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PAPER

Geometrical self-testing of partially entangled two-qubit states

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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 $a=\pm 1$ ($b=\pm 1$). 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 $p(ab|xy)=\frac{1}{4}[1+aC_x^A+bC_y^B+abC_{xy}]$ for no-signaling correlations, with C_x^A (C_y^B) being a bias of the marginal $p(a|x)$ [$p(b|y)$], any no-signaling correlation can be described by a behavior $\{C_x^A, C_y^B, C_{xy}\}$. Such a behavior specifies a point in the 8-dimensional no-signaling space, which we denote by the C-space.

A behavior $\{C_x^A, C_y^B, C_{xy}\}$ 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 $A_x^2=B_y^2=I$, $C_x^A=\langle\psi|A_x|\psi\rangle$, $C_y^B=\langle\psi|B_y|\psi\rangle$, and $C_{xy}=\langle\psi|A_xB_y|\psi\rangle$. 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 $c_i\in\mathbb{C}$, $\vec{\psi}=(\mathrm{Re}\, c_0, \mathrm{Im}\, c_0, \mathrm{Re}\, c_1, \mathrm{Im}\, c_1, \cdots)$ 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 $C_x^A=C_y^B=0$, a behavior belongs to $\mathcal{Q}_C$, if and only if the TLM inequality [20–22]

$$|\tilde{C}_{00}\tilde{C}_{01}-\tilde{C}_{10}\tilde{C}_{11}|\leqslant\sqrt{(1-\tilde{C}_{00}^2)(1-\tilde{C}_{01}^2)}+\sqrt{(1-\tilde{C}_{10}^2)(1-\tilde{C}_{11}^2)}, \tag{1}$$

is satisfied for $\tilde{C}_{xy}=C_{xy}$ [together with $p(ab|xy)\geqslant 0$].

Using the correlators of a behavior $\{C_x^A, C_y^B, C_{xy}\}$, let us introduce the quantities $S_{xy}^{\pm}$ given by

$$\begin{aligned} S_{xy}^{\pm} &\equiv \frac{1}{2}[J_{xy}\pm\sqrt{J_{xy}^2-4K_{xy}^2}], \\ J_{xy} &\equiv C_{xy}^2-(C_x^A)^2-(C_y^B)^2+1, \\ K_{xy} &\equiv C_{xy}-C_x^AC_y^B. \end{aligned} \tag{2}$$

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

$$\begin{aligned} S_{00}^{p_{00}}=S_{01}^{p_{01}}=S_{10}^{p_{10}}=S_{11}^{p_{11}}, \\ H\equiv\textstyle\prod_{xy}[(1-S_{xy}^{p_{xy}})C_{xy}-C_x^AC_y^B]\geqslant 0, \end{aligned} \tag{3}$$

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

$$d_x^B \equiv (C_x^A)^2 + \sin^2 2\chi, \quad d_y^A \equiv (C_y^B)^2 + \sin^2 2\chi. \tag{4}$$

Then, to identify the nonlocal extremal points of $\mathcal{Q}_C$, the following criterion has been conjectured in [23].

Conjecture 1. A nonlocal behavior $\{C_x^A, C_y^B, C_{xy}\}$ is an extremal point of $\mathcal{Q}_C$, if and only if equation (3) holds as $S_{00}^+ = S_{01}^+ = S_{10}^+ = S_{11}^+$, and inequality (1) is saturated for both scaled correlators $\tilde{C}_{xy} = C_{xy}/\sqrt{d_x^B}$ and $\tilde{C}_{xy} = C_{xy}/\sqrt{d_y^A}$.

Note that the fulfillment of equation (3) for some $\{p_{xy}\}$ (not necessarily as $S_{00}^+ = S_{01}^+ = S_{10}^+ = S_{11}^+$) 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

$$A_x = \sin\theta_x^A \sigma_1 + \cos\theta_x^A \sigma_3, \quad B_y = \sin\theta_y^B \sigma_1 + \cos\theta_y^B \sigma_3,$$
$$|\psi\rangle = \cos\chi|00\rangle + \sin\chi|11\rangle, \tag{5}$$

where $(\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices (but there is no σ_2 term), and hence also necessary for the extremality of $\mathcal{Q}_C$ (see the supplemental material of [23]). Note further that the definition of θ_x^A and θ_y^B are changed from [32, 33, 23] for convenience ($\theta_x^A \to \pi/2 - \theta_x^A$ and $\theta_y^B \to \pi/2 - \theta_y^B$).

Moreover, for a given $\{C_x^A, C_y^B, C_{xy}\}$, the quantity D_x^B and D_y^A (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 $\{C_x^A, C_y^B, C_{xy}\}$ satisfies the same condition as Conjecture 1, d_x^B and d_y^A coincides with the device-independent upper bound of $(D_x^B)^2$ and $(D_y^A)^2$, respectively.

3. Quantum set in *D*-space

As mentioned, C_x^A 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 $\rho_{a|x}$ (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 $\rho_{a|x}$. For this purpose, we focus on the quantities introduced in [32, 33]

$$D_x^B \equiv \max_{\langle X_B^2\rangle=1} \langle A_x X_B\rangle, \quad D_y^A \equiv \max_{\langle X_A^2\rangle=1} \langle X_A B_y\rangle, \tag{6}$$

where the maximization is taken over any Hermite operator X_B (X_A) on Bob's (Alice's) side. Indeed, when $\rho_{1|x}$ and $\rho_{-1|x}$ are both pure states, the maximum in the definition of D_x^B is attained when $X_B^2 = I$ [32]; hence D_x^B becomes equal to $\mathrm{tr}|\rho_{1|x} - \rho_{-1|x}|$, coinciding with the bias of Bob's optimal guessing probability [34].

Let us then describe a correlation by a behavior $\{\delta_x^B, \delta_y^A, C_{xy}\}$, such that it is realized by quantum mechanics if and only if there exist $|\psi\rangle$, $A_x^2 = B_y^2 = I$, $\delta_x^B = (D_x^B)^2$, $\delta_y^A = (D_y^A)^2$, and $C_{xy} = \langle\psi|A_x B_y|\psi\rangle$. The reason for taking the square of D_x^B and D_y^A 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 $\{C_x^A = 0, C_y^B = 0, C_{xy} = 0\}$ in the C-space but represented in the D-space by $\{\delta_x^B = 0, \delta_y^A = 0, C_{xy} = 0\}$ and $\{\delta_x^B = 1, \delta_y^A = 1, C_{xy} = 0\}$. The former is realized by $A_x = B_y = \sigma_1$ on $|\psi\rangle = |00\rangle$, and the latter is realized by $A_x = \sigma_1$, $B_y = \sigma_3$ on $|\psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$.

Now, let us investigate the properties of the behaviors in the D-space. When the behaviors $\mathbf{p}_i$ are realized by quantum mechanics, there always exists a realization of the behavior $\mathbf{p} = \sum_i \lambda_i \mathbf{p}_i$ for any $\lambda_i \geqslant 0$ such that $\sum_i \lambda_i = 1$. This is because, as shown in appendix A, although $(D_x^B)^2$ and $(D_y^A)^2$ are convex in general such that

$$[D_x^B(\mathbf{p})]^2 \leqslant \sum_i \lambda_i [D_x^B(\mathbf{p}_i)]^2, \tag{7}$$

the equality holds, at least when each local state of the realization of $\mathbf{p}_i$ has orthogonal support, and hence,

Lemma 1. *The behaviors $\{\delta_x^B, \delta_y^A, C_{xy}\}$, which are realized by quantum mechanics, constitute a convex set.*

This set, denoted by $\mathcal{Q}_D$, is then at least enclosed by the hyperplanes in the D-space defined from the following inequalities:

$$\mathcal{B}^B \equiv -\sum_x V_x^B \delta_x^B + \sum_{xy} V_{xy}^B C_{xy} \leqslant \frac{1}{4q^B}, \tag{8}$$

$$\mathcal{B}^A \equiv -\sum_y V_y^A \delta_y^A + \sum_{xy} V_{yx}^A C_{xy} \leqslant \frac{1}{4q^A}, \tag{9}$$

where the coefficients satisfy $V_x^c \geqslant 0$, $\prod_{xy} V_{xy}^c \leqslant 0$, and $V_1^c V_{00}^c V_{01}^c = -V_0^c V_{10}^c V_{11}^c$ for both $c = A, B$. Note that V_{01}^B is the coefficient of C_{01}, but V_{01}^A is the coefficient of C_{10}. The quantum bound of the inequalities is given by

$$q^c = \frac{V_0^c}{(s_0^c)^2} = \frac{V_1^c}{(s_1^c)^2}, \quad s_0^c \equiv \sqrt{\frac{\mathcal{X}^c}{V_{10}^c V_{11}^c}}, \quad s_1^c \equiv \sqrt{\frac{-\mathcal{X}^c}{V_{01}^c V_{00}^c}},$$
$$\mathcal{X}^c \equiv V_{10}^c V_{11}^c[(V_{00}^c)^2 + (V_{01}^c)^2] - V_{00}^c V_{01}^c[(V_{10}^c)^2 + (V_{11}^c)^2]. \tag{10}$$

This is due to the cryptographic quantum bound shown in [32]. Indeed, $u_{xy}^B = (-1)^{xy} V_{xy}^B / s_x^B$ fulfills $\sum_{xy} (u_{xy}^B)^2 = 1$ and $u_{00}^B u_{01}^B = u_{10}^B u_{11}^B$; hence any realization obeys

$$\begin{aligned}\mathcal{B}^B &= -q^B \textstyle\sum_x (s_x^B D_x^B)^2 + \sum_{xy} s_x^B u_{xy}^B (-1)^{xy} \langle A_x B_y \rangle \\ &\leqslant -q^B \textstyle\sum_x (s_x^B D_x^B)^2 + \left[\sum_x (s_x^B D_x^B)^2\right]^{\frac{1}{2}} \leqslant \dfrac{1}{4q^B}.\end{aligned} \tag{11}$$

The same holds for $\mathcal{B}^A$ by using $u_{yx}^A = (-1)^{xy} V_{yx}^A / s_y^A$. 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 convex set, which is enclosed by inequalities (8) and (9). As inequality (11) holds whenever the first inequality due to the cryptographic quantum bound holds, the behaviors in this set are those satisfying the TLM inequality (1) for both scaled correlators $\tilde{C}_{xy} = C_{xy} / \sqrt{\delta_x^B}$ and $\tilde{C}_{xy} = C_{xy} / \sqrt{\delta_y^A}$ [32] (together with the obvious constraint of $C_{xy}^2 \leqslant \delta_x^B, \delta_y^A \leqslant 1$). This convex set, denoted by $\mathcal{Q}_{\text{crypt}}$, is a superset of $\mathcal{Q}_D$.

Let us now search for the extremal points of $\mathcal{Q}_D$. It is known that each extremal point of $\mathcal{Q}_C$ 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 $\mathcal{Q}_D$ due to the convexity of $(D_x^B)^2$ and $(D_y^A)^2$ as in inequality (7). Fortunately, however, we have the following:

Lemma 2. *A behavior in $\mathcal{Q}_D$, which simultaneously saturates the quantum Bell inequalities (8) and (9), has a two-qubit realization.*

Proof. As the maximization in D_x^B is rewritten by using the Lagrange multiplier l as $D_x^B = \max[\langle\psi|A_x X_B|\psi\rangle - l(\langle\psi|X_B^2|\psi\rangle - 1)]$, any realization must satisfy

$$\mathrm{tr}_A A_x |\psi\rangle\langle\psi| = \frac{D_x^B}{2} \mathrm{tr}_A (F_x |\psi\rangle\langle\psi| + |\psi\rangle\langle\psi| F_x), \tag{12}$$

where F_x is an optimal operator attaining the maximum. Let $\vec{\psi}$, $\vec{A}_x$, $\vec{B}_y$, and $\vec{F}_x$ be the real-vector representation for $|\psi\rangle$, $A_x|\psi\rangle$, $B_y|\psi\rangle$, and $F_x|\psi\rangle$, respectively, which are all unit vectors. Then, equation (12) implies

$$\vec{A}_x \cdot \vec{F}_x = D_x^B, \quad \vec{A}_x \cdot \vec{B}_y = D_x^B \vec{F}_x \cdot \vec{B}_y, \quad \vec{A}_x \cdot \vec{\psi} = D_x^B \vec{F}_x \cdot \vec{\psi}. \tag{13}$$

On the other hand, the saturation of inequality (8) implies that inequality (1) is saturated for $\tilde{C}_{xy} \equiv \vec{A}_x \cdot \vec{B}_y / D_x^B = \vec{F}_x \cdot \vec{B}_y$, which ensures that four real vectors $\vec{B}_0$, $\vec{B}_1$, $\vec{F}_0$, and $\vec{F}_1$ lie in the same B-plane [19] as shown in figure 1. Similarly, the saturation of inequality (9) implies that four real vectors $\vec{A}_0$, $\vec{A}_1$, $\vec{E}_0$, and $\vec{E}_1$ lie in the same A-plane, where $\vec{E}_y$ is the real vector optimizing D_y^A. However, as a high-dimensional vector space is considered, the relationship between the two planes has not been determined yet.

Suppose that $\vec{A}_0 \neq \pm\vec{A}_1$ and $\vec{B}_0 \neq \pm\vec{B}_1$. Let the projection of $\vec{\psi}$ to the A-plane (B-plane) be $\vec{\psi}_A$ ($\vec{\psi}_B$). Moreover, let the projection of $\vec{\psi}_B$ to the A-plane be $\vec{\psi}_{BA}$. From the laws of sines and cosines, $|\vec{\psi}_{BA}|^2$ is given by

$$\frac{(\vec{A}_0 \cdot \vec{\psi}_B)^2 + (\vec{A}_1 \cdot \vec{\psi}_B)^2 - 2(\vec{A}_0 \cdot \vec{\psi}_B)(\vec{A}_1 \cdot \vec{\psi}_B)\cos\Delta}{\sin^2\Delta}, \tag{14}$$

where Δ is the angle between $\vec{A}_0$ and $\vec{A}_1$. From equation (13),

$$\vec{A}_x \cdot \vec{\psi}_B = D_x^B \vec{F}_x \cdot \vec{\psi}_B = D_x^B \vec{F}_x \cdot \vec{\psi} = \vec{A}_x \cdot \vec{\psi} = \vec{A}_x \cdot \vec{\psi}_A, \tag{15}$$

and consequently we have $|\vec{\psi}_{BA}| = |\vec{\psi}_A|$. Similarly, we have $|\vec{\psi}_{AB}| = |\vec{\psi}_B|$. This implies that the two planes intersect with $\vec{\psi}' \equiv \vec{\psi}_A = \vec{\psi}_B$ being a common vector as shown in figure 1. The two-qubit realization of equation (5) can realize the same geometry of real vectors.

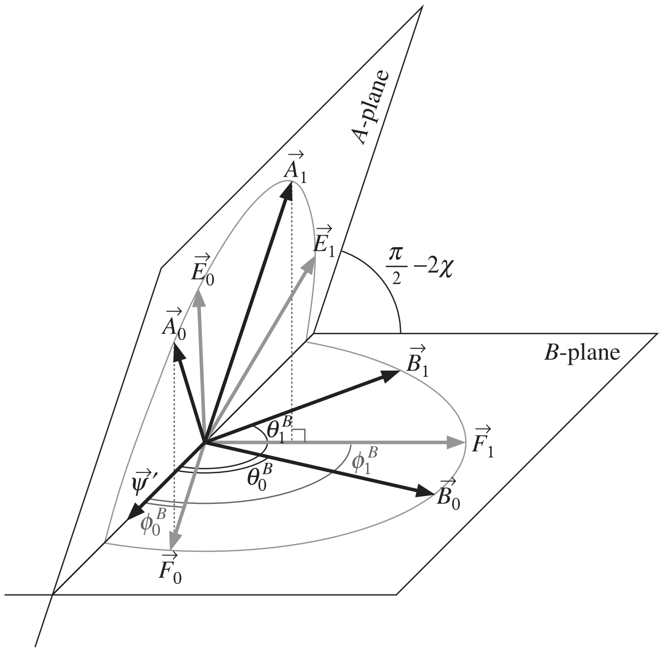

Figure 1. Geometry of real vectors, where $\vec{F}_0$, $\vec{B}_0$, $\vec{F}_1$, and $\vec{B}_1$ ($\vec{E}_0$, $\vec{A}_0$, $\vec{E}_1$, and $\vec{A}_1$) lie in the B-plane (A-plane), and $\vec{F}_x$ ($\vec{E}_y$) is directed along the projection of $\vec{A}_x$ ($\vec{B}_y$) to the B-plane (A-plane), respectively. The two planes intersect at the angle of $\pi/2 - 2\chi$, with $\vec{\psi}'$ being a common vector. The angle between $\vec{\psi}'$ and $\vec{B}_x$ ($\vec{F}_x$) is denoted by θ_x^B (ϕ_x^B), and that between $\vec{\psi}'$ and $\vec{A}_y$ ($\vec{E}_y$) is denoted by θ_y^A (ϕ_y^A). As inequality (1) is saturated by scaled correlators, inequality (17) holds in this geometry. We assume, without loss of generality, $0 \leqslant \chi \leqslant \pi/4$ throughout this paper.

When $\vec{A}_0 = \pm\vec{A}_1$, $\vec{A}_x$ and $\vec{B}_y$ lie in a 3-dimensional subspace. Moreover, the saturation of inequality (1) for scaled correlators occurs only when $\vec{A}_0$ coincides with $\pm\vec{E}_0$ or $\pm\vec{E}_1$, and $\vec{F}_0$ coincides with $\pm\vec{B}_0$ or $\pm\vec{B}_1$. The behavior in the D-space realized by such a simple geometry can be realized by equation (5). Similarly, when $\vec{B}_0 = \pm\vec{B}_1$. □

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

Lemma 3. *$\mathcal{Q}_D$ is a strict subset of $\mathcal{Q}_{\text{crypt}}$.*

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

$$\Delta_{ij}^c \equiv \phi_i^c - \theta_j^c, \quad \Delta\theta^c \equiv \theta_0^c - \theta_1^c, \quad \Delta\phi^c \equiv \phi_0^c - \phi_1^c, \tag{16}$$

for both $c = A, B$. See figure 1 for the definition of ϕ_0^c and ϕ_1^c. Note that, as inequality (1) is saturated for scaled correlators, the geometry of figure 1 satisfies [23]

$$\prod_{xy} \sin\Delta_{xy}^B \leqslant 0 \text{ and } \prod_{xy} \sin\Delta_{yx}^A \leqslant 0. \tag{17}$$

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 $\{\theta_x^A, \theta_y^B, \chi\}$, $\{-\theta_x^A, -\theta_y^B, \chi\}$, $\{\pi - \theta_x^A, \pi - \theta_y^B, \chi\}$, and $\{\pi + \theta_x^A, \pi + \theta_y^B, \bar{\chi}\}$ 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 Δ_{xy}^B and Δ_{yx}^A is determined for a given $\Delta\theta^B$ and $\Delta\theta^A$, respectively. However, $\langle A_x B_y\rangle = D_x^B \cos\Delta_{xy}^B = D_y^A \cos\Delta_{yx}^A$ 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

$$\frac{(1+\alpha^A\cos\Delta\theta^A)^2}{(1+\alpha^A\cos\Delta\bar{\theta}^A)^2}=\frac{(1+\alpha^B\cos\Delta\theta^B)^2}{(1+\alpha^B\cos\Delta\bar{\theta}^B)^2},$$
$$\frac{(\cos\Delta\theta^A+\alpha^A)^2}{(\cos\Delta\bar{\theta}^A+\alpha^A)^2}=\frac{(\cos\Delta\theta^B+\alpha^B)^2}{(\cos\Delta\bar{\theta}^B+\alpha^B)^2},$$
$$\frac{\left(1-\frac{1}{\beta^A}\cos\Delta\theta^A\right)^2}{\left(1-\frac{1}{\beta^A}\cos\Delta\bar{\theta}^A\right)^2}=\frac{\left(1-\frac{1}{\beta^B}\cos\Delta\theta^B\right)^2}{\left(1-\frac{1}{\beta^B}\cos\Delta\bar{\theta}^B\right)^2},$$
$$\frac{\left(\cos\Delta\theta^A-\frac{1}{\beta^A}\right)^2}{\left(\cos\Delta\bar{\theta}^A-\frac{1}{\beta^A}\right)^2}=\frac{\left(\cos\Delta\theta^B-\frac{1}{\beta^B}\right)^2}{\left(\cos\Delta\bar{\theta}^B-\frac{1}{\beta^B}\right)^2}, \tag{18}$$

where the parameters of the original geometry used for constructing a given pair of the Bell inequalities are indicated by an overline such as $\Delta\bar{\theta}^c$. The parameters α^c and β^c are given by $-\sin\bar{\Delta}_{00}^c/\sin\bar{\Delta}_{01}^c$ and $\sin\bar{\Delta}_{11}^c/\sin\bar{\Delta}_{10}^c$, respectively. As details are given in appendix B, when equation (18) only has a trivial solution of $\cos\Delta\theta^c=\cos\Delta\bar{\theta}^c$ 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* $\mathcal{Q}_D$.

For a given pair of quantum Bell inequalities, no pair of α^c and β^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 $\mathcal{Q}_D$, 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 $\mathcal{Q}_D$ 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_x^B and D_y^A is determined by experiments). The first is that $|\vec{\psi}'|$ in figure 1 is undetermined; $|\vec{\psi}'|$ can be determined through $\langle A_x\rangle=|\vec{\psi}'|\cos\theta_x^A$ or $\langle B_y\rangle=|\vec{\psi}'|\cos\theta_y^B$, but these are unspecified in the D-space. The second relates to the convexity of $(D_x^B)^2$ and $(D_y^A)^2$. As shown in appendix C, there exists an example in which the correlation $\mathbf{P}$, despite being an extremal point of $\mathcal{Q}_D$, 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_x^B and D_y^A.

Suppose that Conjecture 2 holds true. As inequality (1) is saturated for scaled correlators, $(D_x^B)^2$ and $(D_y^A)^2$ are also lower bounded by d_x^B and d_y^A [23]; hence those are certifiable, and we have $(D_x^B)^2=d_x^B$ and $(D_y^A)^2=d_y^A$. This correlation, denoted by $\mathbf{p}$, is then found to be an extremal point of $\mathcal{Q}_D$ by lemma 4. When a realization of $\mathbf{p}$ is decomposed into two-qubit realizations of $\mathbf{p}_i$, based on the block-diagonalization [37], $(D_x^B)^2$ and $(D_y^A)^2$ must not be strictly convex; otherwise we would construct a realization whose D_x^B or D_y^A exceeds the device-independent upper bound by using orthogonal bases. Moreover, because the correlation $\mathbf{p}$ is an extremal point of $\mathcal{Q}_D$, all $\mathbf{p}_i$ must exhibit the same behavior $\{d_x^B, d_y^A, C_{xy}\}$ 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 $\{C_x^A, C_y^B\}$ and $\{-C_x^A, -C_y^B\}$, but the latter is clearly inappropriate. In this way, the extremality of $\mathcal{Q}_D$, combined with the certifiability of D_x^B and D_y^A, makes the realization unique; hence,

Lemma 5. *If Conjecture 2 holds true, the extremal behaviors of* $\mathcal{Q}_D$ *by lemma 4 are self-testable extremal points of* $\mathcal{Q}_C$.

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 $\mathcal{Q}_C$ by lemma 5 are such that inequality (3) is satisfied as $S_{00}^+=S_{01}^+=S_{10}^+=S_{11}^+$, inequality (1) is saturated by both $\tilde{C}_{xy}=C_{xy}\Big/\sqrt{d_x^B}$ and $\tilde{C}_{xy}=C_{xy}\Big/\sqrt{d_y^A}$, and equation (18) only has a trivial solution. As mentioned above, the information of $\{C_x^A, C_y^B\}$ 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* $\{C_x^A, C_y^B, C_{xy}\}$*, which satisfies inequality (3) for some* $\{p_{xy}\}$ *(not necessarily as* $S_{00}^+ = S_{01}^+ = S_{10}^+ = S_{11}^+$*) and saturates inequality (1) for both* $\tilde{C}_{xy} = C_{xy}/\sqrt{d_x^B}$ *and* $\tilde{C}_{xy} = C_{xy}/\sqrt{d_y^A}$*, 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 $(D_x^B)^2$ and $(D_y^A)^2$, and we cannot use equation (12). For the same reason, $\vec{F}_x$ and $\vec{E}_y$ in figure 1 are now not ensured to attain D_x^B and D_y^A; $\sqrt{d_x^B}\,\vec{F}_x$ is merely the projection of $\vec{A}_x$ 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 $\mathcal{Q}_C$. This is in contrast to lemma 4, where quantum Bell inequalities are maximized by a unique geometry, and the extremality of $\mathcal{Q}_D$ 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 $|\psi'| = \cos 2\chi$ is ensured 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_x^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* $\{C_x^A, C_y^B, C_{xy}\}$*, which has a unique geometry by lemma 6, the realization is self-testable, if and only if a real vector representation* $\vec{G}$ *of* $G|\psi\rangle$*, with* G *being a local unitary observable, exists in either* A*-plane or* B*-plane (other than* $\pm\vec{A}_x$ *and* $\pm\vec{B}_y$*).*

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 $\vec{F}_x$ and $\vec{E}_y$ can be regarded as $\vec{G}$ 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_B defined by

$$Z_B = \frac{\sin\theta_0^B B_1 - \sin\theta_1^B B_0}{\sin\Delta\theta^B}, \tag{19}$$

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

$$G|\psi\rangle = \frac{\sin\eta^B B_y|\psi\rangle - \sin(\eta^B - \theta_y^B)Z_B|\psi\rangle}{\sin\theta_y^B}, \tag{20}$$

for $y = 0, 1$. Moreover, as G commutes with Z_A and $G^2 = I$, we have $\langle\psi|GZ_AZ_AG|\psi\rangle = \langle\psi|Z_A^2|\psi\rangle = 1$ and

$$\begin{aligned}\sin^2\theta_y^B = {} & \sin^2\eta^B + \sin^2(\eta^B - \theta_y^B)\langle\psi|Z_B^4|\psi\rangle \\ & - 2\sin\eta^B\sin(\eta^B - \theta_y^B)\langle\psi|Z_B^3B_y|\psi\rangle.\end{aligned} \tag{21}$$

From this and equation (19), we have $\langle\psi|Z_B^4|\psi\rangle = 1$; hence $Z_B^2|\psi\rangle$ is a unit vector. As $\langle\psi|Z_B^2|\psi\rangle = 1$, we have $Z_B^2|\psi\rangle = |\psi\rangle$, which proves the anti-commutation relation of

$$(B_0B_1 + B_1B_0)|\psi\rangle = 2\cos\Delta\theta^B|\psi\rangle. \tag{22}$$

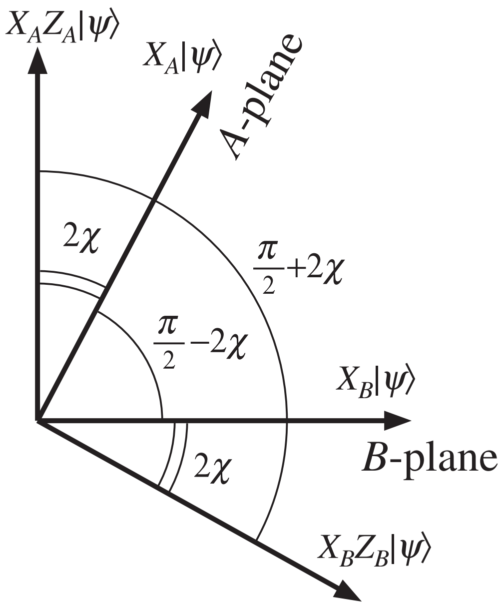

Figure 2. Four state vectors lie in the same plane, and $X_B|\psi\rangle$ and $X_A Z_A|\psi\rangle$ are orthogonal, which also implies that $Z_A|\psi\rangle$ and $X_A X_B|\psi\rangle$ are orthogonal because $\langle\psi|X_B X_A Z_A|\psi\rangle = 0$.

As $Z_A^2|\psi\rangle = Z_B^2|\psi\rangle = |\psi\rangle$, the anti-commutation relation between A_0 and A_1 is also proven. Let us define X_B by

$$X_B = \frac{\cos\theta_0^B B_1 - \cos\theta_1^B B_0}{\sin\Delta\theta^B} \tag{23}$$

and similarly X_A. With the anti-commutation relations of B_y and A_x, 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

$$\begin{aligned}\langle\psi|Z_A X_A X_B Z_B|\psi\rangle &= -\langle\psi|Z_A X_A Z_B X_B|\psi\rangle\\ &= -\langle\psi|X_A X_B|\psi\rangle = -\sin 2\chi,\\ \langle\psi|X_A X_A Z_A|\psi\rangle &= \langle\psi|X_B X_B Z_B|\psi\rangle = \cos 2\chi.\end{aligned} \tag{24}$$

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 $\langle\psi|X_B X_A Z_A|\psi\rangle = 0$; 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 $\langle\psi|Z_A|\psi\rangle = \cos 2\chi$ and $\langle\psi|X_A X_B|\psi\rangle = \sin\chi$, we can conclude

$$|\psi\rangle = \sin 2\chi X_A X_B|\psi\rangle + \cos 2\chi Z_A|\psi\rangle. \tag{25}$$

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

$$\begin{aligned}\sin 2\chi X_A X_B Z_A|\psi\rangle &= \frac{\sin 2\chi X_A X_B|\psi\rangle - \sin^2 2\chi|\psi\rangle}{\cos 2\chi}\\ &= \cos 2\chi|\psi\rangle - Z_A|\psi\rangle,\end{aligned} \tag{26}$$

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

$$\begin{aligned}\Phi|\psi\rangle|00\rangle &= \frac{1}{4}[(I + Z_A)(I + Z_B)|\psi\rangle|00\rangle\\ &\quad + X_B(I + Z_A)(I - Z_B)|\psi\rangle|01\rangle\\ &\quad + X_A(I - Z_A)(I + Z_B)|\psi\rangle|10\rangle\\ &\quad + X_A X_B(I - Z_A)(I - Z_B)|\psi\rangle|11\rangle]\\ &= \frac{(I + Z_A)|\psi\rangle}{2\cos\chi}(\cos\chi|00\rangle + \sin\chi|11\rangle),\end{aligned} \tag{27}$$

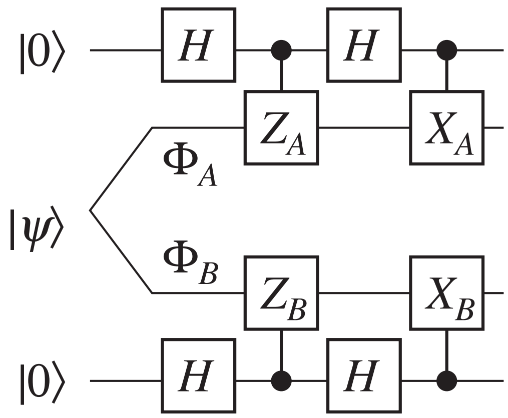

Figure 3. Local unitary transformation used for self-testing.

and consequently $|\psi\rangle$ is locally equivalent to $\cos\chi|00\rangle + \sin\chi|11\rangle$. Similarly, we also have

$$\Phi X_A X_B|\psi\rangle\,|00\rangle = |\mathrm{junk}\rangle(\cos\chi|11\rangle + \sin\chi|00\rangle), \tag{28}$$

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 $0 < \chi < \pi/4$, $\vec{A}_0$ 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^B 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_x^B and D_y^A, 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 ($B_2^2 = I$). 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

$$\langle A_x B_2\rangle = \cos\theta_x^A = \langle A_x\rangle/\cos 2\chi,\quad \langle B_2\rangle = \cos 2\chi, \tag{29}$$

for both $x = 0, 1$, $\vec{B}_2$ is ensured to lie in the A-plane and is directed along $\vec{\psi}'$. Then, in this protocol, $B_2|\psi\rangle = Z_B|\psi\rangle = Z_A|\psi\rangle$ can be directly used for proving the anti-commutation relation of B_y (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 $\{A_0,\ A_1,\ B_0,\ B_2\}$ also satisfy the condition in lemma 6, in addition to the original $\{A_0,\ A_1,\ B_0,\ B_1\}$. Then, as $\vec{\psi}'$, $\vec{B}_0$, $\vec{B}_2$ 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 $\mathcal{Q}_D$, 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 $\mathcal{Q}_C$. Indeed, there exists a two-qubit realization such that, despite being an extremal point of $\mathcal{Q}_D$, it is not an extremal point of $\mathcal{Q}_C$ due to the convexity of guessing probabilities. This suggests that the structure of $\mathcal{Q}_D$ is simpler than $\mathcal{Q}_C$. The complete characterization of the extremal points of $\mathcal{Q}_D$ 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 $\mathcal{Q}_C$) comes to be ensured by the extremality of $\mathcal{Q}_D$ (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

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Appendix A. Convexity of D_x^B

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

$$\begin{aligned} D_x^B &= \max_{X_B} \mathrm{tr}(\rho_{1|x} - \rho_{-1|x})X_B \\ &= \max_{X_B} \textstyle\sum_i \lambda_i \mathrm{tr}(\rho_{1|x}^{(i)} - \rho_{-1|x}^{(i)})X_B \\ &= \max_{X_B} \textstyle\sum_i \lambda_i \mathrm{tr}[(\rho_{1|x}^{(i)} - \rho_{-1|x}^{(i)}) \otimes (|i\rangle\langle i|)_a](X_B \otimes I_a) \\ &\leqslant \max_{X_{Ba}} \textstyle\sum_i \lambda_i \mathrm{tr}[(\rho_{1|x}^{(i)} - \rho_{-1|x}^{(i)}) \otimes (|i\rangle\langle i|)_a]X_{Ba} \\ &= \left[\textstyle\sum_i \lambda_i \left[\max_{X_B^{(i)}} \mathrm{tr}(\rho_{1|x}^{(i)} - \rho_{-1|x}^{(i)})X_B^{(i)}\right]^2\right]^{1/2}, \end{aligned} \tag{A1}$$

where a denotes the ancilla. At the last equality, we used the formula $(D_x^B)^2 = \sum_{kk'} 2|a_{kk'}|^2/(m_k + m_{k'})$, where $a_{kk'} = \langle k|(\rho_{1|x} - \rho_{-1|x})|k'\rangle$ are the matrix elements with respect to the eigenstates of $\rho_{1|x} + \rho_{-1|x}$ 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 $\{\theta_x^A, \theta_y^B, \chi\}$). The saturation condition for the first inequality in inequality (11) is that, for $X_x \equiv \sum_y u_{xy}^B (-1)^{xy} B_y$,

$$X_x \propto F_x = \frac{(\sin\Delta_{x1}^B B_0 - \sin\Delta_{x0}^B B_1)}{\sin\Delta\theta^B},$$
$$(s_0^B D_0^B)^2\langle X_1^2\rangle = (s_1^B D_1^B)^2\langle X_0^2\rangle, \tag{B1}$$

and the coefficients of the quantum Bell inequalities must satisfy

$$\begin{aligned} &u_{00}^c \sin\Delta_{00}^c = -u_{01}^c \sin\Delta_{01}^c, \quad u_{10}^c \sin\Delta_{10}^c = u_{11}^c \sin\Delta_{11}^c,\\ &(s_0^c D_0^c)^2 |\sin\Delta_{01}^c \sin\Delta_{00}^c| = (s_1^c D_1^c)^2 |\sin\Delta_{11}^c \sin\Delta_{10}^c|,\\ &(s_0^c D_0^c)^2 + (s_1^c D_1^c)^2 = \frac{1}{4(q^c)^2}, \end{aligned} \tag{B2}$$

where the last equation is the saturation condition for the second inequality of inequality (11). It is then sufficient to choose for both $c = A, B$ as follows:

$$\begin{aligned} &u_{00}^c = a\sin\Delta_{01}^c, \quad u_{01}^c = -a\sin\Delta_{00}^c,\\ &u_{10}^c = b\sin\Delta_{11}^c, \quad u_{11}^c = b\sin\Delta_{10}^c,\\ &s_0^c = D_1^c a, \quad s_1^c = D_0^c b, \quad 1/q^c = 2\sqrt{(s_0^c D_0^c)^2 + (s_1^c D_1^c)^2},\\ &a = \frac{1}{\sin\Delta\theta^c}\sqrt{\frac{\sin\Delta_{11}^c \sin\Delta_{10}^c}{\sin\Delta_{11}^c\sin\Delta_{10}^c - \sin\Delta_{01}^c\sin\Delta_{00}^c}},\\ &b = \frac{1}{\sin\Delta\theta^c}\sqrt{\frac{-\sin\Delta_{01}^c \sin\Delta_{00}^c}{\sin\Delta_{11}^c\sin\Delta_{10}^c - \sin\Delta_{01}^c\sin\Delta_{00}^c}}. \end{aligned} \tag{B3}$$

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 $\alpha^c \equiv u_{01}^c/u_{00}^c$ and $\beta^c \equiv u_{10}^c/u_{11}^c$. Once we choose $\Delta\theta^c$, $\tan\Delta_{ij}^c$ is determined from equation (B2) as

$$\tan\Delta_{00}^c = \frac{-\alpha^c\sin\Delta\theta^c}{1+\alpha^c\cos\Delta\theta^c}, \quad \tan\Delta_{01}^c = \frac{\sin\Delta\theta^c}{\cos\Delta\theta^c + \alpha^c},$$
$$\tan\Delta_{10}^c = \frac{\frac{1}{\beta^c}\sin\Delta\theta^c}{1-\frac{1}{\beta^c}\cos\Delta\theta^c}, \quad \tan\Delta_{11}^c = \frac{\sin\Delta\theta^c}{\cos\Delta\theta^c - \frac{1}{\beta^c}},$$

and as a result, D_0^c and D_1^c is also determined by $\Delta\theta^c$ as

$$(D_0^c)^2 = \frac{1}{4(s_0^c q^c)^2}\frac{\alpha^c + \frac{1}{\alpha^c} + 2\cos\Delta\theta^c}{\alpha^c + \frac{1}{\alpha^c} + \beta^c + \frac{1}{\beta^c}},$$
$$(D_1^c)^2 = \frac{1}{4(s_1^c q^c)^2}\frac{\beta^c + \frac{1}{\beta^c} - 2\cos\Delta\theta^c}{\alpha^c + \frac{1}{\alpha^c} + \beta^c + \frac{1}{\beta^c}}. \tag{B4}$$

For these solutions to represent the same realization, $\langle A_x B_y\rangle^2 = (D_x^B\cos\Delta_{xy}^B)^2 = (D_y^A\cos\Delta_{yx}^A)^2$ must hold for every x and y; 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 $\cos\Delta\theta^c = \cos\Delta\bar{\theta}^c$, we have $D_0^c = \bar{D}_0^c$ and $D_1^c = \bar{D}_1^c$ from equation (B4). Moreover, from $D_0^B D_1^B \sin\Delta\phi^B = \sin 2\chi \sin\Delta\theta^A$ and $0 \leqslant \chi \leqslant \pi/4$, we have $\chi = \bar{\chi}$ as $\tan\Delta\phi^c = \tan(\Delta_{00}^c - \Delta_{10}^c) = \pm\tan\Delta\bar{\phi}^c$. From $(D_x^B)^2 = \cos^2 2\chi\cos^2\theta_y^A + \sin^2 2\chi$, we have $\cos^2\theta_y^A = \cos^2\bar{\theta}_y^A$, and similarly $\cos^2\theta_x^B = \cos^2\bar{\theta}_x^B$. Considering the possible combination of signs carefully, it is found that the allowed solutions of equation (B2) are only $\{\bar{\theta}_x^A, \bar{\theta}_y^B, \bar{\chi}\}$, $\{-\bar{\theta}_x^A, -\bar{\theta}_y^B, \bar{\chi}\}$, $\{\pi - \bar{\theta}_x^A, \pi - \bar{\theta}_y^B, \bar{\chi}\}$, and $\{\pi + \bar{\theta}_x^A, \pi + \bar{\theta}_y^B, \bar{\chi}\}$.

Appendix C. Example of strict convexity

Let us consider the two nonlocal correlations **P** and **Q** realized by equation (5) using the following parameters:

$$\mathbf{P}\colon\ \theta_0^A = 0,\ \ \theta_1^A = \pi/2,\ \ \theta_0^B = \epsilon,\ \ \theta_1^B = -\pi/4,\ \ 2\chi = \pi/6,$$
$$\mathbf{Q}\colon\ \theta_0^A = 0,\ \ \theta_1^A = \pi/2,\ \ \theta_0^B = \epsilon,\ \ \theta_1^B = -\pi/4,\ \ 2\chi = \pi/4,$$

where ϵ is a small angle $(0 < \epsilon < \pi/40)$ to ensure that equation (18) only has a trivial solution. As **P** and **Q** saturate equation (1) for scaled correlators, they are the extremal points of $\mathcal{Q}_D$. Let us then consider **L** extrapolated from **P** and **Q** as

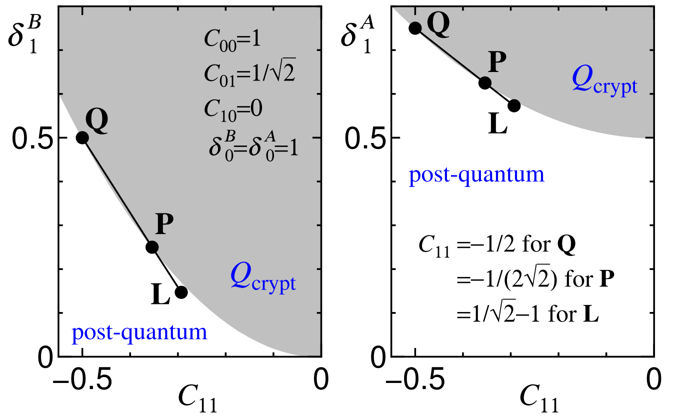

Figure 4. Two cross sections of the D-space, C_{11}-δ_1^B and C_{11}-δ_1^A, which contain **P**, **Q**, and **L**. The behaviors in the gray region belong to $\mathcal{Q}_{\rm crypt}$. When $\mathbf{P} = \lambda\mathbf{Q} + (1-\lambda)\mathbf{L}$ with $\lambda = 1 - \frac{1}{\sqrt{2}}$ (in the limit of $\epsilon \to 0$), the behavior of **L** in the D-space is not quantum realizable, whereas the behavior in the C-space is locally realizable.

$$\mathbf{P} = \lambda\mathbf{Q} + (1-\lambda)\mathbf{L}, \tag{C1}$$

where λ is chosen such that $C_{00} + C_{01} + C_{10} - C_{11} = 2$ at **L**. Suppose that $\{C_x^A, C_y^B, C_{xy}\}$ is extrapolated by equation (C1). Because the behavior of **L** in the C-space satisfies the positivity constraint $p(ab|xy) \geqslant 0$, **L** is a local correlation. 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 $\mathcal{Q}_D$. On the other hand, when $\{\delta_x^B, \delta_y^A, C_{xy}\}$ is extrapolated by equation (C1), **L** is not allowed in quantum mechanics as shown in figure 4. This implies that $(D_x^B)^2$ and $(D_y^A)^2$ must be strictly convex for equation (C1). Although it is unknown that this convex-sum realization certainly realizes $\{\delta_x^B, \delta_y^A, C_{xy}\}$ of **P**, even an extremal point of $\mathcal{Q}_D$ may be realized as a convex sum due to the convexity of D_x^B and D_y^A. Interestingly, as $\{C_x^A, C_y^B, C_{xy}\}$ of **P** in the C-space is realized by equation (C1), **P** is not an extremal point of $\mathcal{Q}_C$, despite being an extremal point of $\mathcal{Q}_D$.

Appendix D. Uniqueness of geometry II

As a nonlocal behavior is considered, the measurement operators in the realization satisfy $A_0 \neq \pm A_1$ and $B_0 \neq \pm B_1$ [41]. In the case of $\sin^2 2\chi = S_{xy}^{P_{xy}} = 1$, the geometry of real vectors is uniquely determined by the TLM criterion as shown in [19]. In the other cases, $\sin^2 2\chi = S_{xy}^{P_{xy}}$ 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

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

Let us introduce θ_x^A and θ_y^B by

$$\langle A_x\rangle = \cos 2\chi\cos\theta_x^A, \quad \langle B_y\rangle = \cos 2\chi\cos\theta_y^B. \tag{D2}$$

Under this parameterization,

$$d_x^B = \cos^2 2\chi\cos^2\theta_x^A + \sin^2 2\chi. \tag{D3}$$

As $H \geqslant 0$, 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 $\sin\theta_x^A$ and $\sin\theta_y^B$, $\langle A_x B_y\rangle$ is always written as

$$\langle A_x B_y\rangle = \cos\theta_x^A\cos\theta_y^B + \sin\theta_x^A\sin\theta_y^B\sin 2\chi. \tag{D4}$$

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

$$\vec{A}_x\cdot\vec{B}_y = \sqrt{d_x^B}\,\vec{F}_x\cdot\vec{B}_y, \quad \vec{A}_x\cdot\vec{B}_y = \sqrt{d_y^A}\,\vec{E}_x\cdot\vec{A}_x, \tag{D5}$$

and $\vec{F}_x$ and $\vec{B}_y$ ($\vec{E}_y$ and $\vec{A}_x$) 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, $\sqrt{d_x^B}$ is the length of the projection of $\vec{A}_x$ to the B-plane, and from the laws of sines and cosines,

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

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

$$[\cos\Delta - \cos\Delta\theta^B][\cos\Delta - \cos(2\phi_x^B - \theta_0^B - \theta_1^B)] = 0. \tag{D7}$$

As this must hold for both $x = 0, 1$, the solution of $\cos\Delta = \cos(2\phi_x^B - \theta_0^B - \theta_1^B)$ 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 $\vec{\psi}$ to the B-plane be $\vec{\psi}_B$. As $\vec{\psi} \cdot \vec{B}_y = \langle B_y \rangle$,

$$|\vec{\psi}_B|^2 = \frac{\langle B_0\rangle^2 + \langle B_1\rangle^2 - 2\langle B_0\rangle\langle B_1\rangle\cos\Delta\theta^B}{\sin^2\Delta\theta^B} = \cos^2 2\chi, \tag{D8}$$

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

$$\vec{\psi}_B = \cos 2\chi \frac{\sin\theta_0^B \vec{B}_1 - \sin\theta_1^B \vec{B}_0}{\sin\Delta\theta^B}, \tag{D9}$$

and from equation (D4) we have $\vec{A}_x \cdot \vec{\psi}_B = \cos 2\chi \cos\theta_x^A$, which implies that the angle between $\vec{A}_x$ and $\vec{\psi}_B$ is θ_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 $\vec{\psi}_B$ lie in the same plane. Similarly, we know that $\vec{B}_0$, $\vec{B}_1$, and $\vec{\psi}_A$ 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 $\{\theta_x^A, \theta_y^B, \chi\}$ and $\{-\theta_x^A, -\theta_y^B, \chi\}$, which arises from the ambiguity in adjusting the sign of $\sin\theta_x^A$ and $\sin\theta_y^B$.

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 $\sin^2 2\chi$. 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 $C_x^A = C_y^B = 0$ 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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