Example of strict convexity**

Let us consider the two nonlocal correlations \( \mathbf{P} \) and \( \mathbf{Q} \) realized by equation (5) using the following parameters:
\[ \mathbf{P}: \theta_0^A = 0, \theta_0^B = \epsilon, \theta_1^A = \pi/2, \theta_1^B = -\pi/4, \quad 2\chi = \pi/6, \]
\[ \mathbf{Q}: \theta_0^A = 0, \theta_0^B = \epsilon, \theta_1^A = \pi/2, \theta_1^B = -\pi/4, \quad 2\chi = \pi/4, \]
where \( \epsilon \) is a small angle \( (0 < \epsilon < \pi/40) \) to ensure that equation (18) only has a trivial solution. As \( \mathbf{P} \) and \( \mathbf{Q} \) saturate equation (1) for scaled correlators, they are the extremal points of \( \mathbf{Q}_D \). Let us then consider \( \mathbf{L} \), extrapolated from \( \mathbf{P} \) and \( \mathbf{Q} \) as...
where $\lambda$ is chosen such that $C_{00} + C_{01} + C_{10} - C_{11} = 2$ at $L$. Suppose that $\{C_A^A, C_B^B, C_{xy}^p\}$ is extrapolated by equation (C1). Because the behavior of $P$ in the $C$-space satisfies the positivity constraint $p(ab|xy) \geq 0$, $L$ is a local correlator. This implies that $P$ can also be realized by a convex sum of $Q$ and deterministic correlations, despite that $P$ is an extremal point of $Q_{D2}$. On the other hand, when $\{\delta_A^B, \delta_B^A, C_{xy}^q\}$ is extrapolated by equation (C1), $L$ is not allowed in quantum mechanics as shown in figure 4. This implies that $(D_B^p)^2$ and $(D_A^A)^2$ must be strictly convex for equation (C1). Although it is unknown that this convex-sum realization certainly realizes $\{\delta_A^B, \delta_B^A, C_{xy}^q\}$ of $P$, even an extremal point of $Q_{D2}$ may be realized as a convex sum due to the convexity of $D_B^p$ and $D_A^A$. Interestingly, as $\{C_A^A, C_B^B, C_{xy}^p\}$ of $P$ in the $C$-space is realized by equation (C1), $P$ is not an extremal point of $Q_{C1}$, despite being an extremal point of $Q_{D2}$.

Appendix D. Uniqueness of geometry II

As a nonlocal behavior is considered, the measurement operators in the realization satisfy $A_\theta \approx \pm A_\chi$ and $B_\phi \approx \pm B_\phi$ [41]. In the case of $\sin^2 2\chi = \delta_{xy}^B = 1$, the geometry of real vectors is uniquely determined by the TLM criterion as shown in [19]. In the other cases, $\sin^2 2\chi = s_{xy}^B$ is a solution of

$$\left(\langle A_x B_y \rangle - \frac{\langle A_x \rangle \langle B_y \rangle}{\cos^2 2\chi}\right)^2 = \sin^2 2\chi \left(1 - \frac{\langle A_x \rangle^2}{\cos^2 2\chi}\right) \left(1 - \frac{\langle B_y \rangle^2}{\cos^2 2\chi}\right),$$

and $\langle A_x B_y \rangle$ is equal to either one of

$$\frac{\langle A_x \rangle \langle B_y \rangle}{\cos^2 2\chi} \pm \sin 2\chi \sqrt{1 - \frac{\langle A_x \rangle^2}{\cos^2 2\chi}} \sqrt{1 - \frac{\langle B_y \rangle^2}{\cos^2 2\chi}}.$$  \hspace{1cm} (D1)

Let us introduce $\theta_A^x$ and $\theta_B^y$ by

$$\langle A_x \rangle = \cos 2\chi \cos \theta_A^x, \quad \langle B_y \rangle = \cos 2\chi \cos \theta_B^y.$$  \hspace{1cm} (D2)

Under this parameterization,

$$d_B^p = \cos^2 2\chi \cos^2 \theta_A^x + \sin^2 2\chi.$$  \hspace{1cm} (D3)

As $H \geq 0$, the double sign of the second term in inequality (D1) can be negative for even pairs among the four possible $(x,y)$, and hence, by adjusting the sign of $\sin \theta_A^x$ and $\sin \theta_B^y$, $\langle A_x B_y \rangle$ is always written as

$$\langle A_x B_y \rangle = \cos \theta_A^x \cos \theta_B^y + \sin \theta_A^x \sin \theta_B^y \sin 2\chi.$$  \hspace{1cm} (D4)

Let us then consider the real-vector representation. Because the scaled correlators saturate equation (1), there exists real unit vectors $\vec{A}_x$ and $\vec{A}_y$ such that

$$\vec{A}_x \cdot \vec{B}_y = \sqrt{d_B^p} \vec{A}_x \cdot \vec{A}_y, \quad \vec{A}_x \cdot \vec{B}_y = \sqrt{d_B^p} \vec{E}_x \cdot \vec{A}_x,$$

and $\vec{A}_x$ and $\vec{B}_y$ (or $\vec{E}_y$) are ensured to lie in the same $B$-plane ($A$-plane) [19]. However, the relationship between the two planes has not been determined yet.
Clearly, $\sqrt{d_B^2}$ is the length of the projection of $\vec{A}_x$ to the $B$-plane, and from the laws of sines and cosines,

$$d_B^2 = \frac{(\vec{A}_x \cdot \vec{B}_0)^2 + (\vec{A}_x \cdot \vec{B}_1)^2 - 2(\vec{A}_x \cdot \vec{B}_0)(\vec{A}_x \cdot \vec{B}_1) \cos \Delta}{\sin^2 \Delta}, \quad (D6)$$

must hold, where $\Delta$ is the angle between $\vec{B}_0$ and $\vec{B}_1$ (not yet determined). From equations (D3) and (D4), we can introduce $\phi_x^B$ to express $\vec{A}_x \cdot \vec{B}_0$ as $\sqrt{d_B^2} \cos (\phi_x^B - \theta_0^B)$, and we have from equation (D6)

$$[\cos \Delta - \cos \Delta \theta_B] \{\cos \Delta - \cos (2\phi_x^B - \theta_0^B - \theta_0^B)\} = 0. \quad (D7)$$

As this must hold for both $x = 0, 1$, the solution of $\cos \Delta = \cos (2\phi_x^B - \theta_0^B - \theta_0^B)$ is inappropriate unless the two-planes are perpendicular (and the correlation is local). We then have $\vec{B}_0 \cdot \vec{B}_1 = \cos \Delta = \cos \Delta \theta_B$. Let the projector of $\psi$ to the $B$-plane be $\vec{B}_B$. As $\psi \cdot \vec{B}_B = \langle \vec{B}_B \rangle$,

$$|\psi_B|^2 = \frac{\langle \vec{B}_0 \rangle^2 + \langle \vec{B}_1 \rangle^2 - 2\langle \vec{B}_0 \rangle \langle \vec{B}_1 \rangle \cos \Delta \theta_B}{\sin^2 \Delta \theta_B} = \cos^2 2\chi, \quad (D8)$$

and hence we know from equation (D2) that the angle between $\vec{B}_B$ and $\vec{B}_1$ is $\theta_0^B$. As $\vec{B}_B$ lies in the $B$-plane, 

$$\vec{B}_B = \cos 2\chi \frac{\sin \theta_0^B \vec{B}_1 - \sin \theta_0^B \vec{B}_0}{\sin \Delta \theta_B}, \quad (D9)$$

and from equation (D4) we have $\vec{A}_x \cdot \vec{B}_B = \cos 2\chi \cos \theta_x^A$, which implies that the angle between $\vec{A}_x$ and $\vec{B}_B$ is $\theta_x^A$. From the same argument as above, we have $\vec{A}_0 \cdot \vec{A}_1 = \cos \Delta \theta_A$, which implies that $\vec{A}_0$, $\vec{A}_1$, and $\vec{B}_B$ lie in the same plane. Similarly, we know that $\vec{B}_0$, $\vec{B}_1$, and $\vec{B}_B$ lie in the same plane. After all, the geometry of real vectors is determined as figure 1 with $|\psi'| = \cos 2\chi$. The obvious symmetry is $\{\theta_x^A, \theta_0^B, \chi\}$ and $\{-\theta_x^A, -\theta_0^B, -\chi\}$, which arises from the ambiguity in adjusting the sign of $\theta_x^A$ and $\sin \theta_0^B$.

In this way, without any assumption, the geometry is determined; hence it is unique. In the special case where $S_{00} = S_{01} = S_{10} = S_{11}$ and $S_{00} = S_{01} = S_{10} = S_{11}$, there seem to exist two possible choices for $2 \chi$. However, as this contradicts the uniqueness of the geometry, some condition is not satisfied for either choice. For example, the correlation of the Tsirelson bound, where $C_A^x = C_B^y = 0$ and $C_{xy} = (-1)^{xy}/\sqrt{2}$, we also have $S_{00} = S_{01} = S_{10} = S_{11} = 1/2$, but $H < 0$ for this choice.

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