Graph-Theoretic Framework for Self-Testing in Bell Scenarios

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Quantum self-testing is the task of certifying quantum states and measurements using the output statistics solely, with minimal assumptions about the underlying quantum system. It is based on the observation that some extremal points in the set of quantum correlations can only be achieved, up to isometries, with specific states and measurements. Here, we present a new approach for quantum self-testing in Bell non-locality scenarios, motivated by the following observation: the quantum maximum of a given Bell inequality is, in general, difficult to characterize. However, it is strictly contained in an easy-to-characterize set: the theta body of a vertex-weighted induced subgraph \((G_{\text{ex}}, w)\) of the graph in which vertices represent the events and edges join mutually exclusive events. This implies that, for the cases where the quantum maximum and the maximum within the theta body (known as the Lovász theta number) of \((G_{\text{ex}}, w)\) coincide, self-testing can be demonstrated by just proving self-testability with the theta body of \(G_{\text{ex}}\). This graph-theoretic framework allows us to: (i) recover the self-testability of several quantum correlations that are known to permit self-testing (like those violating the Clauser-Horne-Shimony-Holt (CHSH) and three-party Mermin Bell inequalities for projective measurements of arbitrary rank, and chained Bell inequalities for rank-one projective measurements), (ii) prove the self-testability of quantum correlations that were not known using existing self-testing techniques (e.g., those violating the Abner Shimony Bell inequality for rank-one projective measurements). Additionally, the analysis of the chained Bell inequalities, along with prior results in Bell non-locality literature, gives us a closed form expression of the Lovász theta number for a family of well studied graphs known as the Möbius ladders, which might be of independent interest in the community of discrete mathematics.

I. INTRODUCTION

In many information processing tasks, quantum systems render a distinct advantage over classical systems. Motivated by this observation, there has been a rapid development of quantum technologies with potentially new real-world communication and computation applications. We have also recently witnessed “quantum supremacy” [AAB+19, ZWD+20] and early hints of the quantum internet [WEH18]. With the increasing importance of quantum technologies, it becomes pertinent to develop tools for certifying, verifying, and benchmarking quantum devices with minimal assumptions regarding their inner working mechanisms [EHW+19]. This is a challenging task due to the enormous dimensionality of the Hilbert space associated with the quantum systems.

One of the prominent approaches to device certification is self-testing [MY04]. The idea of self-testing is to certify underlying measurement settings and quantum states using solely measurement statistics. The notion was initially put forward for Bell non-local correlations. The concept has since been extended to prepare-and-measure scenarios [TSV+20, FK19], contextuality [BRV+19b, BRV+19a], and steering [SASA16, GKW15, SBK20]. Self-testing has also been applied to quantum gates and circuits [VDMMS07, MMM06]. A great amount of work has also been done in making self-testing protocols robust against experimental noise [MYS12, YN13, WCY+14, MS13]. While the Ref. [MY04] considered the noiseless case for the CHSH self-testing, the authors in [MYS12] extended it to the noisy case. In [HH18], the authors proposed the mixture of CHSH test and stabilizer test, which has better noise tolerance than the CHSH test. The authors in [McK11] proposed a robust self testing method for Bell states. Self-testing with Bell states of higher dimensions has been studied in [KST+19, SSKA19]. In [Kam16], tripartite...
Mermin inequality was used for robust self-testing of the three party GHZ state. Robust self-testing protocols based on Chained Bell inequalities have been investigated in Ref. [SASA16]. Comprehensive studies have been carried on for self-testing of single quantum device based on contextuality [BRV19b, BRV19a] and via computational assumptions [MV20]. The idea of self-testing has been used for device-independent randomness generation [CY14, Col09, DPA13, SASA16], entanglement detection [BSCAla, BSAlb], delegated quantum computing [RUV13, McK13], and in several computational complexity proofs, such as the recent breakthrough result of $\text{MIP}^* = \text{RE}$ [JNV20]. For a thorough review of self-testing, refer to [SB19].

Recently, graph-theoretic techniques have been widely used to study the set of quantum correlations [CSW14, Sto20]. In [CSW14], the authors provide a graph-theoretic characterization of classical and quantum sets in correlation experiments with well-studied objects in graph theory (and combinatorial optimization). In particular, the authors in [CSW14] study Bell inequalities and non-contextuality inequalities (a generalization of Bell inequalities). The techniques from [CSW14] have been used to provide robust self-testing schemes in the framework of non-contextuality inequalities for single systems [BRV19b]. However, a systematic treatment for Bell scenarios is still lacking. Here, we provide a graph-theoretic approach to study Bell self-testing for multi-partite scenarios by combining techniques from combinatorial optimization and results from [CSW14].

Given a Bell scenario, the set of quantum correlations $\mathcal{B}_Q$ is, in general, difficult to characterize. However, $\mathcal{B}_Q$ is a strict subset of an easy-to-characterize set, i.e., the theta body $\mathcal{G}_{\text{ex}}(V, E)$ of the graph of exclusivity $\mathcal{G}_{\text{ex}}(V, E)$ of all the events of the scenario. The vertices in $\mathcal{G}_{\text{ex}}(V, E)$ represent the events produced in the scenario [CSW14]. The edges in $\mathcal{G}_{\text{ex}}(V, E)$ connect the nodes corresponding to mutually exclusive events. Using the normalization conditions, every Bell non-locality witness can be written as $S = \sum w_i p_i$, where $w_i > 0$ and $p_i$ are probabilities of events. Therefore, $S$ can be associated to a vertex-weighted graph $(G, w)$ where weights correspond to the $w_i$ and $G$ is an induced subgraph of $\mathcal{G}_{\text{ex}}(V, E)$ [CSW14]. The quantum maximum of $S$ must be in the theta body of $G$, which is an even easier to characterize set, as $G$ is a subgraph of $\mathcal{G}_{\text{ex}}(V, E)$. Therefore, for the cases where the quantum maximum of a Bell non-locality witness is equal to the maximum of the theta body of $G$, one can prove the self-testing of the Bell inequality by analyzing the theta body of $G$.

We have two sets of assumptions. Our first key assumption is that the quantum maximum for the Bell witness is equal to the Lovász theta number of the vertex-weighted induced subgraph $\mathcal{G}_{\text{ex}}(V, E)$ corresponding to the events and their respective weights when the Bell witness is written as a positive linear combination of probabilities of events. The Lovász theta number $\theta(G)$ is a graph invariant defined in (2) (see section II), of the aforementioned induced subgraph. Our second set of assumptions involve some particular relation among the local projective measurements involved in the scenario. We elaborate on the second set of assumptions in subsection II.E. Our results for bipartite and tripartite cases have been stated as Theorems 7, 8, 10 and 11 (see subsection II.E). Since induced subgraph with weights is still a graph of exclusivity, we will use $\mathcal{G}_{\text{ex}}(w)$ throughout the paper in place of $(G, w)$.

We apply our techniques to quantum correlations which are known to allow for self-testing: those maximally violating the CHSH [CHSH69], chained [Pea70, BC90], and three-party Mermin [Mer90] Bell inequalities. For CHSH and tripartite Mermin Bell inequalities, we recover self-testing statements for projectors of arbitrary rank. For the family of chained Bell inequalities, we recover self-testing statement for rank-one projective measurements. Our method leads to intriguing insights concerning the dimensionality of the shared quantum state and measurement settings. We also furnish a self-testing statement for the previously not known case of the Abner Shimony (AS) inequality [Gis09] for the case of rank-one projective measurements. In addition, we provide the closed-form expression for the Lovász theta number for Möbius ladder graphs [GH67] using the aforementioned connections. The previous closed-form expression was conjectured in [Ara14]. Our result, thus, renders a proof for this conjecture.

The structure of the paper is as follows. We discuss the background literature needed for our work and prove our results in section II. The test cases are presented in section III. There, we discuss the CHSH, chained, Mermin, and AS Bell inequalities. Finally, in section IV, we discuss the implications of our work and provide some open problems for future study.

II. BACKGROUND AND RESULTS

A. The graph of exclusivity framework

A measurement $M$, together with its outcome $a$, is called a measurement event (or event, for brevity) and denoted $(a|M)$. Two events, $e_i$ and $e_j$ are mutually exclusive (or exclusive, for brevity) if there exists a measurement $M$ such that $e_i$ and $e_j$ correspond to different outcomes of $M$. To any set of events $\{e_i\}_{i=1}^n$, we associate a simple undirected graph $\mathcal{G}_{\text{ex}} = ([N], E)$, where $[N]$ refers to the set $\{1, 2, \ldots, N\}$. This graph, referred to as the graph of exclusivity, has vertex set $[N]$ and two vertices $i, j$ are adjacent (denoted $i \sim j$) if the corresponding events $e_i$ and $e_j$ are exclusive.

We now consider theories that assign probabilities to events. A behavior for $\mathcal{G}_{\text{ex}}$ is a mapping $p: [N] \rightarrow [0, 1]$, such that $p_i + p_j \leq 1$, for all $i \sim j$, where we denote $p(i)$ by $p_i$. Here, the non-negative scalar $p_i \in [0, 1]$ encodes the probability that event $e_i$ occurs. The linear constraint $p_i + p_j \leq 1$ enforces that, if $p_i = 1$, then $p_j = 0$. Our results for bipartite and tripartite cases have been stated as Theorems 7, 8, 10 and 11 (see subsection II.E). Since induced subgraph with weights is still a graph of exclusivity, we will use $\mathcal{G}_{\text{ex}}(w)$ throughout the paper in place of $(G, w)$.

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A behavior $p: [N] \to [0,1]$ is deterministic non-contextual if all events have pre-determined binary values (0 or 1) that do not depend on the occurrence of other events. In other words, a deterministic non-contextual behavior $p$ is a mapping $p: [N] \to \{0, 1\}$ such that $p_i + p_j \leq 1$, for all $i \sim j$. A deterministic non-contextual behavior can be considered a vector in $\mathbb{R}^N$. The convex hull of all deterministic non-contextual behaviors is called the set of non-contextual behaviors, denoted by $\mathcal{P}_{NC}(\mathcal{G}_{ex})$. The set $\mathcal{P}_{NC}(\mathcal{G}_{ex})$ is a polytope with its vertices being the deterministic non-contextual behaviors. Behaviors that do not lie in $\mathcal{P}_{NC}(\mathcal{G}_{ex})$ are called contextual.

It is worth mentioning that, in combinatorial optimisation, one often encounters the stable set polytope of a graph $\mathcal{G}_{ex}$, denoted by $\mathcal{STAB}(\mathcal{G}_{ex})$ (see Appendix A). It is quite easy to see that stable sets of $\mathcal{G}_{ex}$ (a subset of vertices, where no two vertices share an edge between them) and non-contextual behaviors coincide.

Lastly, a behavior $p: [N] \to [0,1]$ is called quantum behavior if there exists a quantum state $|\psi\rangle$ and projectors $\Pi_1, \ldots, \Pi_N$ acting on a Hilbert space $\mathcal{H}$ such that

$$p_i = \langle \psi | \Pi_i | \psi \rangle, \forall i \in [N] \text{ and } \text{tr}(\Pi_i \Pi_j) = 0, \text{ for } i \sim j.$$  \hspace{1cm} (1)

We refer to the ensemble $|\psi\rangle, \{\Pi_i\}_{i=1}^N$ as a quantum realization of the behavior $p$. The set of all quantum behaviors is a convex set, denoted by $\mathcal{P}_Q(\mathcal{G}_{ex})$. It turns out that $\mathcal{P}_Q(\mathcal{G}_{ex})$ is also a well-studied entity in combinatorial optimisation, namely the theta body, denoted by $\mathcal{TH}(\mathcal{G}_{ex})$ and is formally defined in Appendix A definition 21.

Now, suppose that we are interested in the maximum value of the sum $S = w_1 p_1 + w_2 p_2 + \cdots + w_N p_N$, where $w_i \geq 0$ are weights for $i \in [N]$ and

1. $p \in \mathcal{P}_{NC}(\mathcal{G}_{ex})$ is a non-contextual behavior. In this case, the maximum (henceforth referred to as the classical bound) is given by the independence number of the vertex weighted graph of exclusivity, $\alpha(\mathcal{G}_{ex}, w)$, that is, the size of the largest clique in the complement graph. Here, $w$ refers to the $N$ dimensional vector of non-negative weights.

2. $p \in \mathcal{P}_Q(\mathcal{G}_{ex})$ is a quantum behavior. In this case, the maximum (henceforth referred to as the quantum bound) is given by the Lovász theta number of the vertex weighted graph of exclusivity, $\vartheta(\mathcal{G}_{ex}, w)$, defined by the following semidefinite program:

$$\vartheta(\mathcal{G}_{ex}, w) = \max \sum_{i=1}^N w_i X_{ii} \hspace{1cm} (2)$$

s.t. $X_{ii} = X_{0i}, \forall i \in [N],$

$X_{ij} = 0, \forall i \sim j,$

$X_{00} = 1, X \in S_+^{1+N},$

where $S_+^{1+N}$ denotes positive semidefinite matrices of size $(N+1) \times (N+1)$. From the definition of the theta body and Lemma 27 (see Appendix A), one can note that $p_i = X_{ii}$ for all $i \in [N]$.

Proofs of the above statements follow quite straightforwardly from the definitions and were first observed in [CSW14]. The Gram-Schmidt decomposition of matrix $X$ corresponding to (2) gives the quantum realization for the underlying behaviour $p$ [BRV + 19b] (see Appendix A for the definition of Gram-Schmidt decomposition).

Note that, for a fixed $X$, its different Gram-Schmidt decompositions are related to one another via isometry.

**Definition 1. (Non-contextuality inequality)** For a given graph of exclusivity $\mathcal{G}_{ex}$, a non-contextuality inequality corresponds to a halfspace that contains the set of non-contextual behaviors, i.e.,

$$\sum_i w_i p_i \leq \alpha(\mathcal{G}_{ex}, w), \forall p \in \mathcal{P}_{NC}(\mathcal{G}_{ex}),$$  \hspace{1cm} (3)

and $w_i \geq 0 \forall i \in [N]$.

### B. The CHSH experiment in the graph of exclusivity framework

In the CHSH Bell experiment, an arbitrator generates two maximally entangled quantum systems and transmits them to two spatially separated parties: Alice and Bob. Alice has two measurement settings, $x = 0$ and $x = 1$, and Bob has likewise two measurement settings, $y = 0$ and $y = 1$. These local measurements are binary observables, each having outcomes, say 0 and 1. Each party (Alice and Bob) measures in every round in either the 0 or the 1 setting. The selections of settings made by each party must be random and independent of those of the other party. Let $(a, b | x, y)$ represent the event where Alice measures in the setting $x$, Bob measures in the setting $y$, and they get $a \in \{0,1\}$ and $b \in \{0,1\}$, respectively. Let the probability of the corresponding event be $p(a, b | x, y)$. There are sixteen different events corresponding to all possible combinations of inputs...
and outputs. They repeat this exercise a considerable enough times, once they are finished, to determine the probabilities of these events.

In the CHSH test, eight out of the sixteen events are of relevance, as one is interested in maximizing the Bell witness given by

$$S_{\text{CHSH}} = p(0,0|0,0) + p(1,1|0,1) + p(1,0|1,1) + p(0,0|1,0) + p(1,1|0,0) + p(0,0|0,1) + p(1,0|1,1) + p(1,1|1,0).$$  \hspace{1cm} (4)

Notice that the aforementioned witness necessitates Alice and Bob to output same answers unless they both are asked $x = y = 1$. In cases they are asked $x = y = 1$, they should oppose answers. The graph of exclusivity corresponding to these eight events is shown in Fig. 14, and is denoted as $C_{8\text{a}}(1,4)$. The weights on each of the vertices is 1 and thus the weight vector is an eight dimensional all 1 vector. Notice that $\alpha(C_{8\text{a}}(1,4)) = 3$ and, thus, the classical bound of $S_{\text{CHSH}} \leq 3$. Whereas, $\vartheta(C_{8\text{a}}(1,4)) = 2 + \sqrt{2} \approx 3.414$, see [CSW14], and therefore the quantum bound of $S_{\text{CHSH}} \leq 2 + \sqrt{2}$.

![Fig. 1: Induced subgraph (of the 16-vertex graph of exclusivity of the events in the CHSH scenario) corresponding to the 8 events involved in the expression of the Bell witness given by Eq. (4). This graph is called the 8-vertex circulant graph (1,4) and is denoted $C_{8\text{a}}[1,4]$ (see definition 14 for a definition of circulant graphs), and is isomorphic to the Möbius ladder graph of order 2.](image)

C. Self-Testing

Bell inequalities are special instances of non-contextuality inequalities. Consider an $n$-partite Bell scenario, characterized by a number $n$ of distant observers or parties, their respective measurement settings, and their possible outcomes. Suppose party $j$ possesses $k_j$ different settings with $K_j$ different outcomes for each measurement. In such a scenario, one can compute the probability of a particular string of outcomes given a string of measurements, that is, $p[a_1, a_2, \ldots, a_n|x_1, x_2, \ldots, x_n]$, where $a_j \in [K_j]$ and $x_j \in [k_j]$ for all $j \in [n]$. We use the notation $\vec{a}$ to refer to the $n$-tuple string $a_1, a_2, \ldots, a_n$. Similarly, we use $\vec{x}$ for the measurement settings.

A $n$-partite Bell inequality is of the following form:

$$\sum_{\vec{a}, \vec{x}} s_{\vec{a}, \vec{x}}^2 p[\vec{a}|\vec{x}] \leq S_\mathcal{L},$$  \hspace{1cm} (5)

for some coefficients $s_{\vec{a}, \vec{x}}^2$ and where $S_\mathcal{L}$ is the largest possible value allowed in local hidden variable (LHV) models [BCP+14]. The quantum supremum of the Bell expression, i.e., the left hand side of (5), denoted by $S_\mathcal{Q}$, is the largest possible value of the above expression when $p[\vec{a}|\vec{x}]$ ranges over the set of quantum behaviors, i.e.,

$$p[\vec{a}|\vec{x}] = \langle \psi | \bigotimes_{j=1}^n M_{a_j|x_j}^j | \psi \rangle,$$  \hspace{1cm} (6)

for a shared quantum state $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \ldots \otimes \mathcal{H}_n$ and quantum projective measurements $\{M_{a_j|x_j}^j\}$ acting on $\mathcal{H}_j$ for all $j \in [n]$. We refer to the state and the set of measurements that reproduce the quantum behavior, collectively as a quantum realization.

**Definition 2.** *(Bell self-testing)* The quantum supremum $S_\mathcal{Q}$ of a Bell inequality is a self-test for the realization $(\psi, \{M_{a_j|x_j}^j\})$, if for any other realization $(\psi', \{M_{a_j|x_j}^j\})$ that also attains $S_\mathcal{Q}$, there exists a local unitary...
\( V = V_1 \otimes V_2, \ldots, \otimes V_n \) and an ancilla state \(|\text{junk}\rangle\) such that
\[
V|\psi\rangle = |\text{junk}\rangle \otimes |\psi\rangle,
\]
\[
V(\bigotimes_{j=1}^{n} M_{u_j|x_j})|\psi\rangle = |\text{junk}\rangle \otimes (\bigotimes_{j=1}^{n} M_{u_j|x_j})|\psi\rangle.
\]

**D. Relevant background from Semidefinite programs**

**Definition 3.** *(Semidefinite programs)* A pair of primal and dual SDPs is given by an optimisation problem of the following form:
\[
\sup_X \{\langle C, X \rangle : X \in S^n_+ \}, \quad (A_i, X) = b_i \quad (i \in [m]) \},
\]
\[
\inf_{y, Z} \left\{ \sum_{i=1}^{m} b_i y_i : \sum_{i=1}^{m} y_i A_i - C = Z \in S^n_+ \right\},
\]

where \( C, A_i \) (for all \( i \in [m] \)) are Hermitian \( n \times n \) matrices and \( b \in \mathbb{C}^m \).

We have introduced the primal formulation of the Lovász theta SDP in (2).
The dual formulation for (2) is given by
\[
\min t : t E_{00} + \sum_{i=1}^{n} (\lambda_i - 1)E_{ii} - \sum_{i=1}^{n} \lambda_i E_{0i} + \sum_{i<j} \mu_{ij} E_{ij} \equiv Z \succeq 0,
\]

where \( E_{ij} = e_i e_j^T + e_j e_i^T \). We make crucial use of the following Theorem due to Alizadeh et al. [AHO97, Theorem 4] to show that the optimiser of (2) is unique.

**Theorem 4.** *[AHO97]* Let \( Z^* \) be a dual optimal and nondegenerate solution of a semidefinite program. Then, there exists a unique primal optimal solution for that SDP.

The notion of dual nondegeneracy is given by the following definition.

**Definition 5.** *(Dual nondegeneracy)* Let \( Z^* \) be an optimal dual solution and let \( M \) be any symmetric matrix. If the homogeneous linear system
\[
MZ^* = 0,
\]
\[
\text{tr}(MA_i) = 0 \quad (\forall i \in [m]),
\]
only admits the trivial solution \( M = 0 \), then \( Z^* \) is said to be dual nondegenerate.

A key ingredient for proving the results in this paper is the following lemma:

**Lemma 6.** *(BRV'19)* Let \( X^* \) be the unique optimal solution for the primal and let \( \{\{u_i\}, \{\|i\|\}\}_{i=0}^{n} \) be a quantum realization achieving the maximum quantum value of \( \sum_{i=1}^{n} w_i p_i : p \in \mathcal{P}_Q(\mathcal{G}_{\text{ex}}) \). Then, the non-contextuality inequality \( \sum_{i=1}^{n} w_i p_i \leq B_{nc}(\mathcal{G}_{\text{ex}}, \psi) \), for all \( p \in \mathcal{P}_{nc}(\mathcal{G}_{\text{ex}}) \) is a self-test for the realisation \( \{\{u_i\}, \{\|i\|\}\}_{i=0}^{n} \).

E. Results

We are given a Bell inequality of the form (5) and we consider the set of events \( p[a|x] \) such that \( s_E^2 \neq 0 \). We shall index this set by \( i \) and denote the corresponding event as \( e_i \). Suppose we are given a \( n \)-partite Bell inequality with Bell witness \( \mathcal{B} = \sum_i w_i p_i \), with \( w_i > 0 \) and \( p_i = p(e_i) \), and a quantum realization \( (\psi, \{M_{u_j|x_j}\}) \) (let us call this the reference system) that achieves the quantum supremum, \( S_Q \) of \( \mathcal{B} \). Let \( \mathcal{G}_{\text{ex}}(\psi, w) \) be the weighted graph capturing the weights \( \{w_i\} \) and mutual exclusivity relationships among the events \( \{e_i\} \) in \( \mathcal{B} \).

We have two sets of assumptions in this manuscript. The first set of assumptions is following:

(i) \( S_Q = \vartheta(\mathcal{G}_{\text{ex}}, w) \).

(ii) The Lovász theta SDP in (2) corresponding to \( (\mathcal{G}_{\text{ex}}, w) \) has a unique maximizer. This assumption is a consequence of assumption (i) for the scenarios of interest in this paper.
We consider two types of sets of indexes $\mathcal{I}$ and $\mathcal{I}_0 = \mathcal{I} \cup \{0\}$. We consider the matrix $X_{ij} := \langle \psi | \Pi_i \Pi_j | \psi \rangle$, where $\Pi_i$ is a projection and $\Pi_0$ is the identity operator. We set $n := |\mathcal{I}|$. The assumption $\text{ii}$ means that the following SDP has unique solution.

$$\vartheta(G_{ex}, w) = \max \sum_{i \in \mathcal{I}} w_i X_{ii}$$

s.t. \( X_{ii} = X_{0i}, \forall i \in [n], \)
\( X_{ij} = 0, \forall i \sim j, \)
\( X_{00} = 1, X \in S^{1+n}. \) \hspace{1cm} (13)

The second set of assumptions depend on the scenarios of interest and have been mentioned in the following subsections. Our results for bipartite and tripartite cases have been summarized as Theorems 7, 8, 10 and 11.

1. Bipartite case

Suppose the unique optimal maximizer $X^* = (X_{ij})$ is given by $\eta_i \eta_j \langle v_j, v_i \rangle$ with the following: For $i = (i_A, i_B) \in \mathcal{I}$,

$$v_i = a_{i_A} \otimes b_{i_B}, \hspace{1cm} (14)$$

where $a_{i_A} \in \mathcal{H}_A = C^{d_A}$, $b_{i_B} \in \mathcal{H}_B = C^{d_B}$. Also, for simplicity, $a_{i_A}$ and $b_{i_B}$ are assumed to be normalized and $\eta_i > 0$. Now, we consider a state $|\psi'\rangle$ on $\mathcal{H}_A' \otimes \mathcal{H}_B'$, and projections $\Pi_{i_A}^A$ and $\Pi_{i_B}^B$ on $\mathcal{H}_A'$ and $\mathcal{H}_B'$. Here, when $i_A = i_A'$ ($i_B = i_B'$) for $i \neq i'$, $\Pi_{i_A}^A = \Pi_{i_A'}^A$ ($\Pi_{i_B}^B = \Pi_{i_B'}^B$). Then, we define the projection $\Pi_i := \Pi_{i_A}^A \otimes \Pi_{i_B}^B$.

In the following, we discuss how the state $|\psi'\rangle$ is locally converted to $|\psi\rangle$ when the vectors $\Pi_i |\psi'\rangle$ realize the optimal solution in the SDP (13). We define $|\tilde{v}_i\rangle := \eta_i^{-1} \Pi_i |\psi'\rangle$.

First, we consider the case that the ranks of the projections $\Pi_{i_A}^A$ and $\Pi_{i_B}^B$ are one. We introduce the following conditions.

A1 The set $\{v_i\}_{i \in \mathcal{I}_0}$ of vectors spans the vector space $\mathcal{H}_A \otimes \mathcal{H}_B$.

A2 There exist a subset $\mathcal{I}_{i_B}$ of indexes of the space $\mathcal{H}_B$ with $|\mathcal{I}_{i_B}| = d_B = \dim \mathcal{H}_B$ and $d_B$ sets $\{\mathcal{I}_{A,i_B}\}_{i_B \in \mathcal{I}_{i_B}}$ of indexes of the space $\mathcal{H}_A$ $|\mathcal{I}_{A,i_B}| = d_A = \dim \mathcal{H}_A$ to satisfy the following conditions B1-B4.

B1 $\bigcup_{i_B \in \mathcal{I}_{i_B}} \mathcal{I}_{A,i_B} \times \{i_B\} \subset \mathcal{I}$.

B2 $\{b_{i_B}\}_{i_B \in \mathcal{I}_{i_B}}$ spans the space $\mathcal{H}_B$.

B3 $\{a_{i_A}\}_{i_A \in \mathcal{I}_{A,i_B}}$ spans the space $\mathcal{H}_A$ for any $i_B \in \mathcal{I}_{i_B}$.

B4 We define the graph on $\mathcal{I}_{i_B}$ in the following way. The node $i_B \in \mathcal{I}_{i_B}$ is connected to $i_B' \in \mathcal{I}_{i_B}$ when the following two conditions holds:

B4-1 The relation $\langle b_{i_B}, b_{i_B'} \rangle \neq 0$ holds.

B4-2 The relation $\mathcal{I}_{A,i_B} \cap \mathcal{I}_{A,i_B'} \neq \emptyset$ holds.

In the two qubit case, if the set $\{v_i\}_{i \in \mathcal{I}}$ of vectors contains the following 4 vectors, then the conditions A1 and A2 hold;

$$a_0 \otimes b_0, \quad a_1 \otimes b_0, \quad a_0 \otimes b_1, \quad a_2 \otimes b_1, \hspace{1cm} (15)$$

where $a_0 \neq a_1, a_2, (b_0, b_1) \neq 0$.

**Theorem 7.** Assume that the optimal maximizer given in (14) satisfies conditions A1 and A2 and the vectors $(\Pi_i |\psi'\rangle)_{i \in \mathcal{I}}$ realize the optimal solution in the SDP (13). In addition, the ranks of the projections $\Pi_{i_A}^A$ and $\Pi_{i_B}^B$ are assumed to be one. Then, there exist isometries $V_A : \mathcal{H}_A \to \mathcal{H}_A$ and $V_B : \mathcal{H}_B \to \mathcal{H}_B$ such that

$$V_A \otimes V_B |\psi\rangle = |\psi'\rangle, \hspace{1cm} (16)$$

$$V_A \otimes V_B |v_i\rangle = |\tilde{v}_i\rangle, \hspace{1cm} (17)$$

for $i \in \mathcal{I}$. □

**Proof.** The proof has been deferred to Appendix D. □

Now we consider the general case. In addition to A1 and A2, we assume the following condition.
A3 Ideal systems $\mathcal{H}_A$ and $\mathcal{H}_B$ are two-dimensional.

A4 Each system has only two measurements. That is, the set $\tilde{I}_A$ ($\tilde{I}_B$) of all indexes of the space $\mathcal{H}_A$ ($\mathcal{H}_B$) is composed of 4 elements. For any element $i_A \in \tilde{I}_A$ ($i_B \in \tilde{I}_B$), there exists an element $i'_A \in \tilde{I}_A$ ($i'_B \in \tilde{I}_B$) such that $\langle a_{i_A} | a_{i'_A} \rangle = 0$ ($\langle b_{i_B} | b_{i'_B} \rangle = 0$).

When A3 and A4 hold, $\tilde{I}_A$ ($\tilde{I}_B$) is written as $B_{A,0} \cup B_{A,1}$ ($B_{B,0} \cup B_{B,1}$), where $B_{A,j} = \{(0,j),(1,j)\}$ ($B_{B,j} = \{(0,j),(1,j)\}$) and $\langle a_{(0,j)} | a_{(1,j)} \rangle = 0$ ($\langle b_{(0,j)} | b_{(1,j)} \rangle = 0$) for $j = 0,1$.

We also consider the following condition for $\Pi_i = \Pi_{i_A} \otimes \Pi_{i_B}$.

C1 When $i_A, i'_A \in \tilde{I}_A$ ($i_B, i'_B \in \tilde{I}_B$) satisfy $\langle a_{i_A} | a_{i'_A} \rangle = 0$ ($\langle b_{i_B} | b_{i'_B} \rangle = 0$), we have $\Pi_{i_A}^A + \Pi_{i'_A}^A = I$ ($\Pi_{i_B}^B + \Pi_{i'_B}^B = I$).

Let $\mathcal{H}_{i_A}^A$ and $\mathcal{H}_{i_B}^B$ be the image of the projections $\Pi_{i_A}^A$ and $\Pi_{i_B}^B$.

Theorem 8. Assume that the optimal maximizer given in (14) satisfies conditions A1, A2, A3, and A4, the vectors $(\Pi_i | \psi') \in \mathbb{E}$ realize the optimal solution in the SDP (13), and condition C1 holds. Then, there exist isometries $V_A$ from $\mathcal{H}_A \otimes \mathcal{K}_A$ to $\mathcal{H}'_A$ and $V_B$ from $\mathcal{H}_B \otimes \mathcal{K}_B$ to $\mathcal{H}'_B$ such that
\begin{align}
V_A \otimes V_B | \psi \rangle &\otimes | \text{junk} \rangle = | \psi' \rangle, \\
V_A \otimes V_B | v_i \rangle &\otimes | \text{junk} \rangle = | v'_i \rangle,
\end{align}
for $i \in \mathbb{I}$, where $| \text{junk} \rangle$ is a state on $\mathcal{K}_A \otimes \mathcal{K}_B$.

Proof. The proof has been deferred to Appendix D.

2. Tripartite case

We assume that the unique optimal maximizer $X^* = (X_{ij})$ is given by $\eta_i \eta_j (v_j, v_i)$ with the following: For $i = (i_A, i_B, i_C) \in \mathbb{I}$,
\begin{equation}
\eta_i = a_{i_A} \otimes b_{i_B} \otimes c_{i_C},
\end{equation}
where $a_{i_A} \in \mathcal{H}_A = \mathbb{C}^{d_A}$, $b_{i_B} \in \mathcal{H}_B = \mathbb{C}^{d_B}$, $c_{i_C} \in \mathcal{H}_C = \mathbb{C}^{d_C}$. Also, for simplicity, $a_{i_A}$, $b_{i_B}$, and $c_{i_C}$ are assumed to be normalized and $\eta_i > 0$.

Now, we consider a state $| \psi' \rangle$ on $\mathcal{H}'_A \otimes \mathcal{H}'_B \otimes \mathcal{H}'_C$, and projections $\Pi_{i_A}^A$, $\Pi_{i_B}^B$, $\Pi_{i_C}^C$ on $\mathcal{H}'_A$, $\mathcal{H}'_B$, and $\mathcal{H}'_C$. Then, we define the projection $\Pi_i \doteq \Pi_{i_A}^A \otimes \Pi_{i_B}^B \otimes \Pi_{i_C}^C$.

In the following, we discuss how the state $| \psi' \rangle$ is locally converted to $| \psi \rangle$ when the vectors $\Pi_i | \psi' \rangle$ realize the optimal solution in the SDP (13). We define $| \psi'_i \rangle \doteq \eta_i^{-1} \Pi_i | \psi' \rangle$.

We consider the case that the ranks of the projections $\Pi_{i_A}^A$, $\Pi_{i_B}^B$ and $\Pi_{i_C}^C$ are one. We introduce the following conditions.

Definition 9. Three distinct elements $i, j, k \in \mathbb{I}$ are called linked when the following two conditions holds.

C1 The relations $(v_i, v_j) \neq 0$, $(v_j, v_k) \neq 0$, and $(v_j, v_k) \neq 0$ hold.

C2 $v_i, v_j$ shares a $t_{i,j}$-th common element for $t_{i,j} \in \{A, B, C\}$. Other components of $v_i, v_j$ are different. That is, when $t_{i,j} = A$, $i_A = j_A, i_B \neq j_B$, and $i_C \neq j_C$. $v_i$ and $v_k$ share a $t_{i,k}$-th common element for $t_{i,k} \in \{A, B, C\} \setminus \{t_{i,j}\}$. $v_j$ and $v_k$ share a $t_{j,k}$-th common element for $t_{j,k} \in \{A, B, C\} \setminus \{t_{i,j}, t_{i,k}\}$. In this case, there exist elements $x_A, x'_A, x_B, x'_B, x_C, x'_C$ such that $i,j,k \in \{x_A, x'_A\} \times \{x_B, x'_B\} \times \{x_C, x'_C\}$.

In addition, two distinct elements $x_A, x'_A$ for index of a vectors of $\mathbb{C}^{d_A}$ are called connected when there exist three linked elements $i, j, k \in \mathbb{I}$ such that the first components of $i, j, k \in \mathbb{I}$ are $x_A, x'_A$.

For $i_B, i_C$, we use notation
\begin{equation}
\psi(i_B, i_C) \doteq b_{i_B} \otimes c_{i_C}.
\end{equation}

Then, we introduce the following conditions for the optimal maximizer given in (20).

A5 The vectors $\{v_i\}_{i \in \mathbb{I}}$ span the vector space $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$.

A6 There exist a subset $\mathcal{I}_A$ of indecies of the space $\mathcal{H}_A$ with $|\mathcal{I}_A| = d_A$ and $d_A$ sets $\mathcal{I}_{BC,i_A}$ for $i_A \in \mathcal{I}_A$ of indecies of the space $\mathcal{H}_B \otimes \mathcal{H}_C$ to satisfy the following conditions. The set $\{a_{i_A}\}_{i_A \in \mathcal{I}_A}$ spans the space $\mathcal{H}_A$. The set $\{\psi_{i_A}\}_{i_A \in \mathcal{I}_{BC,i_A}}$ spans the space $\mathcal{H}_B \otimes \mathcal{H}_C$ and $\mathcal{I}_0 = \cup_{i_A \in \mathcal{I}_A} \times \{i_A\} \times \mathcal{I}_{BC,i_A}$. We consider the graph $G_A$ with the set $\mathcal{I}_A$ of vertices such that the edges are given as the the pair of all connected elements in $\mathcal{I}_A$ in the sense of the end of Definition 9. The graph $G_A$ is not divided into two disconnected parts.
The vectors \( \{b_{ia} \otimes c_{ic}\}_{(iB, iC) \in \mathcal{I}_B \times \mathcal{I}_C} \) satisfy condition A2 by substituting \( c_{ic} \) into \( a_{ia} \). That is, there exist a subset \( \mathcal{I}_B \) of the second indecies and subsets \( \mathcal{I}_{C,i} \) of the third indecies such that they satisfy conditions B1, B2, B3, and B4. We denote the graph defined in this condition by \( GB \).

**Theorem 10.** Assume that the optimal maximizer given in (20) satisfies conditions A5, A6, and A7, and the vectors \( \{\Pi_i | \psi_i^\prime\}_{i \in \mathcal{I}} \) realize the optimal solution in the SDP (13). In addition, the ranks of the projections \( \Pi_{iA}^A, \Pi_{iB}^B, \) and \( \Pi_{iC}^C \) are assumed to be one.

Then, there exist isometries \( V_A : \mathcal{H}_A \to \mathcal{H}_A', V_B : \mathcal{H}_B \to \mathcal{H}_B', \) and \( V_C : \mathcal{H}_C \to \mathcal{H}_C' \) such that

\[
V_A \otimes V_B \otimes V_C | \psi_i^\prime \rangle = | \psi_i' \rangle,
\]
\[
V_A \otimes V_B \otimes V_C | v_i \rangle = | v_i' \rangle,
\]

for \( i \in \mathcal{I} \).

**Proof.** The proof has been deferred to Appendix D.

Now we consider the general case. We define \( | v_i' \rangle := \eta_i^{-1} \Pi_{iA}^A \otimes \Pi_{iB}^B \otimes \Pi_{iC}^C | \psi_i \rangle \).

Let \( \mathcal{I}_A, \mathcal{I}_B, \) and \( \mathcal{I}_C \) be the sets of indecies of the spaces \( \mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C \).

We introduce other conditions for the optimal maximizer given in (20) as a generalization of A3 and A4.

**A8** Ideal systems \( \mathcal{H}_A, \mathcal{H}_B, \) and \( \mathcal{H}_C \) are two-dimensional.

**A9** Each system has only two measurements. That is, the sets \( \mathcal{I}_A, \mathcal{I}_B, \) and \( \mathcal{I}_C \) is composed of 4 elements. For any element \( i_A \in \mathcal{I}_A \), \( i_B \in \mathcal{I}_B \), and \( i_C \in \mathcal{I}_C \), there exists an element \( i_A' \in \mathcal{I}_A \), \( i_B' \in \mathcal{I}_B \), \( i_C' \in \mathcal{I}_C \) such that \( \langle a_{i_A} | a_{i_A}' \rangle = 0 \). \( \langle b_{i_B} | b_{i_B}' \rangle = 0 \), \( \langle c_{i_C} | c_{i_C}' \rangle = 0 \).

When A3 and A4 hold, \( \mathcal{I}_A \) \( \mathcal{I}_B \), and \( \mathcal{I}_C \) is written as \( \mathcal{B}_{A,0} \cup \mathcal{B}_{A,1} \) \( \mathcal{B}_{B,0} \cup \mathcal{B}_{B,1} \), \( \mathcal{B}_{C,0} \cup \mathcal{B}_{C,1} \), where \( \mathcal{B}_{A,j} = \{(0, 0), (0, 1)\} \), \( \mathcal{B}_{B,j} = \{(0, 0), (0, 1)\} \), \( \mathcal{B}_{C,j} = \{(0, 0), (0, 1)\} \) and \( \langle a_{i_{A,j}} | a_{i_{A,j}} \rangle = 0 \), \( \langle b_{i_{B,j}} | b_{i_{B,j}} \rangle = 0 \), \( \langle c_{i_{C,j}} | c_{i_{C,j}} \rangle = 0 \).

We also consider the following condition for \( \Pi_i = \Pi_{iA}^A \otimes \Pi_{iB}^B \otimes \Pi_{iC}^C \).

**C1** When \( i_A, i_A' \in \mathcal{I}_A \), \( i_B, i_B' \in \mathcal{I}_B \), \( i_C, i_C' \in \mathcal{I}_C \) satisfy \( \langle a_{i_A} | a_{i_A}' \rangle = 0 \), \( \langle b_{i_B} | b_{i_B}' \rangle = 0 \), \( \langle c_{i_C} | c_{i_C}' \rangle = 0 \), we have \( \Pi_{iA}^A + \Pi_{iA}' = I \), \( \Pi_{iB}^B + \Pi_{iB}' = I \), \( \Pi_{iC}^C + \Pi_{iC}' = I \).

Let \( \mathcal{H}_{iA}, \mathcal{H}_{iB}, \) and \( \mathcal{H}_{iC} \) be the image of the projections \( \Pi_{iA}^A, \Pi_{iB}^B, \) and \( \Pi_{iC}^C \).

**Theorem 11.** Assume that the optimal maximizer given in (20) satisfies conditions A5, A6, A5, A7, A8, and A9, and the vectors \( \{\Pi_i | \psi_i^\prime\}_{i \in \mathcal{I}} \) realize the optimal solution in the SDP (13). Then, there exist isometries \( V_A \) from \( \mathcal{H}_A \otimes \mathcal{K}_A \) to \( \mathcal{H}_A' \), \( V_B \) from \( \mathcal{H}_B \otimes \mathcal{K}_B \) to \( \mathcal{H}_B' \), and \( V_C \) from \( \mathcal{H}_C \otimes \mathcal{K}_C \) to \( \mathcal{H}_C' \) such that

\[
V_A \otimes V_B \otimes V_C | \psi_i \rangle \otimes | \text{junk} \rangle = | \psi_i' \rangle \otimes | \text{junk} \rangle,
\]
\[
V_A \otimes V_B \otimes V_C | v_i \rangle \otimes | \text{junk} \rangle = | v_i' \rangle \otimes | \text{junk} \rangle,
\]

for \( i \in \mathcal{I} \), where \( | \text{junk} \rangle \) is a state on \( \mathcal{K}_A \otimes \mathcal{K}_B \otimes \mathcal{K}_C \).

**Proof.** The proof has been deferred to Appendix D.

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**III. TEST CASES**

In the following subsections we apply our techniques to the CHSH, chained, Mermin, and AS Bell inequalities.

**A. CHSH Self-Testing**

Self-testing is known to hold for the maximum quantum violation of the CHSH inequality [MY04]. Here, we study the CHSH inequality in the graph of exclusivity framework [CSW14].

Recall that the graph of exclusivity corresponding to the Bell witness given by Eq. (4) is given by the \( C_{ia}(1,4) \) graph (see figure 14). We claim that the optimal solution to dual (10) for \( C_{ia}(1,4) \) is given by

\[
Z_{\text{CHSH}} = \begin{pmatrix}
2 + \sqrt{3} & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & 1 & h & 0 & 0 & k & 0 & 0 \\
-1 & h & 1 & h & 0 & 0 & k & 0 \\
-1 & 0 & h & 1 & h & 0 & 0 & k \\
-1 & 0 & 0 & h & 1 & h & 0 & 0 \\
-1 & k & 0 & 0 & h & 1 & h & 0 \\
-1 & 0 & k & 0 & 0 & h & 1 & h \\
-1 & 0 & 0 & k & 0 & 0 & h & 1
\end{pmatrix},
\]
where $k = 3 - 2\sqrt{2}$ and $h = 2 - \sqrt{2}$. Lovász theta SDP has zero duality gap, that is, the primal optimal solution and optimal dual solution yield the same program value. It can be easily verified that (26) is a feasible solution to (10) for the graph $C_4(1, 4)$. The dual solution (26) achieves $2 + \sqrt{2}$ and is thus dual optimal. In order to show the uniqueness of the primal optimal, we show that $Z_{\text{CHSH}}$ is nondegenerate. That requires us to show that $M = 0$ is the only symmetric $9 \times 9$ matrix satisfying equations (11) and (12) corresponding to the Lovász theta SDP. That is, the linear system

$$M_{ii} = 0, \quad M_{ij} = 0 (\forall \ i \sim j), \quad MZ^* = 0$$

has a unique solution $M = 0$. Barring the $MZ^* = 0$ constraint, the rest of the constraints already guarantee that several entries of $M$ must be zeros. Thus the $M$ matrix has the following form:

$$M = \begin{pmatrix}
0 & m_1 & m_2 & m_3 & m_4 & m_5 & m_6 & m_7 & m_8 \\
m_1 & m_{15} & 0 & m_{20} & m_{21} & m_{23} & 0 & 0 & 0 \\
m_2 & 0 & m_{10} & 0 & m_{16} & 0 & m_{21} & m_{24} & 0 \\
m_3 & m_{15} & 0 & m_{40} & m_{10} & m_{12} & m_{18} & 0 & 0 \\
m_4 & m_{10} & m_{11} & 0 & m_{50} & 0 & x_{13} & m_{19} & 0 \\
m_5 & m_{20} & m_{12} & 0 & m_{60} & m_{10} & 0 & m_{14} & 0 \\
m_6 & m_{21} & m_{18} & m_{13} & 0 & mn & 0 & 0 & 0 \\
m_7 & 0 & m_{24} & m_{22} & 0 & m_{19} & 0 & m_{14} & 0 \\
m_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.$$  

(28)

It can be easily checked that the only solution to the system of linear equations $M \cdot Z_{\text{CHSH}} = 0$ is $M = 0$.

The optimal solution for primal (2) is given by

$$P_{\text{CHSH}} = \begin{pmatrix}
1 & x & x & x & x & x & x & x & x \\
x & x & 0 & \frac{1}{2}x & \xi & 0 & \xi & \frac{1}{2}x & 0 \\
x & \frac{1}{2}x & 0 & x & 0 & \frac{1}{2}x & \xi & 0 & \xi \\
x & \xi & \frac{1}{2}x & 0 & x & 0 & \frac{1}{2}x & \xi & 0 \\
x & 0 & \xi & \frac{1}{2}x & 0 & x & 0 & \frac{1}{2}x & \xi \\
x & \xi & 0 & \xi & \frac{1}{2}x & 0 & x & 0 & \frac{1}{2}x \\
x & \frac{1}{2}x & \xi & 0 & \xi & \frac{1}{2}x & 0 & x & 0 \\
x & 0 & \frac{1}{2}x & \xi & 0 & \xi & \frac{1}{2}x & 0 & x
\end{pmatrix},$$

(29)

where $x = 2 + \sqrt{2}$ and $\xi = 1 + \sqrt{2}$. The configurations corresponding to the primal optimal matrix $P_{\text{CHSH}}$ correspond to different Gram decomposition of $P_{\text{CHSH}}$ and are related to each other via global isometry. A quantum realization is achieved with the two-qubit maximally entangled state $|\psi\rangle = (\frac{1}{\sqrt{2}}, 0, 0, \frac{1}{\sqrt{2}})^T$ and the vectors corresponding to the 8 projective measurements given by

$$|v_1\rangle = |A_{1,1}\rangle \otimes |B_{1,1}\rangle,$$

$$|v_2\rangle = |A_{0,0}\rangle \otimes |B_{1,0}\rangle,$$

$$|v_3\rangle = |A_{0,1}\rangle \otimes |B_{0,1}\rangle,$$

$$|v_4\rangle = |A_{1,0}\rangle \otimes |B_{0,0}\rangle,$$

$$|v_5\rangle = |A_{1,1}\rangle \otimes |B_{1,0}\rangle,$$

$$|v_6\rangle = |A_{0,1}\rangle \otimes |B_{1,1}\rangle,$$

$$|v_7\rangle = |A_{0,0}\rangle \otimes |B_{0,0}\rangle,$$

$$|v_8\rangle = |A_{1,1}\rangle \otimes |B_{0,1}\rangle,$$

(30)

where the kets corresponding to the local measurements are given by

$$|A_{0,0}\rangle = (1, 0)^T,$$

$$|A_{0,1}\rangle = (0, -1)^T,$$

$$|A_{1,0}\rangle = (a, a)^T,$$

$$|A_{1,1}\rangle = (a, -a)^T,$$

$$|B_{0,0}\rangle = (c, d)^T,$$

$$|B_{0,1}\rangle = (d, -c)^T,$$

$$|B_{1,0}\rangle = (c, -d)^T,$$

$$|B_{1,1}\rangle = (-d, -c)^T,$$

(31)
FIG. 2: Graph of exclusivity of the 16 events in the Bell witness (B6) of the Mermin inequality. Here, Z and X are denoted 0 and 1, respectively, while −1 and 1 are denoted 0 and 1, respectively. We will refer to this graph as \( G_M \). It is the complement of Shrikhande graph \([Str59]\).

with \( a = \frac{1}{\sqrt{2}} \), \( c = \cos \left( \frac{\pi}{8} \right) \), and \( d = \sin \left( \frac{\pi}{8} \right) \).

For the CHSH case, the vector \( v_i \) corresponds to \(|v_i\rangle\). The dimension of the canonical realization is 4 with \( d_1 = d_2 = 2 \). CHSH inequality satisfies Conditions A1 and A2, which can be checked by choosing the vectors in (15) as follows:

\[
a_0 = |A_{0,0}\rangle, \quad a_1 = a_2 = |A_{0,1}\rangle, \\
 b_0 = |B_{0,0}\rangle, \quad b_1 = |B_{1,0}\rangle.
\]

Moreover, the local measurements for the CHSH case satisfy condition A3, A4 and C1 as well. Thus, the CHSH case satisfies all the conditions for Theorem 8, which implies there exist isometries \( V_A \) from \( \mathcal{H}_A \otimes \mathcal{K}_A \) to \( \mathcal{H}_A' \) and \( V_B \) from \( \mathcal{H}_B \otimes \mathcal{K}_B \) to \( \mathcal{H}_B' \) such that

\[
V_A \otimes V_B|\psi\rangle \otimes |\text{junk}\rangle = |\psi'\rangle, \\
V_A \otimes V_B|v_i\rangle \otimes |\text{junk}\rangle = |v'_i\rangle,
\]

for \( i \in \mathcal{I} \), where \( |\text{junk}\rangle \) is a state on \( \mathcal{K}_A \otimes \mathcal{K}_B \).

Therefore, any two tensored realizations attaining the maximum quantum violation of the CHSH inequality are related via local isometries.

B. Mermin Self-Testing

Here, we examine the case of Mermin’s Bell inequality for three parties [Mer90]. As detailed in Appendix B, the Bell witness of this inequality includes 16 events. Their graph of exclusivity, denoted \( G_M \), is shown in Fig. IIIB.

The primal optimal for the SDP corresponding to the quantum violation of the Mermin inequality for three parties is given by

\[
P_{\text{Mermin}} = \begin{bmatrix}
1 & a \cdot e_{16}^T \\
a \cdot I_{16} + b \cdot E_{GM} & a \cdot I_{16}^T
\end{bmatrix} \in \mathbb{R}^{(17 \times 17)},
\]

where \( a = 0.25 \), \( b = 0.125 \), \( e_{16} \) is the all one column vector of size 16, and \( E_{GM} \) is the adjacency matrix of the complement of \( G_M \), and \( I_{16} \) is the identity matrix of size 16. The proof of the uniqueness of the primal optimal \( P_{\text{Mermin}} \) is trivially similar to the CHSH case. The quantum state and measurement settings can be obtained via Gram decomposition of \( P_{\text{Mermin}} \). A quantum realization is achieved with the three-qubit GHZ
state $|u_0\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$ and the projective measurements

\[ |u_1\rangle = |Z\rangle \otimes |P\rangle \otimes |P\rangle, \]
\[ |u_2\rangle = |O\rangle \otimes |M\rangle \otimes |P\rangle, \]
\[ |u_3\rangle = |O\rangle \otimes |P\rangle \otimes |M\rangle, \]
\[ |u_4\rangle = |Z\rangle \otimes |M\rangle \otimes |M\rangle, \]
\[ |u_5\rangle = |P\rangle \otimes |Z\rangle \otimes |P\rangle, \]
\[ |u_6\rangle = |M\rangle \otimes |O\rangle \otimes |P\rangle, \]
\[ |u_7\rangle = |M\rangle \otimes |Z\rangle \otimes |M\rangle, \]
\[ |u_8\rangle = |P\rangle \otimes |O\rangle \otimes |M\rangle, \]
\[ |u_9\rangle = |P\rangle \otimes |P\rangle \otimes |Z\rangle, \]
\[ |u_{10}\rangle = |M\rangle \otimes |M\rangle \otimes |Z\rangle, \]
\[ |u_{11}\rangle = |M\rangle \otimes |P\rangle \otimes |O\rangle, \]
\[ |u_{12}\rangle = |P\rangle \otimes |M\rangle \otimes |O\rangle, \]
\[ |u_{13}\rangle = |O\rangle \otimes |O\rangle \otimes |O\rangle, \]
\[ |u_{14}\rangle = |Z\rangle \otimes |Z\rangle \otimes |O\rangle, \]
\[ |u_{15}\rangle = |Z\rangle \otimes |O\rangle \otimes |Z\rangle, \]
\[ |u_{16}\rangle = |O\rangle \otimes |Z\rangle \otimes |Z\rangle. \]  

where $|Z\rangle = |0\rangle$, $|O\rangle = |1\rangle$, $|P\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$, and $|M\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$. This quantum realization achieves the quantum bound of the Bell witness (given by Eq. (B6) in Appendix B), i.e., 4, which is equal to the Lovász theta number of $G_M$ (Fig. IIIb). The local bound is 3 and is equal to the independence number of $G_M$. We can check that local measurement settings for the tripartite Mermin case satisfy Conditions A5, A6, and A7 as follows. In this example, $a_O, b_O, c_O$ means $|O\rangle$. This notation is applied to $Z, P, M$.

We choose the subset $\mathcal{I}_A := \{O, P\}$. Then, we have

\[ \mathcal{I}_{BC,O} = \{(O, O), (Z, Z), (M, P), (P, M)\}, \]  
\[ \mathcal{I}_{BC,P} = \{(Z, P), (P, Z), (O, M), (M, O)\}. \]  

Two elements $O, P \in \mathcal{I}_A$ are connected in the sense of the end of Definition 9 by choosing \{i, j, k\} = \{(P, Z, P), (O, Z, Z), (O, M, P)\}. Based on (38) and (39), we choose the subsets $\mathcal{I}_B$, $\mathcal{I}_{C,Z}$, and $\mathcal{I}_{C,P}$ as

\[ \mathcal{I}_B := \{Z, P\}, \mathcal{I}_{C,Z} := \{Z, P\}, \mathcal{I}_{C,P} := \{Z, M\}. \]  

The subsets $\mathcal{I}_B$, $\mathcal{I}_{C,Z}$, and $\mathcal{I}_{C,P}$ satisfy conditions B1, B2, B3, and B4. The Mermin case satisfies Conditions A8 and A9 in addition to Conditions A5, A6, and A7. Thus, given the vectors $(\Pi_i |\psi\rangle)\in\mathbb{R}$ which realize the optimal solution in the SDP (13), there exist isometries $V_A$ from $\mathcal{H}_A \otimes \mathcal{K}_A$ to $\mathcal{H}_A'$, $V_B$ from $\mathcal{H}_B \otimes \mathcal{K}_B$ to $\mathcal{H}_B'$, and $V_C$ from $\mathcal{H}_C \otimes \mathcal{K}_C$ to $\mathcal{H}_C'$ such that

\[ V_A \otimes V_B \otimes V_C |\psi\rangle \otimes |junk\rangle = |\psi'\rangle, \]
\[ V_A \otimes V_B \otimes V_C |u_i\rangle \otimes |junk\rangle = |u_i'\rangle, \]

for $i \in \mathcal{I}$, where $|junk\rangle$ is a state on $\mathcal{K}_A \otimes \mathcal{K}_B \otimes \mathcal{K}_C$.

Since $P_{\text{Mermin}}$ is a Gram matrix of vectors $|u_0\rangle, |u_1\rangle, \ldots, |u_{16}\rangle$, rank of $P_{\text{Mermin}}$ is equal to the dimension of the span of $|u_0\rangle, |u_1\rangle, \ldots, |u_{16}\rangle$. As it turns out, the rank of $P_{\text{Mermin}}$ is seven. Thus, a seven-dimensional configuration can achieve the maximal violation of the Mermin inequality. We append a seven-dimensional configuration corresponding to $P_{\text{Mermin}}$ in Appendix C. In the tripartite Bell scenario, one obtains maximal violation of the Mermin inequality using three qubits and thus dimension eight. This is purely because the seven dimensional state can not be realized as tensor product of three two-dimensional subsystems. Moreover, as one can expect, the dimension of the span of the measurement settings in the tensored case, i.e., $\dim(\text{span}(|u_0\rangle, |u_1\rangle, \ldots, |u_{16}\rangle))$ is still seven!

The graph $G_M$ is the complement of Shrikhande graph $[\text{Shr}59]$. Since Shrikhande Graph is vertex transitive, it implies that $G_M$ is also vertex transitive. We observe that there is a unique behaviour in QSTAB $(G_M)$ which achieves $\alpha^*(G_M)$. Moreover, by vertex transitivity in the theta body, we also observe that there is a unique behavior which achieves $\theta(G_M)$.

C. Self-Testing Chained Bell Inequalities

The chained Bell inequalities $[\text{Pea}70, \text{BC}90]$ are defined for the bipartite Bell scenario with N dichotomic measurements per party. In terms of correlations between the observables of Alice and Bob, the chained Bell
inequality for \( N \) settings is given by

\[
I_N^{\text{Refl}} = \langle A_1 B_2 \rangle + \langle A_3 B_2 \rangle + \langle A_3 B_4 \rangle + \langle A_5 B_4 \rangle + \cdots + \langle A_{2N-1} B_{2N} \rangle - \langle A_1 B_2 \rangle \leq_{LHV} 2N - 2. \tag{43}
\]

Here, “LHV” indicates that the local hidden variable bound is \( 2N - 2 \). The observables \( A_i \) and \( B_j \), measured by Alice and Bob, respectively, have outcomes 1 or -1. The correlation terms \( \langle A_i B_j \rangle \) denote the expectation value of the product of outcomes for \( A_i \) and \( B_j \). The maximum quantum value of \( I_N^{\text{Refl}} \) is \( 2N \cos \left( \frac{\pi}{2N} \right) \).

Suppose Alice measures \( A_x \) on her particle and obtains \( a \). Similarly, assume Bob measures \( B_y \) on his particle and obtains \( b \). The probability for the aforementioned event is denoted by \( P(a, b|x, y) \). We can use these probabilities to re-express the correlations as follows:

\[
\langle A_i B_j \rangle = 2P(1, 1|i, j) + 2P(-1, -1|i, j) - 1, \tag{44}
\]

\[
-\langle A_i B_j \rangle = 2P(1, -1|i, j) + 2P(-1, 1|i, j) - 1. \tag{45}
\]

Using Eqs. (44) and (45), we can re-express the inequality in equation (43) as

\[
I_N^{\text{CSW}} = P(1, 1|1, 2) + P(-1, -1|1, 2) + P(1, 1|3, 2) + P(-1, -1|3, 2) + \cdots
\]

\[
+ P(1, 1|2N - 1, 2N) + P(-1, -1|2N - 1, 2N) + P(1, -1|1, 2N) + P(-1, 1|1, 2N) \leq_{LHV} 2N - 1. \tag{46}
\]

The graph of exclusivity for the events in \( I_N^{\text{CSW}} \) is \( C_4 \times N \) and is isomorphic to the Möbius ladder graph of order \( 4N \). The independence number of \( C_4 \times N \) is \( 2N - 1 \). The Lovász theta number, however, remains unknown and has been conjectured \([\text{Ara}14]\) to be equal to

\[
\vartheta(C_4 \times N) = N \left[ 1 + \cos \left( \frac{\pi}{2N} \right) \right]. \tag{47}
\]

Here, we prove that the above conjecture is correct by simple semidefinite programming duality arguments. Moreover, we recover Bell self-testing statements for the chained Bell inequalities for arbitrary \( N \). For the purposes of the proof, we introduce the matrix

\[
Z_N = \begin{bmatrix}
\frac{N}{l} & l \cdot A_{C_4 N} & -e_{1N}^T \\
-e_{1N} & l \cdot f & f \cdot I_{2N} \\
& f \cdot I_{2N} & I_{2N}
\end{bmatrix} \in \mathbb{R}^{(4N+1) \times (4N+1)}, \tag{48}
\]

where \( e_{1N} \) denotes the all-ones column vector of length \( 4N \), \( k = \cos \left( \frac{\pi}{2N} \right) \), \( f = \frac{1-k}{1+k} \), \( l = \frac{1}{1+k} \), \( A_{C_4 N} \) is the adjacency matrix of the cycle graph \( C_4 \times N \), and \( I_{2N} \) is a \( 2N \times 2N \) identity matrix.

**Lemma 12.** \( Z_N \succeq 0 \).

**Proof.** Taking the Schur complement of \( Z_N \) with respect to its top left entry, we have that

\[
Z_N \succeq 0 \iff M_N - \frac{1}{N} e_{1N} e_{1N}^T \succeq 0, \tag{49}
\]

where \( M_N = l \cdot A_{C_4 N} + \begin{bmatrix} I_{2N} & f \cdot I_{2N} \\ f \cdot I_{2N} & I_{2N} \end{bmatrix} \). To prove that \( Z_N \) is positive semidefinite, it remains to show that the eigenvalues of \( M_N - \frac{1}{N} e_{1N} e_{1N}^T \) are non-negative. Notice that \( e_{1N} \) is a common eigenvector of \( M_N \) and \( e_{1N} e_{1N}^T \) as both matrices have the property that the sum of the entries across a row is a constant. Hence, it suffices to compute all the eigenvalues of \( M_N \). The eigenvalues of a circulant matrix are well characterised.

**Fact 1.** The eigenvalues of the circulant matrix

\[
C = \begin{bmatrix}
c_0 & c_{n-1} & \cdots & c_2 & c_1 \\
c_1 & c_0 & c_{n-1} & \cdots & c_2 \\
& \vdots & c_1 & c_0 & \cdots \\
& & c_{n-2} & \cdots & c_{n-1} \\
& & c_{n-1} & c_{n-2} & \cdots & c_1 & c_0
\end{bmatrix} \tag{50}
\]

are given by

\[
\lambda_j = c_0 + c_{n-1} \omega^j + c_{n-2} \omega^{2j} + \cdots + c_1 \omega^{(n-1)j}, \quad j = 0, 1, \ldots, n - 1,
\]

where \( \omega = \exp \left( \frac{2\pi i}{n} \right) \) is the \( n^{th} \) root of unity.
Note that the matrix $M_N$ is a circulant matrix with $n = 4N$, $c_0 = 1$, $c_1 = l$, $c_{2N} = f$, $c_{2N-1} = l$, and $c_i = 0$ for $i \notin \{0, 1, 2N, n-1\}$. Therefore, its eigenvalues are given by $\lambda_j = 1 + l(\omega_j^{(n-1)}j) + f\omega_j^{2Nj}$, for $j = 0, 1, \ldots n-1$. Simplifying this, we obtain

$$\lambda_j = \begin{cases} 1 - f + 2l \cos \frac{j\pi}{2N}, & \text{if } j \text{ is odd}, \\ 1 + f + 2l \cos \frac{j\pi}{2N}, & \text{if } j \text{ is even}. \end{cases}$$ (52)

When $j$ is even, the minimum eigenvalue is when $j = 2N$, for which

$$\lambda_{2N} = 1 + f - 2l = 1 + 1 - k - \frac{2}{1+k} = 0.$$ (53)

When $j$ is odd, the minimum eigenvalue is when $j = 2N - 1$, for which

$$\lambda_{2N-1} = 1 - f + 2l \cos \left(\frac{(2N-1)\pi}{2N}\right) = 1 - f - 2l(1 - \frac{1 - k}{1+k} - \frac{2k}{1+k}) = 0. \quad (54)$$

Finally, note that the eigenvalue of $M_N$ corresponding to the eigenvector $e_{4N}$ is $1 + 2l + f$. Whereas $\frac{1}{N}e_{4N}e_{4N}^T$ is a rank-1 matrix with eigenvector $e_{4N}$ with eigenvalue $\frac{1}{N} \times 4N = 4l$. Therefore, the eigenvalue of $M_N - \frac{1}{N}e_{4N}e_{4N}^T$ corresponding to the eigenvector $e_{4N}$ is $1 + 2l + f - 4l = 1 + f - 2l = 1 + \frac{1 - k}{1+k} - \frac{2k}{1+k} = 0$. The rest of the eigenvalues of $M_N - \frac{1}{N}e_{4N}e_{4N}^T$ are the same as those of $M_N$ and are non-negative as shown above. Hence, all the eigenvalues are non-negative. ■

**Claim 1.** The dual optimal corresponding to the optimization program (10) for $C_{i4N}(1, 2N)$ is $Z^*_N$ (expression 48).

**Proof.** We need to show that

1. $Z^*_N$ is dual feasible for the program in (10).
2. $Z^*_N$ corresponds to dual optimal value.

To show feasibility, we need to show that $Z^*_N$ is of the form as in (10), that is, $Z^*_N = tE_{00} + \sum_{i=1}^n(\lambda_i - 1)E_{ii} - \sum_{i=1}^n\lambda_iE_{0i} + \sum_{i<j}\mu_{ij}E_{ij}$. This is indeed true for the following choice of values: $t = \frac{N}{2}$, $\lambda_i = 2$ for $i = 1, 2, \ldots, 4N$ and $\mu_{ij} = 2f$ whenever $i$ and $j$ share an edge in $C_{4N}$ and $\mu_{ij} = 2f$ for $|i - j| = 2N$. Finally, using Lemma 12, we have $Z^*_N \succ 0$.

Using the measurement settings for chained Bell inequalities in [AQB⁺13], one obtains the output of the primal SDP (2) for $I_{N}^{SW}$ equal to $N[1 + \cos\left(\frac{\pi}{2N}\right)]$. Strong duality for the SDP in (2) implies that $Z^*_N$ corresponds to dual optimal value. ■

The proof of the uniqueness of the primal optimal is similar to the proof corresponding to $n$-cycle graphs in [BRV⁺19b]. Chained Bell Inequalities satisfies Conditions A1 and A2, which can be checked by choosing the vectors in (D3) as follows:

$$a_0 = |A_1 = 1\rangle, \quad a_1 = |A_3 = 1\rangle, \quad a_2 = |A_{2N-1} = -1\rangle, \quad b_0 = |B_2 = 1\rangle, \quad b_1 = |B_{2N} = -1\rangle.$$ (55) (56)

Here, $|A_1 = 1\rangle$ expresses the eigenvector of $A_1$ with eigenvalue 1. This notation is applied to other observables. Since the optimal maximizer given in (14) satisfies conditions A1 and A2 and the vectors $(\Pi_i|\psi')_{i \in \mathcal{I}}$ realize the optimal solution in the SDP (13). In addition, we the ranks of the projections $\Pi^A_i$ and $\Pi^B_i$ are assumed to be one. Thus, there exist isometries $V_A : \mathcal{H}_A \rightarrow \mathcal{H}_A^*$ and $V_B : \mathcal{H}_B \rightarrow \mathcal{H}_B^*$ such that

$$V_A \otimes V_B|\psi\rangle = |\psi'\rangle,$$ (57)

$$V_A \otimes V_B|v_i\rangle = |v'_i\rangle,$$ (58)

for $i \in \mathcal{I}$. This completes the proof of self-testability for the chained Bell inequalities for rank-one projectors.

Since $Z^*_N$ corresponds to dual optimal value, we have $\Psi(C_{i4N}(1, 2N)) = N[1 + \cos\left(\frac{\pi}{2N}\right)]$ as conjectured in [Aral.14].

**D. Abner Shimony Self-Testing**

The Abner Shimony (AS) Bell inequalities [Gis09] refer to a bipartite Bell scenario with an even number $n$ of measurement settings per party. Each measurement has two outcomes. It can be written as

$$AS_n = \sum_{i+j<n} \langle A_iB_j \rangle - \sum_{i+j=n} \min\{i-1, j-1\} \langle A_iB_j \rangle \leq \frac{n(n+2)}{4}. \quad (59)$$

This inequality is satisfied only if the measurement settings corresponding to the left-hand side (LHS) of the inequality are not independent. If the settings are independent, then the inequality is violated by Bell's theorem, which is a new bound on correlations. This inequality is a new bound on correlations and is used to test the Bell inequality.
By taking into account that
\[
\langle A_i B_j \rangle = 2[2P(0,0|i,j) + P(1,1|i,j)] - 1, \tag{60}
\]
\[
-\langle A_i B_j \rangle = 2[2P(0,1|i,j) + P(1,0|i,j)] - 1, \tag{61}
\]
Eq. (59) can be rewritten as
\[
AS_n^c = \sum_{i+j<n} [P(0,0|i,j) + P(1,1|i,j)]
+ \sum_{i+j=n} \min\{i-1, j-1\} [P(0,1|i,j) + P(1,0|i,j)] \leq \frac{n(n+1)}{2}. \tag{62}
\]
For example, for the case \( n = 4 \),
\[
AS_4^c = P(0,0|0,0) + P(1,1|0,0) + P(0,0|0,1) + P(1,1|0,1) + P(0,0|0,2) + P(1,1|0,2)
+ P(0,0|0,3) + P(1,1|0,3) + P(0,0|1,0) + P(1,1|1,0) + P(0,0|1,1) + P(1,1|1,1)
+ P(0,0|1,2) + P(1,1|1,2) + P(0,0|1,3) + P(1,1|1,3) + P(0,0|2,0) + P(1,1|2,0)
+ P(0,0|2,1) + P(1,1|2,1) + 2[P(0,0|2,2) + P(1,1|2,2)] + P(0,0|3,0) + P(1,1|3,0)
+ P(0,0|3,1) + P(1,1|3,1). \tag{63}
\]
The (vertex-weighted) graph of exclusivity of the 26 events in Eq. (63) is shown in Fig. III D and has \( \alpha(G, w) = 10, \ \vartheta(G, w) = 7 + \frac{2\sqrt{21}}{3}, \) and \( \alpha^*(G, w) = 14. \) Notice that the vertex weight is 2 for events \([0,0|2,2]\) and \([1,1|2,2]\) and 1 otherwise.

\[
\left| w_1 \right| = \left| A_0 \right| \otimes \left| A_0 \right|,
\left| w_2 \right| = \left| B_0 \right| \otimes \left| B_0 \right|,
\left| w_3 \right| = \left| A_0 \right| \otimes \left| A_1 \right|,
\left| w_4 \right| = \left| B_0 \right| \otimes \left| B_1 \right|,
\left| w_5 \right| = \left| A_0 \right| \otimes \left| A_2 \right|,
\left| w_6 \right| = \left| B_0 \right| \otimes \left| B_2 \right|,
\left| w_7 \right| = \left| A_0 \right| \otimes \left| A_3 \right|,
\left| w_8 \right| = \left| B_0 \right| \otimes \left| B_3 \right|,
\left| w_9 \right| = \left| A_1 \right| \otimes \left| A_0 \right|,
\left| w_{10} \right| = \left| B_1 \right| \otimes \left| B_0 \right|,
\left| w_{11} \right| = \left| A_1 \right| \otimes \left| A_1 \right|,
\left| w_{12} \right| = \left| B_1 \right| \otimes \left| B_1 \right|,
\left| w_{13} \right| = \left| A_1 \right| \otimes \left| A_2 \right|,
\left| w_{14} \right| = \left| B_1 \right| \otimes \left| B_2 \right|,
\left| w_{15} \right| = \left| A_1 \right| \otimes \left| A_3 \right|,
\left| w_{16} \right| = \left| B_1 \right| \otimes \left| B_3 \right|,
\left| w_{17} \right| = \left| A_2 \right| \otimes \left| A_0 \right|,
\left| w_{18} \right| = \left| B_2 \right| \otimes \left| B_0 \right|,
\left| w_{19} \right| = \left| A_2 \right| \otimes \left| A_1 \right|,
\left| w_{20} \right| = \left| B_2 \right| \otimes \left| B_1 \right|,
\left| w_{21} \right| = \left| A_2 \right| \otimes \left| A_2 \right|,
\left| w_{22} \right| = \left| B_2 \right| \otimes \left| B_2 \right|,
\left| w_{23} \right| = \left| A_3 \right| \otimes \left| A_0 \right|,
\left| w_{24} \right| = \left| B_3 \right| \otimes \left| B_0 \right|,
\left| w_{25} \right| = \left| A_3 \right| \otimes \left| A_1 \right|,
\left| w_{26} \right| = \left| B_3 \right| \otimes \left| B_1 \right|. \tag{64}
\]

The violation of the Bell inequality \( AS_n^c \) can achieve \( \vartheta(G, w) \) by choosing as initial state
\[
|s\rangle = \cos t(|00\rangle - |11\rangle) + \sin t(|01\rangle - |10\rangle), \tag{65}
\]
and as local measurements
\[
A_i = |m(\alpha_i)\rangle, B_i = |m(\pi/2 + \alpha_i)\rangle. \tag{66}
\]
with $i = 0, 1, 2, 3$, $m(\alpha) = \cos \alpha |0\rangle + \sin \alpha |1\rangle$, and

$$
\alpha_0 = 0, \quad \alpha_1 = \arcsin \left( \frac{1}{\sqrt{6}} \right), \quad \alpha_2 = \frac{1}{2} \left( \pi - \arctan \left( \frac{5\sqrt{145}}{8} + \frac{77}{8} \right) \right),
$$

$$
\alpha_3 = \frac{1}{2} \left( \pi - \arctan \left( 48 \sqrt{\frac{2}{275\sqrt{145} + 3317}} \right) \right), \quad t = \frac{1}{8} \left( \alpha_2 + 2\alpha_4 - \frac{\pi}{2} \right).
$$

The primal optimal for the SDP corresponding to the quantum violation of $AS_c^4$ can be obtained by the state and measurement directions given in Eqs. (65)–(67). Here, we omit its expression, as it is lengthy and complex. The proof of the uniqueness of the primal optimal is similar as in previous cases.

The local projective measurements satisfy Conditions A1 and A2, which can be checked by choosing the vectors in (D3) as follows:

$$
a_0 = |A_2 = 0\rangle, \quad a_1 = a_2 = |A_3 = 0\rangle, \quad b_0 = |B_0 = 0\rangle, \quad b_1 = |B_1 = 0\rangle.
$$

Here, $|A_1 = 1\rangle$ expresses the eigenvector of $A_1$ with eigenvalue 1. This notation is applied to other observables. Since the optimal maximizer given in (14) satisfies conditions A1 and A2 and the vectors $(\Pi_i |\psi\rangle)_{i \in I}$ realize the optimal solution in the SDP (13). In addition, we the ranks of the projections $\Pi_A^i$ and $\Pi_B^i$ are assumed to be one. Thus, there exist isometries $V_A : \mathcal{H}_A \to \mathcal{H}'_A$ and $V_B : \mathcal{H}_B \to \mathcal{H}'_B$ such that

$$
V_A \otimes V_B |\psi\rangle = |\psi\rangle',
$$

$$
V_A \otimes V_B |\nu_i\rangle = |\nu_i\rangle',
$$

for $i \in I$. This completes the proof of self-testability for the $AS_c^4$ Bell inequality for rank-one projectors.

### IV. SUMMARY AND OPEN PROBLEMS

In this work, we introduced a graph-theoretic approach to self-testing in Bell scenarios, combining ideas from graph theory and semidefinite programming. The motivation was the observation that the set of quantum correlations for a Bell scenario is, in general, difficult to characterize while, using ideas from [CSW14], one can provide an easy to characterize single SDP-based relaxation of this set. By proving self-testing for the maximizer of a Bell inequality with respect to the aforementioned set, we furnish self-testing for the set of quantum correlations for the underlying Bell scenario.

Our method requires that the quantum bound of the Bell inequality is equal to the Lovász theta number of the vertex-weighted graph of exclusivity of the events appearing in the Bell witness, when written as a positive linear combination of probabilities of events. As we have seen, this is frequently the case. Our other assumptions
involves some particular relation among the local projective measurements involved in the scenario as mentioned in Theorems 7, 8, 10 and 11. In future, it would be interesting to simplify our assumptions involving relation among local projective measurements.

We applied our technique to the CHSH, chained and three-party Mermin Bell inequalities. For CHSH and the trpartite Mermin case, we recovered self-testing results for projectors of arbitrary rank. For chained Bell inequalities, our self-testing statements hold for rank-one projectors. For the Mermin three-party case, the primal optimal matrix’s rank is seven, indicating that the self-testing preparation dimension can be seven. However, in the Bell scenario, the underlying dimension has to be eight due to the tensor structure. We also applied our method to the previously not-known case of AS inequalities and provided a self-testing statement for the case of rank-one projectors.

While delivering the self-testing statement for the chained-Bell inequality via our graph-theoretic framework, we also obtained a closed-form expression for the Lovász theta number for Möbius ladder graphs. Our closed-form expression matches with the conjecture of [Ara14].

Our methods belong in the intersection region of graph theory, Bell non-locality, and contextuality. Our results provide further motivation to study Bell self-testing via the graph-theoretic framework in the future. Furthermore, we believe that techniques such as ours could be used in the future to study open problems in graph theory taking advantage of ideas from quantum theory.

A natural next step in our program would be to generalize our result for scenarios with noise. In other words, a graph-theoretic approach to robust Bell self-testing.

The graph-theoretic approach has been employed to study self-testing in Bell scenarios and in contextuality scenarios with sequential measurements. It will be interesting to see if the techniques based on graph theory could be also useful for self-testing in prepare and measure scenarios. In future, it would be interesting to extend our self-testing statements for chained Bell and AS inequalities for arbitrary rank projectors.

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A graph $G = (V,E)$ consists of a set of vertices $V$ and edges $E$ \cite{W01}. Two vertices are adjacent if they share an edge between them. The complement graph $\bar{G}$ has same vertices as $G$, but its edge set is complement of the set $E$. A clique of a graph is set of pairwise adjacent vertices. The complement of clique is a set of vertices that are pairwise non-adjacent. A natural generalization of graph is hypergraph with generalized edges connecting more than two vertices. These generalized edges are called hyperedges.

**Definition 13.** (Cyclic graph) Given a graph with $n$ vertices such that every $i$th vertex of the graph is connected to $(i+1)\mod n$th vertex and $(i-1)\mod n$th vertex is called cyclic graph and denoted as $C_n$.

An elegant generalization of the concept of cyclic graph is the concept of circulant graph, which is defined below.

**Definition 14.** (Circulant graph) Given a list $[L]$ of integers, a graph with $n$ vertices where $i$th vertex is connected to $(i+1)\mod n$th and $(i-l)\mod n$th vertices for all $l \in [L]$, is referred as circulant graph $Ci_n[L]$. $Ci_n[1]$ graphs are called cyclic graphs.

**Definition 15.** (Orthonormal representation of a graph \cite{Lov79}) An orthonormal representation of a graph is an assignment of unit vectors $|v_i\rangle \in \mathbb{R}^d$ to every vertex $i \in V$ such that
\begin{equation}
\langle v_i|v_j \rangle = 0, \forall i, j \notin E. \tag{A1}
\end{equation}
We will use the notation $\text{OR}(G)$ to represent the orthonormal representation of $G$.

**Definition 16.** (Stable set) Stable set is a set of vertices of a graph such that no two vertices which lie in it share an edge.

**Definition 17.** (Independence number) Independence number of a graph is the cardinality of the largest stable set of the graph. We will denote it by $\alpha(G)$.

**Definition 18.** (Convex hull) Convex hull of a set $A$ is the smallest convex set containing $A$.

**Definition 19.** (Incidence vector) An Incidence vector of a set $B \subset A$ is a vector $P \in \mathbb{R}^{|A|}$ such that for every $i \in A$,
\begin{equation}
P_i = \begin{cases} 
1 & \text{if } i \in B, \\
0 & \text{otherwise}. 
\end{cases} \tag{A2}
\end{equation}

**Definition 20.** (Stable set polytope) The convex hull of all the incidence vectors of stable sets of graph $G$ is called stable set polytope of graph. It is denoted by $\text{STAB}(G)$.

**Definition 21.** (Theta body) Let $\{|v_i\rangle\}$ corresponds to the orthonormal representation of $G$. Given a unit vector $|\phi\rangle = (1,0,0,\cdots,0) \in \mathbb{R}^d$ with only first co-ordinate 1 and rest 0, the Theta body of graph $G$ is defined as
\begin{equation}
\text{TH}(G) = \{P \in \mathbb{R}^{|V|} : P_i = |\langle \psi|v_i \rangle|^2\}. \tag{A3}
\end{equation}

**Definition 22.** (Lovász theta number \cite{Lov79}) The Lovász theta number $\vartheta(G)$ of a graph $G$ is defined as follows:
\begin{equation}
\vartheta(G) = \max_{|\phi\rangle,\{|v_i\rangle\}} \sum_i |\langle \phi|v_i \rangle|^2,
\end{equation}
where $|\phi\rangle$ is a unit vector and $\{|v_i\rangle\}$ is an orthonormal representation of the graph $G$. $|\phi\rangle$ is also known as handle.

**Definition 23.** (Fractional stable set polytope) The fractional stable set polytope is given by
\begin{equation}
\text{QSTAB}(G) = \left\{ P \in \mathbb{R}^{|V|} : \sum_{i \in C} P_i \leq 1 \text{ for every clique } C \text{ of graph } G \right\}. \tag{A4}
\end{equation}
Definition 24. (Fractional packing number) The fractional packing of a graph $G$ is the value of the following linear program:

$$\alpha^*(G) = \max \left\{ \sum_{i=1}^{n} x_i : x \in \text{QSTAB}(G) \right\}.$$

Definition 25. (Gram matrix and Gram decomposition) Given a set of vectors $v_1, v_2, \ldots, v_k$ in an inner product space, the corresponding Gram matrix is a Hermitian matrix $X$, defined via their inner products such that $X_{i,j} = \langle v_i, v_j \rangle$ for $i, j \in \{1, 2, \ldots, n\}$. It is important to note that rank $X = \dim \text{span} (v_1, v_2, \ldots, v_k)$.

Decomposing Gram matrix $X$ such that $X = AA^\dagger$ is called Gram decomposition of $X$. The rows of $A$ are related to $v_i$ up to isometry.

Definition 26. (Vertex-transitive graph) A graph $G = (V, E)$ is called vertex transitive, if given any two vertices $v_1, v_2 \in V$ there exists an automorphism $h: V \to V$ such that $h(v_1) = v_2$.

Fact 2. [Lov79] For a given graph $G$, $\alpha(G) \leq \vartheta(G) \leq \alpha^*(G)$.

It is worthwhile to note that $\text{STAB}(G) \subseteq \text{Th}(G) \subseteq \text{QSTAB}(G)$ [Knu94]. An alternate formulation of the theta body of a graph $G = ([n], E)$ is given by:

$$\text{Th}(G) = \{ x \in \mathbb{R}_+^n : \exists X \in \mathbb{S}^{1+n}_+, X_{00} = 1, X_{ii} = X_{0i}, X_{ij} = 0, \forall ij \in E \}.$$  

(A6)

Lemma 27. [RBBZ21] We have that $x \in \text{Th}(G)$ iff there exist unit vectors $d, w_1, \ldots, w_n$ such that

$$x_i = \langle d, w_i \rangle^2, \forall i \in [n] \text{ and } \langle w_i, w_j \rangle = 0, \text{ for } ij \in E.$$  

(A7)

Appendix B: Mermin inequality

Mermin’s Bell inequality [Mer90] refers to a $n$-partite Bell scenario (with $n \geq 3$ odd; there is also a version for $n$ even [Ard92], but we won’t consider it here). The interest of this Bell inequality is based on the fact that the Bell operator

$$S_n = \frac{1}{2^n} \left[ \bigotimes_{j=1}^{n} (\sigma_x^{(j)} + i\sigma_y^{(j)}) - \bigotimes_{j=1}^{n} (\sigma_x^{(j)} - i\sigma_y^{(j)}) \right],$$  

(B1)

where $\sigma_x^{(j)}$ is the Pauli matrix $x$ for qubit $j$, has an eigenstate with eigenvalue $2^{(n-1)}$. In contrast, for local hidden-variable (LHV) and non-contextual hidden-variable (NCHV) theories, $S_n \leq \sigma^{(n-1)/2}$.

(B2)

For example,

$$S_3 = \sigma_x^{(1)} \otimes \sigma_x^{(2)} \otimes \sigma_x^{(3)} + \sigma_x^{(1)} \otimes \sigma_z^{(2)} \otimes \sigma_z^{(3)} + \sigma_z^{(1)} \otimes \sigma_x^{(2)} \otimes \sigma_z^{(3)}.$$  

(B3)

Therefore, we can write (using obvious notation),

$$\langle S_3 \rangle = \langle ZXX \rangle + \langle XZX \rangle + \langle XZX \rangle - \langle ZZZ \rangle.$$  

(B5)

Then, by taking into account that

$$\langle ZXX \rangle = P(Z = X = X = 1) + P(Z = X = -X = -1) + P(Z = -X = X = -1) + P(-Z = X = X = 1)$$

$$-P(Z = X = X = -1) - P(Z = X = -X = 1) - P(Z = -X = X = 1) - P(-Z = X = X = 1)$$

$$= 2[P(Z = X = X = 1) + P(Z = X = -X = -1) + P(Z = -X = X = -1) + P(-Z = X = X = 1)] - 1,$$

$$\langle XZX \rangle = P(X = Z = X = 1) + P(X = Z = -X = -1) + P(X = -X = Z = -1) + P(-X = Z = Z = 1)$$

$$-P(X = Z = Z = -1) - P(X = Z = Z = 1) - P(X = Z = Z = 1) - P(X = Z = Z = 1)$$

$$= 2[P(X = Z = X = 1) + P(X = Z = -X = -1) + P(X = Z = Z = 1) + P(-X = Z = X = 1)] - 1,$$

$$\langle XZX \rangle = P(X = X = Z = 1) + P(X = Z = Z = 1) + P(X = Z = Z = 1) + P(-X = X = Z = 1)$$

$$-P(X = X = Z = 1) - P(X = X = Z = 1) - P(X = Z = Z = 1) - P(X = Z = Z = 1)$$

$$= 2[P(Z = X = Z = 1) + P(Z = Z = Z = 1) + P(Z = Z = Z = 1) + P(-Z = Z = Z = 1)] - 1,$$

$$-\langle ZZZ \rangle = P(Z = Z = Z = 1) + P(Z = Z = Z = 1) + P(Z = Z = Z = 1) + P(-Z = Z = Z = 1)$$

$$-P(Z = Z = Z = 1) - P(Z = Z = Z = 1) - P(Z = Z = Z = 1) - P(-Z = Z = Z = 1)$$

$$= 2[P(Z = Z = Z = 1) + P(Z = Z = Z = 1) + P(Z = Z = Z = 1) + P(-Z = Z = Z = 1)] - 1,$$
we can rewrite $\langle S_4 \rangle$ as a sum of the probabilities of 16 events. That is,

$$\langle S_4 \rangle = 2 \left[ P(Z = X = X = 1) + P(Z = X = -X = -1) + P(Z = -X = X = -1) + P(-Z = X = X = -1) 
+ P(X = Z = X = 1) + P(X = Z = -X = -1) + P(X = -Z = X = -1) + P(-X = Z = X = -1) 
+ P(X = X = Z = 1) + P(X = X = -Z = -1) + P(X = -X = Z = -1) + P(-X = X = Z = -1) 
+ P(Z = Z = Z = -1) + P(Z = Z = -Z = 1) + P(Z = -Z = Z = 1) + P(-Z = Z = Z = 1) \right] - 4.$$  

The graph of exclusivity of these 16 events is the complement of Shrikhande graph [Shr59].

This graph, shown in Fig. III B, has $\alpha = 3$ and $\theta = \alpha^* = 4$. Similarly, one can obtain the graph corresponding to any $\langle S_n \rangle$.

Appendix C: Seven dimensional configuration for the Mermin case

We have obtained numerically (rounded up to three digits after decimal) the following seven dimensional configuration achieving the Lovázs theta number of the graph in Fig. III B.

$$|u_0\rangle = (1, 0, 0, 0, 0, 0, 0)^T,$$
$$|u_1\rangle = (0.25, -0.113, -0.241, 0.284, 0.088, 0.166, -0.029)^T,$$
$$|u_2\rangle = (0.25, -0.110, -0.251, -0.120, 0.247, -0.021, -0.191)^T,$$
$$|u_3\rangle = (0.25, -0.292, 0.079, 0.151, 0.075, -0.051, -0.255)^T,$$
$$|u_4\rangle = (0.25, 0.182, -0.087, 0.003, 0.311, 0.215, 0.059)^T,$$
$$|u_5\rangle = (0.25, -0.226, 0.069, 0.104, -0.227, 0.262, -0.021)^T,$$
$$|u_6\rangle = (0.25, 0.223, -0.059, 0.300, 0.068, -0.075, 0.184)^T,$$
$$|u_7\rangle = (0.25, -0.004, -0.232, 0.130, -0.298, 0.001, 0.167)^T,$$
$$|u_8\rangle = (0.25, -0.247, 0.049, -0.152, 0.140, -0.278, 0.059)^T,$$
$$|u_9\rangle = (0.25, 0.251, -0.059, -0.252, 0.019, 0.091, -0.222)^T,$$
$$|u_{10}\rangle = (0.25, 0, -0.242, -0.274, -0.139, -0.186, 0.004)^T,$$
$$|u_{11}\rangle = (0.25, 0.069, 0.271, 0.019, -0.154, 0.062, -0.285)^T,$$
$$|u_{12}\rangle = (0.25, 0.044, 0.261, 0.167, 0.054, -0.291, -0.042)^T,$$
$$|u_{13}\rangle = (0.25, 0.069, 0.223, -0.178, -0.004, 0.312, 0.067)^T,$$
$$|u_{14}\rangle = (0.25, 0.045, 0.212, -0.030, 0.204, -0.042, 0.310)^T,$$
$$|u_{15}\rangle = (0.25, -0.182, 0.039, -0.200, -0.161, 0.035, 0.293)^T,$$
$$|u_{16}\rangle = (0.25, 0.291, -0.031, 0.046, -0.225, -0.199, -0.097)^T.$$  

Appendix D: Proofs of Self-testing

We consider two types of sets of indexes $I$ and $I_0 = I \cup \{0\}$. We consider the matrix $X_{ij} := \langle \psi | \Pi_i \Pi_j | \psi \rangle$, where $\Pi_i$ is a projection and $\Pi_0$ is the identity operator. We set $n := |I|$. Then, we assume that the following SDP has the unique solution.

$$\vartheta(G_{\text{ox}}, w) = \max \sum_{i \in I} w_i X_{ii}$$

s.t. $X_{ii} = X_{0i}, \forall i \in [n],$

$$X_{ij} = 0, \forall i \sim j,$$

$$X_{00} = 1, X \in S^{1+n}_+.$$
1. Bipartite case

We assume that the unique optimal maximizer \( X^* = (X_{ij}) \) is given by \( \eta_i \eta_j \langle v_j, v_i \rangle \) with the following: For \( i = (i_A, i_B) \in I \),

\[
v_i = a_{i_A} \otimes b_{i_B},
\]

where \( a_{i_A} \in \mathcal{H}_A = \mathbb{C}^{d_A}, b_{i_B} \in \mathcal{H}_B = \mathbb{C}^{d_B}. \) Also, for simplicity, \( a_{i_A} \) and \( b_{i_B} \) are assumed to be normalized and \( \eta_k > 0. \)

Now, we consider a state \(| \psi' \rangle \) on \( \mathcal{H}_A \otimes \mathcal{H}_B \) and projections \( \Pi^A_i \) and \( \Pi^B_i \) on \( \mathcal{H}_A \) and \( \mathcal{H}_B \). Here, when \( i_A = i_A' \) \( (i_B = i_B') \) for \( i \neq i' \), \( \Pi^A_i = \Pi^A_{i_A} \) \( (\Pi^B_i = \Pi^B_{i_B}) \). Then, we define the projection \( \Pi_i := \Pi^A_i \otimes \Pi^B_i \).

In the following, we discuss how the state \(| \psi' \rangle \) is locally converted to \(| \psi \rangle \) when the vectors \( \Pi_i | \psi' \rangle \) realize the optimal solution in the SDP \( (D1) \). We define \( | \psi' \rangle := \eta_i^{-1} \Pi_i | \psi \rangle \).

a. Rank-one case

First, we consider the case that the ranks of the projections \( \Pi^A_{i_A} \) and \( \Pi^B_{i_B} \) are one. We introduce the following conditions.

A1 The set \( \{v_i\}_{i \in I_0} \) of vectors span the vector space \( \mathcal{H}_A \otimes \mathcal{H}_B \).

A2 There exist a subset \( I_B \) of indexes of the space \( \mathcal{H}_B \) with \( |I_B| = d_B = \dim \mathcal{H}_B \) and \( d_B \) sets \( \{I_A, i_B\}_{i_B \in I_B} \) of indexes of the space \( \mathcal{H}_A |I_A, i_B| = d_A = \dim \mathcal{H}_A \) to satisfy the following conditions B1-B4.

B1 \( \cup_{i_B \in I_B} I_A, i_B \times \{i_B\} \subset I \).

B2 \( \{b_{i_B}\}_{i_B \in I_B} \) spans the space \( \mathcal{H}_B \).

B3 \( \{a_{i_A}\}_{i_A \in I_A, i_B} \) spans the space \( \mathcal{H}_A \) for any \( i_B \in I_B \).

B4 We define the graph on \( I_B \) in the following way. This graph cannot be divided. \( i_B \in I_B \) is connected to \( i_B' \in I_B \) when the following two conditions holds.

B4-1 The relation \( \langle b_{i_B}, b_{i_B'} \rangle \neq 0 \) holds.

B4-2 The relation \( I_{A, i_B} \cap I_{A, i_B'} \neq \emptyset \) holds.

In the two qubit case, if The set \( \{v_i\}_{i \in I} \) of vectors contains the following 4 vectors, then the conditions A1 and A2 hold;

\[
a_0 \otimes b_0, \ a_1 \otimes b_0, \ a_0 \otimes b_1, \ a_2 \otimes b_1,
\]

where \( a_0 \neq a_1, a_2, \ (b_0, b_1) \neq 0. \)

**Example 1.** CHSH inequality satisfies Conditions A1 and A2, which can be checked by choosing the vectors in \( (D3) \) as follows:

\[
a_0 = |A_{0,0} \rangle, \ a_1 = a_2 = |A_{0,1} \rangle, \quad b_0 = |B_{0,0} \rangle, \ b_1 = |B_{1,0} \rangle.
\]

**Example 2.** Chained Bell inequalities satisfies Conditions A1 and A2, which can be checked by choosing the vectors in \( (D3) \) as follows:

\[
a_0 = |A_{1} = 1 \rangle, \ a_1 = |A_{3} = 1 \rangle, \ a_2 = |A_{2N-1} = -1 \rangle, \quad b_0 = |B_{2} = 1 \rangle, \ b_1 = |B_{2N} = -1 \rangle.
\]

In this example and the next example, \(|A_1 = 1 \rangle \) expresses the eigenvector of \( A_1 \) with eigenvalue 1. This notation is applied to other observables.

**Example 3.** Abner Shimony Self-Testing satisfies Conditions A1 and A2, which can be checked by choosing the vectors in \( (D3) \) as follows:

\[
a_0 = |A_{2} = 0 \rangle, \ a_1 = a_2 = |A_{3} = 0 \rangle, \quad b_0 = |B_{0} = 0 \rangle, \ b_1 = |B_{1} = 0 \rangle.
\]
Theorem 28. Assume that the optimal maximizer given in (D2) satisfies conditions A1 and A2 and the vectors $(\Pi_i|\psi')_{i \in \mathcal{I}}$ realize the optimal solution in the SDP (D1). In addition, the ranks of the projections $\Pi^A_{i_A}$ and $\Pi^B_{i_B}$ are assumed to be one. Then, there exist isometries $V_A : \mathcal{H}_A \rightarrow \mathcal{H}'_A$ and $V_B : \mathcal{H}_B \rightarrow \mathcal{H}'_B$ such that

$$V_A \otimes V_B|\psi\rangle = |\psi\rangle, \quad \Pi_i \otimes \Pi_i|\psi\rangle = |\psi\rangle,$$

for $i \in \mathcal{I}$.

Proof. Since the vectors $\Pi_i|\psi\rangle$ realize the optimal solution in the SDP (D1), there exists a isometry $V$ from $\mathcal{H}_A \otimes \mathcal{H}_B$ to $\mathcal{H}'_A \otimes \mathcal{H}'_B$ such that

$$\Pi_i|\psi\rangle = \Pi_i|\psi\rangle$$

for $i \in \mathcal{I}$. We denote $\Pi_i|\psi\rangle = \eta_i |a^\prime_{i_A} \otimes b^\prime_{i_B}\rangle$.

We fix an arbitrary element $i_B \in \mathcal{I}_B$. For $i_A, i'_A \in \mathcal{I}_{A,i_B}$, Condition A1 implies

$$\langle b_{i_B}, b_{i'_B}\rangle = \langle a_{i_A} \otimes b_{i_B}, a'_{i_A} \otimes b_{i'_B}\rangle = \langle a'_{i_A} \otimes b'_{i_B}, a'_{i_A} \otimes b'_{i'_B}\rangle = \langle b'_{i_B}, b'_{i'_B}\rangle.$$

Hence, there exists an isometry $V_{A,i_B} : \mathcal{H}_A \rightarrow \mathcal{H}'_A$ such that

$$V_{A,i_B}|a_{i_A}\rangle = |a'_{i_A}\rangle$$

for $i_A \in \mathcal{I}_{A,i_B}$.

We choose two connected elements $i_B, i'_B \in \mathcal{I}_B$. For $i_A \in \mathcal{I}_{A,i_B} \cap \mathcal{I}_{A,i'_B}$, (D12) implies

$$\langle b_{i_B}, b_{i'_B}\rangle = \langle a_{i_A} \otimes b_{i_B}, a_{i_A} \otimes b_{i'_B}\rangle = \langle a'_{i_A} \otimes b'_{i_B}, a'_{i_A} \otimes b'_{i'_B}\rangle = \langle b'_{i_B}, b'_{i'_B}\rangle.$$

Hence, for $i_A \in \mathcal{I}_{A,i_B}$ and $i'_A \in \mathcal{I}_{A,i'_B}$, (D12) implies

$$\langle a_{i_A}, a'_{i_A}\rangle \langle b_{i_B}, b_{i'_B}\rangle = \langle (a_{i_A} \otimes b_{i_B}), (a_{i_A} \otimes b_{i'_B}) = \langle (a'_{i_A} \otimes b'_{i_B}), (a'_{i_A} \otimes b'_{i'_B}) = \langle (b'_{i_B}, b'_{i'_B}).$$

Since Condition B4-1 guarantees $\langle b_{i_B}, b_{i'_B}\rangle \neq 0$, the combination of (D15) and (D16) implies that

$$\langle a_{i_A}, a'_{i_A}\rangle = \langle a'_{i_A}, a'_{i_A}\rangle.$$

Hence, we find that $V_{A,i_B} = V_{A,i'_B}$. Since the graph defined in B4 is not divided, all isometries $V_{A,i_B}$ are the same. We denote it by $V_A$.

We choose arbitrary two elements $i_B, i'_B \in \mathcal{I}_B$. We choose elements $i_A, i'_A \in \mathcal{I}_{A,i_B}$ and $i'_A \in \mathcal{I}_{A,i'_B}$ such that

$$\langle a_{i_A}, a'_{i_A}\rangle \neq 0.$$

Condition A1 implies

$$\langle a_{i_A}, a'_{i_A}\rangle \langle b_{i_B}, b_{i'_B}\rangle = \langle a_{i_A} \otimes b_{i_B}, a'_{i_A} \otimes b_{i'_B}\rangle = \langle a'_{i_A} \otimes b'_{i_B}, a'_{i_A} \otimes b'_{i'_B}\rangle$$

$$= \langle a'_{i_A}, a'_{i_A}\rangle \langle b'_{i_B}, b'_{i'_B}\rangle = \langle V_A a_{i_A}, V_A a'_{i_A}\langle b'_{i_B}, b'_{i'_B}\rangle = \langle a_{i_A}, a'_{i_A}\rangle \langle b'_{i_B}, b'_{i'_B} \rangle,$$

the combination of (D18) and (D19) implies that

$$\langle b_{i_B}, b_{i'_B}\rangle = \langle b'_{i_B}, b'_{i'_B}\rangle.$$

Hence, there exists an isometry $V_B : \mathcal{H}_B \rightarrow \mathcal{H}'_B$ such that

$$V_B|b_{i_B}\rangle = |b'_{i_B}\rangle$$

for $i_B \in \mathcal{I}_B$.

Since $\{a_{i_A} \otimes b_{i_B}\}_{i_A \in \mathcal{I}_{A,i_B}, i_B \in \mathcal{I}_B}$ spans $\mathcal{H}_A \otimes \mathcal{H}_B$, we have $V = V_A \otimes V_B.$

\[\square\]
We consider the general case. In addition to A1 and A2, we assume the following condition.

**A3** Ideal systems $\mathcal{H}_A$ and $\mathcal{H}_B$ are two-dimensional.

**A4** Each system has only two measurements. That is, the set $\mathcal{I}_A$ ($\mathcal{I}_B$) of all indexes of the space $\mathcal{H}_A$ ($\mathcal{H}_B$) is composed of 4 elements. For any element $i_A \in \mathcal{I}_A$ ($i_B \in \mathcal{I}_B$), there exists an element $i'_A \in \mathcal{I}_A$ ($i'_B \in \mathcal{I}_B$) such that $(a_{i_A}|a_{i'_A}) = 0$ ($|b_{i_B}|b_{i'_B}) = 0$).

When A3 and A4 hold, $\mathcal{I}_A$ ($\mathcal{I}_B$) is written as $B_{A,0} \cup B_{A,1}$ ($B_{B,0} \cup B_{B,1}$), where $B_{A,j} = \{(0,j),(1,j)\}$ ($B_{B,j} = \{(0,j),(1,j)\}$) and $|\langle a_{(0,j)}|a_{(1,j)}\rangle| = 0$ ($|\langle b_{(0,j)}|b_{(1,j)}\rangle| = 0$) for $j = 0, 1$.

While CHSH inequality, Chained Bell inequalities, and Abner Shimony Self-Testing satisfy Conditions A1 and A2, only CHSH inequality satisfies Conditions A3 and A4.

We also consider the following condition for $\Pi = \Pi_{A,n} \otimes \Pi_{B,n}$.

**C1** When $i_A, i'_A \in \mathcal{I}_A$ ($i_B, i'_B \in \mathcal{I}_B$) satisfy $(a_{i_A}|a_{i'_A}) = 0$ ($|b_{i_B}|b_{i'_B}) = 0$), we have $\Pi_{A} + \Pi_{A}' = I$ ($\Pi_{B} + \Pi_{B}' = I$).

Let $\Pi_{A}$ and $\Pi_{B}$ be the image of the projections $\Pi_{A}$ and $\Pi_{B}$.

**Theorem 29.** Assume that the optimal maximizer given in (D2) satisfies conditions A1, A2, A3, and A4, the vectors $(\Pi_i|\psi_i)^{i \in \mathcal{I}}$ realize the optimal solution in the SDP (D1), and condition C1 holds. Then, there exist isometries $V_A$ from $\mathcal{H}_A \otimes K_A$ to $\mathcal{H}_A'$ and $V_B$ from $\mathcal{H}_B \otimes K_B$ to $\mathcal{H}_B'$ such that

$$V_A \otimes V_B|\psi_i\rangle \otimes |junk\rangle = |\psi_i\rangle, \quad (D22)$$

$$V_A \otimes V_B|\psi_i\rangle \otimes |junk\rangle = |\psi_i\rangle, \quad (D23)$$

for $i \in \mathcal{I}$, where $|junk\rangle$ is a state on $K_A \otimes K_B$.

**Lemma 30.** Assume that the vectors $(\Pi_i|\psi_i)^{i \in \mathcal{I}}$ realize the optimal solution in the SDP (D1). Assume that a projection $\Pi_i$ is commutative with $\Pi_j$ for any $i, j \in \mathcal{I}$. Also assume that $\Pi_i \psi_i \neq 0$. Let $\psi_i(\Pi_i)$ be the normalized vector of $\Pi_i \psi_i$. Then, the vectors $\Pi_i|\psi_i(\Pi_i)\rangle$ realize the optimal solution in the SDP (D1).

Proof of Theorem 29:

**Step 1:** Let $P_{A,(0)\{0,1\},(0)}$ be the projection to the eigenspace of $\Pi_{A,(0)}^{(0)} \Pi_{A,(1)}^{(1)} \Pi_{A,(0)}^{(0)}$ with one eigenvalue. Let $P_{A,(0)\{0,1\},(1)}$ be the projection to the eigenspace of $\Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$ with zero eigenvalue. Let $\{e_{j_A}\}$ be orthogonal basis corresponding to orthogonal eigenvectors of $\Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$ with other eigenvalues. We define $f_{j_A}$ as the normalized vector of $\Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$.

For $j_A \neq j'_A$, $f_{j_A}$ is orthogonal to $f_{j'_A}$ due to the choice of $\{e_{j_A}\}$. We define $g_{j_A}$ as the normalized vector of $f_{j_A} - (e_{j_A} | f_{j_A}) e_{j_A}$. $g_{j_A}$ belongs to $\mathcal{H}_{A,(0)}^{(0)}$. For $j_A \neq j'_A$, $g_{j_A}$ is orthogonal to $g_{j'_A}$ because $e_{j_A}$ and $f_{j_A}$ are orthogonal to $e_{j_A}$ and $f_{j_A}$, respectively. We define the projection $\Pi_{j_A} := |\langle e_{j_A}|e_{j_A}\rangle + |\langle g_{j_A}|g_{j_A}\rangle|$. For $j_A \neq j'_A$, we have $\Pi_{j_A} \Pi_{j_A}^{(0)} = 0$. $\Pi_{j_A}$ is commutative with $\Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$, $\Pi_{A,(0)}^{(0)}$, and $\Pi_{A,(0)}^{(0)}$. For $j_A \neq j'_A$, $\Pi_{j_A} \Pi_{j_A}^{(0)} = 0$. $\Pi_{j_A}$ is commutative with $\Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$.

Since $(I - \Pi A^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}) = 0 \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$ and $\Pi_{j_A}$ is commutative with $\Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)} \Pi_{A,(0)}^{(0)}$.
Thus, there exists isometries $\Pi, \psi$. Due to Lemma 30, the vectors $\Pi_i \psi(2, j_B, j_B')$ realize the optimal solution in the SDP (D1). Also, $\Pi, \Pi_1, \psi$ is rank-one. Hence, we can apply Theorem 28 to the vectors $\Pi_1 \psi(2, j_B, j_B')$. Thus, there exists isometries $V_{A, j_B, j_B'}$ such that

$$V_{A, j_B, j_B'} = \Pi_1 \psi(2, j_B, j_B').$$

As shown in Step 3, for $j_B \neq j_B'$, we have $V_{A, j_B, j_B'} = \beta_{j_B, j_B'} V_{A, j_B, j_B'}$ with a constant $\beta_{j_B, j_B'}$ when $\Pi(2, j_B, j_B') \neq 0$ and $\Pi(2, j_B, j_B') \neq 0$. That is,

$$V_{A, j_B, j_B'} = \beta_{j_B, j_B'} V_{A, j_B, j_B'}.$$

Then, for $j_B$, we choose an element $j_B$ such that $\Pi(2, j_B, j_B') \neq 0$. Then, we define $V_{A, j_B} = V_{A, j_B, j_B'}$. Thus, for elements $j_B$ and $j_B'$, there exists an constant $\beta_{j_B, j_B'}$ such that

$$V_{A, j_B} \otimes V_{B, j_B'} = \beta_{j_B, j_B'} V_{A, j_B, j_B'}.$$

Then, we have

$$\beta_{j_B, j_B'} V_{A, j_B} \otimes V_{B, j_B'} = \Pi_{j_B} \psi(1)_{j_B}.$$

We define the spaces $K_A$ and $K_B$ spanned by $\{j_B\}$ and $\{j_B\}$, respectively. We define the junk state on $K_A \otimes K_B$ as

$$|junk\rangle := \sum_{j_B} \beta_{j_B, j_B'} V_{A, j_B} \otimes V_{B, j_B'}. $$

The isometries $V_A$ and $V_B$ satisfy conditions (D22) and (D23).

**Step 3:** We show the following fact; For $j_B \neq j_B'$, we have $V_{A, j_B, j_B'} = \beta_{j_B, j_B'} V_{A, j_B, j_B'}$ with a constant $\beta_{j_B, j_B'}$ when $\Pi(2, j_B, j_B') \neq 0$ and $\Pi(2, j_B, j_B') \neq 0$. We define $a_{i, j_B, j_B'} := V_{A, j_B, j_B'}$. Then, we have

$$\Pi_{j_B} \psi(1)_{j_B} = \Pi_{j_B} \psi(1)_{j_B}.$$

The above vector is a constant times of $\eta a_{i, j_B, j_B'} \otimes b_{i, j_B, j_B'}$. Also, the vectors $\{a_{i, j_B, j_B'} \otimes b_{i, j_B, j_B'}\}$ and the vectors $\{\Pi_{j_B} \psi(1)_{j_B}\}$ are the unique optimal solution in the SDP (D1). Hence, there exists a constant $\beta_{j_B, j_B'}$ such that $\Pi_{j_B} \psi(1)_{j_B} = \beta_{j_B, j_B'} \Pi_{j_B} \psi(1)_{j_B}$, which is the desired statement.

### 2. Trivalent case

We assume that the unique optimal maximizer $X^* = (X_{ij})$ is given by $\eta_i \eta_j (v_i, v_j)$ with the following; For $i = (i_A, i_B, i_C) \in I$,

$$v_i = a_{i_A} \otimes b_{i_B} \otimes c_{i_C},$$

where $a_{i_A} \in H_A = \mathbb{C}^{d_A}$, $b_{i_B} \in H_B = \mathbb{C}^{d_B}$, $c_{i_C} \in H_C = \mathbb{C}^{d_C}$. Also, for simplicity, $a_{i_A}$, $b_{i_B}$, and $c_{i_C}$ are assumed to be normalized and $\eta_i > 0$.

Now, we consider a state $|\psi\rangle$ on $H_A \otimes H_C$, and projections $\Pi_{i_A} = \Pi_{i_B} = \Pi_{i_C}$ on $H_A$, $H_C$. Then, we define the projection $\Pi := \Pi_{i_A} \otimes \Pi_{i_C}$.

In the following, we discuss how the state $|\psi\rangle$ is locally converted to $|\psi\rangle$ when the vectors $\Pi(\psi)$ realize the optimal solution in the SDP (D1). We define $|\psi\rangle := \eta_i^{-1} \Pi(\psi)$.
a. Rank-one case

We consider the case that the ranks of the projections \( \Pi_{A}^{\prime} \), \( \Pi_{B}^{\prime} \), and \( \Pi_{C}^{\prime} \) are one. We introduce the following conditions.

**Definition 32.** Three distinct elements \( i, j, k \in I \) are called linked when the following two conditions holds.

**C1** The relations \( \langle vi, vj \rangle \neq 0, \langle vi, vj \rangle \neq 0, \) and \( \langle vj, vk \rangle \neq 0 \) hold.

**C2** \( vi, vj \) shares a \( ti, j \)-th common element for \( ti, j \in \{ A, B, C \} \). Other components of \( vi, vj \) are different. That is, when \( ti, j = Ai, iA \neq jB, \) and \( ic \neq jC, \) \( vi \) and \( vj \) share a \( ti, j \)-th common element for \( ti, j \in \{ A, B, C \} \). In this case, there exist elements \( xA, xB, xC, x' \) such that \( i, j, k \in \{ xA, x' \} \times \{ xB, x' \} \times \{ xC, x' \} \).

In addition, two distinct elements \( xA, x' \) for index of a vectors of \( C^{i} \) are called connected when there exist three linked elements \( i, j, k \in I \) such that the first components of \( i, j, k \) are \( xA, x' \).

For \( iB, ic \), we use notation

\[
\psi(iB, ic) := b_{iB} \otimes c_{ic}.
\]

Then, we introduce the following conditions for the optimal maximizer given in (D37).

**A5** The vectors \( \{ vi \}_{i} \in \mathcal{I}_{B} \) span the vector space \( \mathcal{H}_{A} \otimes \mathcal{H}_{B} \otimes \mathcal{H}_{C} \).

**A6** There exist a subset \( I_{A} \) of indexes of the space \( \mathcal{H}_{A} \) with \( |I_{A}| = d_{A} \) and \( d_{A} \) sets \( I_{BC,iA} \) for \( iA \in I_{A} \) of indexes of the space \( \mathcal{H}_{B} \otimes \mathcal{H}_{C} \) to satisfy the following conditions. The set \( \{ a_{iA} \}_{iA} \) spans the space \( \mathcal{H}_{A} \). The set \( \{ \psi_{BC} \}_{iBC} \in I_{BC,iA} \) spans the space \( \mathcal{H}_{B} \otimes \mathcal{H}_{C} \) and \( I_{0} = \cup_{iA} I_{A} \). We consider the graph \( G_{A} \) with the set \( I_{A} \) of vertices such that the edges are given as the the pair of all connected elements in \( I_{A} \) in the sense of the end of Definition 32. The graph \( G_{A} \) is not divided into two disconnected parts.

**A7** The vectors \( \{ b_{iB} \otimes c_{ic} \} \in I_{iB} \) satisfy condition A2 by substituting \( c_{ic} \) into \( a_{iA} \). That is, there exist a subset \( I_{B} \) of the second indexes and subsets \( I_{C,iB} \) of the third indexes such that they satisfy conditions B1, B2, B3, and B4. We denote the graph defined in this condition by \( G_{B} \).

**Example 4.** We can check that Mermin Self-testing satisfies Conditions A5, A6, and A7 as follows. In this example, \( a_{O}, b_{O}, c_{O} \) means \( |O \rangle \). This notation is applied to \( Z, P, M \).

We choose the subset \( I_{A} := \{ O, P \} \). Then, we have

\[
I_{BC,O} = \{(O, O), (Z, Z), (M, P), (P, M)\},
\]

\[
I_{BC,P} = \{(Z, P), (P, Z), (O, M), (M, O)\}.
\]

Two elements \( O, P \in I_{A} \) are connected in the sense of the end of Definition 32 by choosing \( i, j, k = \{ (P, Z), (O, Z, Z) \} \). Based on (D39) and (D40), we choose the subsets \( I_{B}, I_{C,Z}, \) and \( I_{C,P} \) as

\[
I_{B} := \{ Z, P \}, \quad I_{C,Z} := \{ Z, P \}, \quad I_{C,P} := \{ Z, M \}.
\]

The subsets \( I_{B}, I_{C,Z}, \) and \( I_{C,P} \) satisfy conditions B1, B2, B3, and B4.

**Lemma 33.** Assume that \( i, j, k \in I_{O} \) are connected by one edge, i.e., satisfy conditions C1 and C2. We choose \( xA, x'B, x''B, xC, x''C \) in the way as Condition C2. We consider three normalized vectors \( v_{l}, v'_{l}, v''_{l} \), where

\[
v_{l} = a_{iA} \otimes b_{iB} \otimes c_{ic}
\]

for \( l = i, j, k \). We assume that \( \langle vi, vl \rangle = \langle v'l, v''l \rangle \) for \( l, l' = i, j, k \). Then, we have

\[
\langle a_{xA}, a_{x'A} \rangle = \langle a'_{x'A}, a''_{x'A} \rangle
\]

\[
\langle b_{xB}, b_{x'B} \rangle = \langle b'_{x'B}, b''_{x'B} \rangle
\]

\[
\langle c_{xC}, c_{x'C} \rangle = \langle c'_{x'C}, c''_{x'C} \rangle
\]

or

\[
\langle a_{xA}, a_{x'A} \rangle = -\langle a'_{x'A}, a''_{x'A} \rangle
\]

\[
\langle b_{xB}, b_{x'B} \rangle = -\langle b'_{x'B}, b''_{x'B} \rangle
\]

\[
\langle c_{xC}, c_{x'C} \rangle = \langle c'_{x'C}, c''_{x'C} \rangle
\]
Proof. For simplicity, without loss of generality, we assume that
\[ i = (x_A', x_B, x_C), j = (x_A, x_B', x_C), k = (x_A, x_B, x_C'). \] (D49)

Since
\[ \langle v_i, v_j \rangle = (v_i', v_j'), \langle v_i, v_k \rangle = (v_i', v_k'), \langle v_k, v_j \rangle = (v_k', v_j'), \] (D50)
we have
\[ \langle a_{x_A}, a_{x_A'} \rangle \langle b_{x_B}, b_{x_B'} \rangle = \langle a_{x_A}, a_{x_A'} \rangle \langle b_{x_B}, b_{x_B'} \rangle, \] (D51)
\[ \langle a_{x_A}, a_{x_A'} \rangle \langle c_{x_C}, c_{x_C'} \rangle = \langle a_{x_A}, a_{x_A'} \rangle \langle c_{x_C}, c_{x_C'} \rangle, \] (D52)
\[ \langle b_{x_B}, b_{x_B'} \rangle \langle c_{x_C}, c_{x_C'} \rangle = \langle b_{x_B}, b_{x_B'} \rangle \langle c_{x_C}, c_{x_C'} \rangle. \] (D53)

Hence,
\[ \langle a_{x_A}, a_{x_A'} \rangle^2 = \langle (a_{x_A}, a_{x_A'} \rangle \langle b_{x_B}, b_{x_B'} \rangle) (\langle a_{x_A}, a_{x_A'} \rangle \langle c_{x_C}, c_{x_C'} \rangle) (\langle b_{x_B}, b_{x_B'} \rangle \langle c_{x_C}, c_{x_C'} \rangle)^{-1} \] (D54)
\[ = \langle (a_{x_A}, a_{x_A'} \rangle \langle b_{x_B}, b_{x_B'} \rangle) (\langle a_{x_A}, a_{x_A'} \rangle \langle c_{x_C}, c_{x_C'} \rangle) (\langle b_{x_B}, b_{x_B'} \rangle \langle c_{x_C}, c_{x_C'} \rangle)^{-1} \] (D55)
\[ = \langle a_{x_A}, a_{x_A'} \rangle^2, \] (D56)
which implies (D43) or (D46). When (D43), we have (D44) and (D45). When (D45), we have (D46) and (D47).

Theorem 34. Assume that the optimal maximizer given in (D37) satisfies conditions A5, A6, and A7, and the vectors \( (\Pi_i|\psi_i^\prime)_{i \in I} \) realize the optimal solution in the SDP (D1). In addition, the ranks of the projections \( \Pi_{\alpha}^A, \Pi_{\beta}^B, \) and \( \Pi_{\gamma}^C \) are assumed to be one.

Then, there exist isometries \( V_A : \mathcal{H}_A \to \mathcal{H}_A', V_B : \mathcal{H}_B \to \mathcal{H}_B', \) and \( V_C : \mathcal{H}_C \to \mathcal{H}_C' \) such that
\[ V_A \otimes V_B \otimes V_C |\psi_i^\prime \rangle = |\psi_i^\prime \rangle, \] (D58)
\[ V_A \otimes V_B \otimes V_C |v_i \rangle = |v_i^\prime \rangle, \] (D59)
for \( i \in I. \)

Proof. Step 1: We fix an arbitrary element \( i_A \in I_A. \) For \( i_{BC}, \iota_{BC} \in I_{BC,i_A}, \) Condition A1 implies
\[ \langle \psi_{i_{BC}}, \psi_{i_{BC}}^\prime \rangle = \langle a_{i_{BC}} \otimes \psi_{i_{BC}}, a_{i_{BC}} \otimes \psi_{i_{BC}}^\prime \rangle = \langle a_{i_{BC}} \otimes \psi_{i_{BC}}^\prime, a_{i_{BC}}^\prime \otimes \psi_{i_{BC}}^\prime \rangle = \langle \psi_{i_{BC}}, \psi_{i_{BC}}^\prime \rangle. \] (D60)

Hence, there exists an isometry \( V_{BC,i_A} : \mathcal{H}_B \otimes \mathcal{H}_C \to \mathcal{H}_B' \otimes \mathcal{H}_C' \) such that
\[ V_{BC,i_A} \psi_{i_{BC}} = \psi_{i_{BC}}^\prime. \] (D61)
for \( i_{BC} \in I_{BC,i_A}. \)

Step 2: We choose a subgraph \( G_{A,0} \subset G_A \) such that the vertecies of \( G_{A,0} \) is \( I_A, G_{A,0} \) has no cycle, and \( G_{A,0} \) cannot be divided into two parts.

We fix the origin \( i_{A,0} \in I_A. \) For any element \( i_A \in I_A, \) we have the unique path to connect \( i_{A,0} \) and \( i_A \) by using \( G_{A,0} \) because \( G_{A,0} \) has no cycle. We denote this path as \( i_{A,0} - i_{A,1} - \cdots - i_{A,n} = i_A. \) We define \( \alpha(i_A) \) as
\[ \alpha(i_A) := \prod_{m=1}^{n} \frac{(a_{i_{A,m-1}}, a_{i_{A,m}})}{(a_{i_{A,m-1}}, a_{i_{A,m}})}. \] (D62)

Lemma 33 guarantees that \( \alpha(i_A) \) takes value 1 or \( -1. \) Due to the above definition and the uniqueness of the above path, we find that
\[ \alpha(i_{A,i}) := \prod_{m=1}^{i} \frac{(a_{i_{A,m-1}}, a_{i_{A,m}})}{(a_{i_{A,m-1}}, a_{i_{A,m}})}. \] (D63)

For \( i_{BC} \in I_{BC,i_A} \) and \( \iota_{BC} \in I_{BC,i_{A,i+1}}, \) we find that
\[ \langle a_{i_{A,1}}, a_{i_{A,i+1}} \rangle \psi_{i_{BC}} = \langle a_{i_{A,1}} \otimes \psi_{i_{BC}}, a_{i_{A,i+1}} \otimes \psi_{i_{BC}} \rangle \] (D64)
\[ = \langle a_{i_{A,1}} \otimes \psi_{i_{BC}}^\prime, a_{i_{A,i+1}} \otimes \psi_{i_{BC}}^\prime \rangle \] (D65)
\[ = \alpha(i_{A,i}) \alpha(i_{A,i+1}) \langle a_{i_{A,1}}, a_{i_{A,i+1}} \rangle \psi_{i_{BC}} \] (D66)
\[ = \alpha(i_{A,i}) \alpha(i_{A,i+1}) \langle \psi_{i_{BC}}, \psi_{i_{BC}} \rangle \] (D67)
\[ \langle \psi_{i_{BC}}, \psi_{i_{BC}} \rangle = \langle \psi_{i_{BC}}, \psi_{i_{BC}} \rangle. \] (D68)
Since \( a_{i,A,l} \neq 0 \) and the sets \( \{ \psi_{BC} \}_{iBC \in \mathcal{I}_{BC,i,A,l}} \) and \( \{ \psi'_{BC} \}_{iBC \in \mathcal{I}_{BC,i,A,l+1}} \) span the space \( C^{d_A d_C} \), we find that \( \alpha(i_A) \alpha(i_{A,l+1}) V^\dagger_{BC,i_A,l} V_{BC,i_A,l+1} \) is identity. Then, we find that
\[
V_{BC} := V_{BC,i_A,0} = \alpha(i_A) V_{BC,i_A,l}. \tag{D69}
\]
That is, we have
\[
V_{BC} = \alpha(i_A) V_{BC,i_A,l}. \tag{D70}
\]
Also, we define the isometry \( V_A : \mathcal{H}_A \to \mathcal{H}'_A \) such that
\[
V_A a_{i_A} = \alpha(i_A) a'_{i_A} \tag{D71}
\]
for \( i_A \in \mathcal{I}_A \).
Therefore, for \( (i_A, i_{BC}) \in \bigcup_{i,A} \mathcal{I}_{BC,i_A,l} \), we have
\[
V_{\alpha i_A} \psi_{iBC} = a'_{i_A} \otimes \psi'_{iBC} = (V_A \otimes V_{BC}) a_{i_A} \otimes \psi_{iBC}. \tag{D72}
\]
Since the set \( \{ a_{i_A} \}_{i_A \in \mathcal{I}_A} \) spans the space \( C^{d_A} \), we have
\[
V = V_A \otimes V_{BC}. \tag{D73}
\]

**Step 3:** For \( i_B \in \mathcal{I}_B \) and \( i_C \in \mathcal{I}_{C,B,l} \), we choose \( i_C \) such that \( (i_B, i_C) \in \mathcal{I}_{BC, i_A,l} \). Then, we define \( \beta(i_B, i_C) := \alpha(i_A) \). We fix an arbitrary element \( i_B \in \mathcal{I}_B \). For \( i_C, i'_C \in \mathcal{I}_{C,B,l} \), Relation (D70) implies
\[
(D74)
\]



\[
(D75)
\]

Hence, there exists an isometry \( V_{C,B,l} : \mathcal{H}_C \to \mathcal{H}'_C \) such that
\[
V_{C,B,l} c_{i_C} = \beta(i_B, i_C) c'_{i_C} \tag{D76}
\]
for \( i_C \in \mathcal{I}_{C,B,l} \).

**Step 4:** We choose a subgraph \( G_{B,0} \subset G_{B} \) such that the vertices of \( G_{B,0} \) is \( \mathcal{I}_B \), \( G_{B,0} \) has no cycle, and \( G_{B,0} \) cannot be divided into two parts.
We fix the origin \( i_{B,0} \in \mathcal{I}_B \). For any element \( i_B \in \mathcal{I}_B \), we have the unique path to connect \( i_{B,0} \) and \( i_B \) by using \( G_{B,0} \) because \( G_{B,0} \) has no cycle. We denote this path as \( i_{B,0} = i_{B,1} \cdots i_{B,n'} = i_B \). We choose a non-zero element \( i_C, i''_C \in \mathcal{I}_{C,B,l-1} \cap \mathcal{I}_{C,B,l} \). We choose \( i_{A,l}, i'_{A,l} \) such that \( (i_{B,l-1}, i_C,l) \in \mathcal{I}_{BC,i_A,l} \) and \( (i_{B,l}, i_C,l) \in \mathcal{I}_{BC,i_A,l} \). We define \( \beta(i_B) \) as
\[
\gamma(i_B) := \prod_{l=1}^{n'} \beta(i_{B,l-1}, i_C,l) \beta(i_{B,l}, i_C,l). \tag{D77}
\]
Then, we have
\[
(D78)
\]

\[
(D79)
\]

\[
(D80)
\]

\[
(D81)
\]

For \( i_C \in \mathcal{I}_{C,B,l} \) and \( i''_C \in \mathcal{I}_{C,B,l+1} \), we find that
\[
(D82)
\]

\[
(D83)
\]

\[
(D84)
\]

\[
(D85)
\]

Since \( \langle b_{i_B,l}, b_{i_B,l+1} \rangle \neq 0 \) and the sets \( \{ c_{i_C} \}_{i_C \in \mathcal{I}_{C,B,l}} \) and \( \{ c'_i \} \in \mathcal{I}_{C,B,l+1} \) span the space \( \mathcal{H}_C \), we find that \( \gamma(i_B) \gamma(i_{B,l+1}) V^\dagger_{C,i_B,l} V_{C,i_B,l+1} \) is identity. Then, we find that
\[
V_C := V_{C,B,0} = \gamma(i_B) V_{C,i_B,l}. \tag{D86}
\]
That is, we have

\[ V_C = \gamma(i_B) V_{C,i_B}. \]  

(D87)

**Step 5:** For elements \( i_B, i'_B \in \mathcal{I}_B \), the sets \( \{ c_{iC} \}_{iC \in \mathcal{I}_{C,i_B}} \) and \( \{ c'_{iC} \}_{iC \in \mathcal{I}_{C,i'_B}} \) span the space \( \mathcal{C}^{d_C} \). We choose \( i_C \in \mathcal{I}_{C,i_B} \) and \( i'_C \in \mathcal{I}_{C,i'_B} \) such that \( \langle c_{iC}, c'_{iC} \rangle \neq 0 \). We have

\[
\langle b_{i_B}, b'_{i_B} \rangle (c_{iC}, c'_{iC}) = \langle b_{i_B} \otimes c_{iC}, b'_{i_B} \otimes c'_{iC} \rangle
\]

\[
= \beta(i_B, i_C) \beta(i'_B, i'_C) (b'_{i_B} \otimes c'_{iC}, b''_{i_B} \otimes c''_{iC})
\]

\[
= \langle b'_{i_B}, b''_{i_B} \rangle \beta(i_B, i_C) \beta(i'_B, i'_C) (c_{iC}, c'_{iC})
\]

\[
= \langle b'_{i_B}, b''_{i_B} \rangle \gamma(i_B) (V_{C,i_C}, V_{C,i'_C})
\]

\[
= \gamma(i_B) (V_{C}, b'_{i_B}, b''_{i_B}) (c_{iC}, c'_{iC}).
\]

Since \( \langle c_{iC}, c'_{iC} \rangle \neq 0 \), we have

\[
\langle b_{i_B}, b'_{i_B} \rangle = \gamma(i_B) (i'_B) (b'_{i_B}, b''_{i_B}) (c_{iC}, c'_{iC}).
\]

(D93)

Also, we define the isometry \( V_B : \mathcal{H}_B \rightarrow \mathcal{H'}_B \) such that

\[
V_B b_{i_B} = \gamma(i_B) b'_{i_B}
\]

(D94)

for \( i_B \in \mathcal{I}_B \).

Therefore, for \( (i_B, i_C) \in \bigcup_{i_B \in \mathcal{I}_B} \{ (i_B) \times \mathcal{I}_{C,i_B} \} \), we have

\[
V_{BC} b_{i_B} \otimes c_{iC} = b'_{i_B} \otimes c'_{iC} = (V_B \otimes V_C) b_{i_B} \otimes c_{iC}.
\]

(D95)

Since \( \{ b_{i_B} \otimes c_{iC} \}_{(i_B, i_C) \in \bigcup_{i_B \in \mathcal{I}_B} \{ (i_B) \times \mathcal{I}_{C,i_B} \}} \) spans \( \mathcal{H}_B \otimes \mathcal{H}_C \), we have

\[
V_{BC} = V_B \otimes V_C.
\]

(D96)

Combining (D73) and (D96), we have

\[
V = V_A \otimes V_B \otimes V_C.
\]

(D97)

**b. General case**

We consider the general case. We define \( |\psi'\rangle := \eta_{i_B}^{-1} \Pi^A_{i_A} \otimes \Pi^B_{i_B} \otimes \Pi^C_{i_C} |\psi\rangle \).

Let \( \tilde{\mathcal{I}}_A, \tilde{\mathcal{I}}_B, \tilde{\mathcal{I}}_C \) be the sets of indexes of the spaces \( \mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C \).

We introduce other conditions for the optimal maximizer given in (D37) as a generalization of A3 and A4.

**A8** Ideal systems \( \mathcal{H}_A, \mathcal{H}_B, \) and \( \mathcal{H}_C \) are two-dimensional.

**A9** Each system has only two measurements. That is, the sets \( \tilde{\mathcal{I}}_A, \tilde{\mathcal{I}}_B, \) and \( \tilde{\mathcal{I}}_C \) is composed of 4 elements. For any element \( i_A \in \tilde{\mathcal{I}}_A \) \((i_B \in \tilde{\mathcal{I}}_B, i_C \in \tilde{\mathcal{I}}_C)\), there exists an element \( i'_A \in \tilde{\mathcal{I}}_A \) \((i'_B \in \tilde{\mathcal{I}}_B, i'_C \in \tilde{\mathcal{I}}_C)\) such that \( \langle a_{i_A} | a'_{i'_A} \rangle = 0 \,(\langle b_{i_B} | b'_{i_B} \rangle = 0, \, \langle c_{i_C} | c'_{i_C} \rangle = 0) \).

**Mermin Self-testing** satisfies Conditions A8 and A9 in addition to Conditions A5, A6, and A7.

When A3 and A4 hold, \( \tilde{\mathcal{I}}_A (\tilde{\mathcal{I}}_B, \tilde{\mathcal{I}}_C) \) is written as \( B_{A,0} \cup B_{A,1} \) \((B_{B,0} \cup B_{B,1}, B_{C,0} \cup B_{C,1})\), where \( B_{A,j} = \{(0,j), (1,j)\} \) \((B_{B,j} = \{(0,j), (1,j)\}, B_{C,j} = \{(0,j), (1,j)\})\) and \( \langle a_{(0,j)} | a_{(1,j)} \rangle = 0 \,(\langle b_{(0,j)} | b_{(1,j)} \rangle = 0, \, \langle c_{(0,j)} | c_{(1,j)} \rangle = 0) \) for \( j = 0, 1 \).

We also consider the following condition for \( \Pi_i = \Pi^A_{i_A} \otimes \Pi^B_{i_B} \otimes \Pi^C_{i_C} \).

**C1** When \( i_A, i'_A \in \tilde{\mathcal{I}}_A \) \((i_B, i'_B \in \tilde{\mathcal{I}}_B, i_C, i'_C \in \tilde{\mathcal{I}}_C)\) satisfy \( \langle a_{i_A} | a'_{i'_A} \rangle = 0 \,(\langle b_{i_B} | b'_{i_B} \rangle = 0, \, \langle c_{i_C} | c'_{i_C} \rangle = 0) \), we have

\[
\Pi^A_{i_A} + \Pi^A_{i'_A} = I \,(\Pi^B_{i_B} + \Pi^B_{i'_B} = I, \, \Pi^C_{i_C} + \Pi^C_{i'_C} = I).
\]

Let \( \mathcal{H}^A_{i_A}, \mathcal{H}^B_{i_B}, \) and \( \mathcal{H}^C_{i_C} \) be the image of the projections \( \Pi^A_{i_A}, \Pi^B_{i_B}, \) and \( \Pi^C_{i_C} \).

**Theorem 35.** Assume that the optimal maximizer given in (D37) satisfies conditions A5, A6, A5, A7, A8, and A9, and the vectors \( (\Pi_i | \psi) \in \mathcal{I}_E \) realize the optimal solution in the SDP (D1). Then, there exist isometries \( V_A \) from \( \mathcal{H}_A \otimes \mathcal{K}_A \) to \( \mathcal{H}^A_{i_A}, V_B \) from \( \mathcal{H}_B \otimes \mathcal{K}_B \) to \( \mathcal{H}^B_{i_B}, \) and \( V_C \) from \( \mathcal{H}_C \otimes \mathcal{K}_C \) to \( \mathcal{H}^C_{i_C} \) such that

\[
V_A \otimes V_B \otimes V_C |\psi\rangle \otimes |\text{junk}\rangle = |\psi'\rangle,
\]

(D98)

\[
V_A \otimes V_B \otimes V_C |v_i\rangle \otimes |\text{junk}\rangle = |v'_i\rangle,
\]

(D99)

for \( i \in \mathcal{I}_B \), where \( |\text{junk}\rangle \) is a state on \( \mathcal{K}_A \otimes \mathcal{K}_B \otimes \mathcal{K}_C \).
Proof. Similar to the proof of Theorem 29, we define orthogonal projections $\bar{\Pi}_X^j$ on $\mathcal{H}_X$ such that the projection $\Pi^X := \sum_j \bar{\Pi}_X^j$ satisfies $\Pi^X \psi' = \psi'$ for $X = A, B, C$. Then, we define the projection $\bar{\Pi}^{(j_A,j_B,j_C)} := \bar{\Pi}_A^j \bar{\Pi}_B^j \bar{\Pi}_C^j$. In the same way as the proof of Theorem 29, we define $\alpha^{(j_A,j_B,j_C)}$, $\beta^{(j_A,j_B,j_C)}$, and $V_{X,j_X}$ for $X = A, B, C$.

We define the space $\mathcal{K}_X$ spanned by $\{|j_X\rangle\}$ for $X = A, B, C$. We define the junk state on $\mathcal{K}_A \otimes \mathcal{K}_B \otimes \mathcal{K}_C$ as

$$|\text{junk}\rangle := \sum_{j_A,j_B,j_C} \beta^{-1}_{j_A,j_B,j_C} \alpha^{-1}_{(j_A,j_B,j_C)} |j_A,j_B,j_C\rangle.$$  \hspace{1cm} (D100)

We define the isometries $V_X : \mathcal{H}_X \otimes \mathcal{K}_X \to \mathcal{H}'_X$ as

$$V_X := \sum_{j_X} V_{X,j_X} |j_X\rangle$$  \hspace{1cm} (D101)

for $X = A, B, C$. The isometries $V_A, V_B,$ and $V_C$ satisfy conditions (D98) and (D99). \hfill \blacksquare