Graph-Theoretic Approach for Self-Testing in Bell Scenarios

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Self-testing is a technology to certify states and measurements using only the statistics of the experiment. Self-testing is possible if some extremal points in the set B_Q of quantum correlations for a Bell experiment are achieved, up to isometries, with specific states and measurements. However, B_Q is difficult to characterize, so it is also difficult to prove whether or not a given matrix of quantum correlations allows for self-testing. Here, we show how some tools from graph theory can help to address this problem. We observe that B_Q is strictly contained in an easy-to-characterize set associated with a graph, $\Theta(G)$. Therefore, whenever the optimum over B_Q and the optimum over $\Theta(G)$ coincide, self-testing can be demonstrated by simply proving self-testability with $\Theta(G)$. Interestingly, these maxima coincide for the quantum correlations that maximally violate many families of Bell-like inequalities. Therefore, we can apply this approach to prove the self-testability of many quantum correlations, including some that are not previously known to allow for self-testing. In addition, this approach connects self-testing to some open problems in discrete mathematics. We use this connection to prove a conjecture [M. Araújo *et al.*, Phys. Rev. A, 88, 022118 (2013)] about the closed-form expression of the Lovász theta number for a family of graphs called the Möbius ladders. Although there are a few remaining issues (e.g., in some cases, the proof requires the assumption that measurements are of rank 1), this approach provides an alternative method to self-testing and draws interesting connections between quantum mechanics and discrete mathematics.

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I. INTRODUCTION

A. Self-testing in Bell scenarios

Quantum systems render a distinct advantage over classical systems in many quantum information processing tasks. Spurred 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" [1,2] and early hints of the quantum internet [3]. 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 [4]. This is a challenging task due to the exploding dimensionality of the Hilbert space associated with many-body quantum systems.

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In the classical system, any certification requires trusted measurement devices. However, for quantum systems, it is possible to provide certification with untrusted measurement devices. This relaxation in the requirement is yet another quantum advantage over classical systems. Such a device certification is called self-testing [5]. The idea of self-testing is to certify the underlying quantum states and measurement settings based solely on the measurement statistics. We do not need to trust the state nor the measurement device in self-testing, whereas conventional verification needs to trust either the measurement device or the state [6]. Self-testing was initially put forward for Bell nonlocal correlations. The concept has since been extended to any prepare-and-measure scenarios [7,8], contextuality [9,10], and steering [11–13]. Self-testing has also been applied to quantum gates and circuits [14,15]. A great amount of work has also been done in making self-testing protocols robust against experimental noise [16–19]. For example, while Mayers and Yao [5] considered the noiseless case for Clauser-Horne-Shimony-Holt (CHSH) self-testing, McKague *et al.* [16] extended it to the noisy case. Hayashi and Hajdušek [20] proposed a blended scheme, juxtaposing the CHSH test and the stabilizer test. The blended version has a better noise tolerance than the CHSH test. McKague [21] proposed a robust self-testing method for graph states. There, the number of required copies increases with order $\mathcal{O}(n^{22})$, where n is the number of qubits of one graph state. To improve the scaling, Hayashi and Hajdušek [20] proposed another self testing method for the same setting with $\mathcal{O}(n^4 \log n)$ copies. Furthermore, Hayashi and Koshiba [22] proposed a robust self-testing protocol for Greenberger-Horne-Zeilinger (GHZ) states. Self-testing with Bell states of higher dimensions has been studied in Refs. [23,24]. In Ref. [25], the 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. [11]. Comprehensive studies have been carried out for self-testing of a single quantum device based on contextuality [9,10] and via computational assumptions [26]. The idea of self-testing has been used for device-independent randomness generation [11,27–29], entanglement detection [30,31], delegated quantum computing [32,33], and in several computational complexity proofs, such as the recent breakthrough result of MIP* = RE [34]. For a thorough review of self-testing, see Ref. [35].

B. An interesting observation

The crucial observation that motivates this work is the following: given a Bell scenario, a set of quantum correlations, B_Q, is difficult to characterize [36]. Consequently, it is also difficult to prove whether or not a given matrix of quantum correlations allows for self-testing. To address this problem, we focus on the uniqueness of the solution of semidefinite programming. We consider the maximization of a linear function using semidefinite matrices under linear constraints. When the solution of the dual problem is nondegenerate, the solution of the primal problem is unique [37]. Because of this property, when a state achieves the maximum value of the above semidefinite programming, the state is guaranteed to be unitarily equivalent to a certain state. Hence, if the set of quantum correlations, B_Q, realizes the above linear constraints, it also realizes a self-testing method.

To find such a set of quantum correlations B_Q, we focus on its exclusivity graph. That is, we employ the *theta body* [38] of the graph of exclusivity $\mathcal{G}_{\rm ex}(V,E)$ of all the events of the scenario, where V is the set of vertices and E is the set of edges. The vertices in $\mathcal{G}_{\rm ex}(V,E)$ represent the events produced in the scenario [39]. The edges in $\mathcal{G}_{\rm ex}(V,E)$ connect the nodes corresponding to mutually exclusive events. Using the normalization conditions, every Bell nonlocality 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 with a vertex-weighted graph (G,w) where weights correspond to the w_i and G is an induced subgraph of $\mathcal{G}_{\rm ex}(V,E)$ [39]. The quantum maximum of S must be in the theta body of G, a set which is even easier to characterize, as G is a subgraph of $\mathcal{G}_{\rm ex}(V,E)$. Therefore, for the cases where the quantum maximum of a Bell nonlocality 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.

Interestingly, these cases have high relevance within the landscape of Bell inequalities, as they include the quantum correlations maximally violating many families of Bell and Bell-like inequalities, including the CHSH Bell inequality [40], all chained Bell inequalities [41,42], all Svetlichny inequalities to detect true n-body nonseparability [43,44], all Mermin-Ardehali-Belinskiĭ-Klyshko Bell inequalities [45–47], all Bell inequalities associated with all-versus-nothing proofs and producing fully nonlocal correlations [48,49], all Bell inequalities for graph states [50–52], Abner Shimony (AS) Bell inequalities [53], and Bell inequalities obtained from Kochen-Specker sets [54].

C. Structure of the paper

The paper is organized as follows. In Sec. II, we review some concepts from different areas used within the article. In Sec. III, we detail the assumptions and present our results. In Sec. IV, we apply the graph-theoretic approach to some test cases. Specifically, we discuss the CHSH, chained, Mermin, and AS Bell inequalities. Application to the case of chained Bell inequalities allows us to prove a conjecture made in Ref. [67], and application to the AS Bell inequalities allows us to identify new quantum correlations, allowing for self-testing. In Sec. V, we compare our results with existing results. In Sec. VII, we summarize our results and point out some remaining issues and open problems. In addition, some technical details are discussed in several appendices.

II. PRELIMINARY CONCEPTS

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 $\mathcal{G}_{\rm ex} = ([N], E)$, 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 $\mathcal{G}_{\rm ex}$ is a mapping $p : [N] \to [0, 1]$, such that $p_i + p_j \le 1$ 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 $p_i + p_j \le 1$ enforces that if $p_i = 1$ then $p_j = 0$.

Behavior $p : [N] \to [0, 1]$ is *deterministic noncontextual* if all events have predetermined binary values (0 or 1) that do not depend on the occurrence of other events. In other words, a deterministic noncontextual behavior p is a mapping $p : [N] \to \{0, 1\}$, such that $p_i + p_j \le 1$ for all $i \sim j$. A *deterministic noncontextual* behavior can be considered a vector in $\mathbb{R}^N$. The convex hull of all deterministic noncontextual behaviors is called the *set of noncontextual behaviors*, denoted $\mathcal{P}_{\rm NC}(\mathcal{G}_{\rm ex})$. The set $\mathcal{P}_{\rm NC}(\mathcal{G}_{\rm ex})$ is a polytope with its vertices being the deterministic noncontextual behaviors. Behaviors that do not lie in $\mathcal{P}_{\rm NC}(\mathcal{G}_{\rm ex})$ are called *contextual*. It is worth mentioning that, in combinatorial optimization, one often encounters the *stable set* polytope of a graph $\mathcal{G}_{\rm ex}$, STAB$(\mathcal{G}_{\rm ex})$ (see Definition 9 in Appendix A). It is quite easy to see that stable sets of $\mathcal{G}_{\rm ex}$ (a subset of vertices, where no two vertices share an edge between them) and *noncontextual* behaviors coincide.

Lastly, 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

$$p_i = \langle\psi|\Pi_i|\psi\rangle \quad \text{for all } i \in [N] \quad \text{and} \quad \mathrm{tr}(\Pi_i\Pi_j) = 0 \quad \text{for } i \sim j. \tag{1}$$

We refer to the ensemble $|\psi\rangle, \{\Pi\}_{i=1}^N$ as a *quantum realization* of behavior p. The set of all quantum behaviors is a convex set, denoted $\mathcal{P}_Q(\mathcal{G}_{\rm ex})$. It turns out that $\mathcal{P}_Q(\mathcal{G}_{\rm ex})$ is also a well-studied entity in combinatorial optimization, namely the *theta body*, denoted $\Theta(\mathcal{G}_{\rm ex})$ and formally defined in Definition 14 in Appendix A.

Now, suppose that we are interested in the maximum value of the sum $S = w_1p_1 + w_2p_2 + \cdots + w_Np_N$, where $w_i \ge 0$ are weights for $i \in [N]$ and

1. $p \in \mathcal{P}_{\rm NC}(\mathcal{G}_{\rm ex})$ is a *noncontextual* behavior (see Definition 10 in Appendix A); 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, $\alpha(\mathcal{G}_{\rm ex}, w)$, that is, the size of the largest clique in the complement graph, where w refers to the N-dimensional vector of non-negative weights;
2. $p \in \mathcal{P}_Q(\mathcal{G}_{\rm ex})$ 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, $\vartheta(\mathcal{G}_{\rm ex}, w)$, defined by the semidefinite program (SDP)

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

$$\text{such that} \quad X_{ii} = X_{0i} \quad \text{for all } i \in [N], \tag{2b}$$

$$X_{ij} = 0 \quad \text{for all } i \sim j, \tag{2c}$$

$$X_{00} = 1, \quad X \in \mathbb{S}_+^{1+N}, \tag{2d}$$

where $\mathbb{S}_+^{1+N}$ denotes positive semidefinite matrices of size $(N + 1) \times (N + 1)$. From the definition of the theta body and Lemma 4 (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 Ref. [39]. The Gram-Schmidt decomposition of matrix X corresponding to Eq. (2) gives the quantum realization for the underlying behavior p [9] (see Appendix A for the definition of the Gram-Schmidt decomposition). Note that, for a fixed X, its different Gram-Schmidt decompositions are related to one another via isometry.

Definition 1 (Noncontextuality inequality): For a given graph of exclusivity $\mathcal{G}_{\rm ex}$, a noncontextuality inequality corresponds to a half space that contains the set of noncontextual behaviors, i.e.,

$$\sum_i w_i p_i \le \alpha(\mathcal{G}_{\rm ex}, w) \quad \text{for all } p \in \mathcal{P}_{\rm NC}(\mathcal{G}_{\rm ex}), \tag{3}$$

and $w_i \ge 0$ for all $i \in [N]$.

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 setting x, Bob measures in 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

$$\begin{aligned}S_{\text{CHSH}} = {} & p(0,0|0,0)+p(1,1|0,1)+p(1,0|1,1)\\ & +p(0,0|1,0)+p(1,1|0,0)+p(0,0|0,1)\\ & +p(0,1|1,1)+p(1,1|1,0).\end{aligned} \tag{4}$$

Note that the aforementioned witness necessitates Alice and Bob to output the same answers unless they are both asked $x=y=1$. In cases where they are asked $x=y=1$, they should give opposite answers. The graph of exclusivity corresponding to these eight events is shown in Fig. 1, and is denoted $C_{i_8}(1,4)$. The weights on each of the vertices is 1 and thus the weight vector is an eight-dimensional all-1 vector. Note that $\alpha[C_{i_8}(1,4)]=3$ and, thus, the classical bound of $S_{\text{CHSH}}\leq 3$. However, $\vartheta[C_{i_8}(1,4)]=2+\sqrt{2}\approx 3.414$ (see Ref. [39]), and therefore the quantum bound of $S_{\text{CHSH}}\leq 2+\sqrt{2}$.

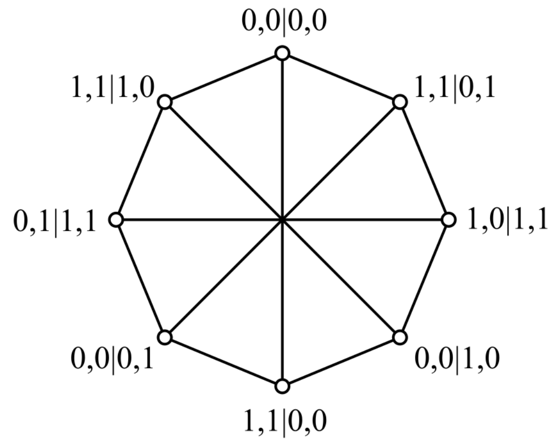

FIG. 1. Induced subgraph (of the 16-vertex graph of exclusivity of the events in the CHSH scenario) corresponding to the eight events involved in the expression of the Bell witness given by Eq. (4). This graph is called the eight-vertex circulant graph (1, 4) and is denoted $\mathrm{Ci}_8[1,4]$ (see Definition 7 in Appendix A for a definition of circulant graphs), and is isomorphic to the Möbius ladder graph of order 2.

C. Self-testing

Bell inequalities are special instances of noncontextuality 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 that 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. An n-partite Bell inequality is of the form

$$\sum_{\vec{a},\vec{x}} s_{\vec{x}}^{\vec{a}}\, p[\vec{a}|\vec{x}] \leq S_{\mathcal{L}} \tag{5}$$

for some coefficients $s_{\vec{x}}^{\vec{a}}$ and where $S_{\mathcal{L}}$ is the largest possible value allowed in *local hidden variable* (LHV) models [68]. The quantum supremum of the Bell expression, i.e., the left-hand side of Eq. (5), denoted $S_{\mathcal{Q}}$, is the largest possible value of the above expression when $p[\vec{a}|\vec{x}]$ ranges over the set of quantum behaviors, i.e.,

$$p[\vec{a}|\vec{x}] = \langle\psi|\bigotimes_{j=1}^{n} M^{j}_{a_j|x_j}|\psi\rangle \tag{6}$$

for a shared quantum state $|\psi\rangle\in\mathcal{H}_1\otimes\mathcal{H}_2\otimes\cdots\otimes\mathcal{H}_n$ and quantum projective measurements $\{M^{j}_{a_j|x_j}\}$ acting on $\mathcal{H}_j$ for all $j\in n$. We collectively refer to the state and the set of measurements that reproduce the quantum behavior 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 $(|\psi\rangle,\{M^{j}_{a_j|x_j}\}_j)$ if, for any other realization $(|\psi\rangle',\{M'^{j}_{a_j|x_j}\})$ that also attains $S_{\mathcal{Q}}$, there exists a local unitary $V=V_1\otimes V_2\otimes\cdots\otimes V_n$ and an ancilla state $|\text{junk}\rangle$ such that

$$\begin{aligned}V|\psi'\rangle &= |\text{junk}\rangle\otimes|\psi\rangle,\\ V\left(\bigotimes_{j=1}^{n} M'^{j}_{a_j|x_j}\right)|\psi'\rangle &= |\text{junk}\rangle\otimes\left(\bigotimes_{j=1}^{n} M^{j}_{a_j|x_j}\right)|\psi\rangle.\end{aligned} \tag{7}$$

D. Concepts from semidefinite programs

Definition 3 (Semidefinite programs): A pair of primal and dual SDPs is given by an optimization problem of the form

$$\sup_X\{\langle C,X\rangle : X \in \mathcal{S}_+^n,\ \langle A_i,X\rangle = b_i\ (i\in[m])\}, \tag{8}$$

$$\inf_{y,Z}\left\{\sum_{i=1}^m b_i y_i :\ \sum_{i=1}^m y_i A_i - C = Z \in \mathcal{S}_+^n\right\}, \tag{9}$$

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 (2). The dual formulation for Eq. (2) is given by

$$\min\left\{t\ \middle|\ tE_{00}+\sum_{i=1}^n(\lambda_i-1)E_{ii}-\sum_{i=1}^n\lambda_i E_{0i} + \sum_{i\sim j}\mu_{ij}E_{ij}\equiv Z\succeq 0\right\}, \tag{10}$$

where $E_{ij}=(e_ie_j^T+e_je_i^T)/2$. We make crucial use of the following theorem due to Alizadeh *et al.* [37, Theorem 4] to show that the optimizer of Eq. (2) is unique.

Theorem 1 (Ref. [37]): *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 4 (Dual nondegeneracy): Let Z^* be an optimal dual solution, and let M be any symmetric matrix. If the homogeneous linear system

$$MZ^* = 0, \tag{11}$$

$$\mathrm{tr}(MA_i) = 0 \quad \text{for all } i\in[m], \tag{12}$$

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 1 (Ref. [9]): *Let X^* be the unique optimal solution for the primal, and let $\{|u_i\rangle\langle u_i|\}_{i=0}^n$ be a quantum realization achieving the maximum quantum value of $\sum_{i=1}^n w_ip_i : p\in\mathcal{P}_q(\mathcal{G}_{\rm ex})$. Then the noncontextuality inequality $\sum_{i=1}^n w_ip_i\le B_{nc}(\mathcal{G}_{\rm ex},w)$ for all $p\in\mathcal{P}_{nc}(\mathcal{G}_{\rm ex})$ is a self-test for the realization $\{|u_i\rangle\langle u_i|\}_{i=0}^n$.*

III. RESULTS

We are given a Bell inequality of the form (5). We consider the set of events $p[\vec{a}|\vec{x}]$ such that $s_{\vec{x}}^{\vec{a}}\neq 0$. We index this set by i and denote the corresponding event as e_i. Then we can write the Bell witness as $\mathcal{B}=\sum_i w_ip_i$ with $w_i>0$ and $p_i=p(e_i)$. In addition, we are given a quantum realization $(|\psi\rangle,\{M^j_{a_j|x_j}\}_j)$ (let us call this the *reference* system) that achieves the quantum supremum S_Q of $\mathcal{B}$. Let $(\mathcal{G}_{\rm ex},w)$ be the weighted graph capturing the weights $\{w_i\}$ and mutual exclusivity relationships among the events $\{e_i\}$ in $\mathcal{B}$.

A. Assumptions

We enforce two sets of assumptions. The first one is the following.

Assumption 1: *(i) It holds that $S_Q=\vartheta(\mathcal{G}_{\rm ex},w)$.*

(ii) The Lovász theta SDP (2) corresponding to $(\mathcal{G}_{\rm ex},w)$ has a unique maximizer. This is a consequence of (i) for the scenarios of interest in this paper.

We consider two types of sets of indices, $\mathcal{I}$ and $\mathcal{I}_0=\mathcal{I}\cup\{0\}$. We consider the matrix $X_{ij}:=\langle\psi|\Pi_j\Pi_i|\psi\rangle$, where Π_i is a projection and Π_0 is the identity operator. We set $n:=|\mathcal{I}|$. Assumption 1(ii) means that the following SDP has a unique solution:

$$\vartheta(\mathcal{G}_{\rm ex},w)=\max\sum_{i\in\mathcal{I}}w_iX_{ii} \tag{13a}$$

$$\text{such that}\quad X_{ii}=X_{0i}\quad\text{for all } i\in[n], \tag{13b}$$

$$X_{ij}=0\quad\text{for all } i\sim j, \tag{13c}$$

$$X_{00}=1,\qquad X\in\mathbb{S}_+^{1+n}. \tag{13d}$$

The second set of assumptions depends on the scenario under study, so we detail them in each of the scenarios discussed.

B. Results

Our results can be summarized in several theorems (Theorems 2, 3, 4, and 5 below).

1. Bipartite case

Suppose 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 $i=(i_A,i_B)\in\mathcal{I}$,

$$v_i=a_{i_A}\otimes b_{i_B}, \tag{14}$$

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 $\eta_i>0$. Now, we consider a state $|\psi'\rangle$ on $\mathcal{H}'_A\otimes\mathcal{H}'_B$, and projections $\Pi^A_{i_A}$ and $\Pi^B_{i_B}$ on $\mathcal{H}'_A$ and $\mathcal{H}'_B$. Here, when $i_A = i'_A$ ($i_B = i'_B$) for $i \neq i'$, $\Pi^A_{i_A} = \Pi^A_{i'_A}$ ($\Pi^B_{i_B} = \Pi^B_{i'_B}$). Then, we define the projection $\Pi_i := \Pi^A_{i_A} \otimes \Pi^B_{i_B}$,

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 SDP (13). We define $|v'_i\rangle := \eta_i^{-1}\Pi_i|\psi'\rangle$.

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 $\{v_i\}_{i\in\mathcal{I}_0}$ of vectors spans the vector space $\mathcal{H}_A \otimes \mathcal{H}_B$.
(A2) There exists a subset $\mathcal{I}_B$ of indices of the space $\mathcal{H}_B$ with $|\mathcal{I}_B| = d_B = \dim \mathcal{H}_B$ and d_B sets $\{\mathcal{I}_{A,i_B}\}_{i_B\in\mathcal{I}_B}$ of indices of the space $\mathcal{H}_A$ $|\mathcal{I}_{A,i_B}| = d_A = \dim \mathcal{H}_A$ to satisfy the following (B1)–(B4) conditions.
(B1) We have $\bigcup_{i_B\in\mathcal{I}_B} \mathcal{I}_{A,i_B} \times \{i_B\} \subset \mathcal{I}$.
(B2) The set $\{b_{i_B}\}_{i_B\in\mathcal{I}_B}$ spans the space $\mathcal{H}_B$.
(B3) The set $\{a_{i_A}\}_{i_A\in\mathcal{I}_{A,i_B}}$ spans the space $\mathcal{H}_A$ for any $i_B \in \mathcal{I}_B$.
(B4) We define the graph on $\mathcal{I}_B$ in the following way. The node $i_B \in \mathcal{I}_B$ is connected to $i'_B \in \mathcal{I}_B$ when the following two conditions hold.
  (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.
  Note that this refers not to an exclusivity graph but to another graph defined on the nodes i_B.

In the two-qubit case if the set $\{v_i\}_{i\in\mathcal{I}}$ of vectors contains the following four vectors then the conditions (A1) and (A2) hold:

$$a_0 \otimes b_0, \quad a_1 \otimes b_0, \quad a_0 \otimes b_1, \quad a_2 \otimes b_1, \tag{15}$$

with $a_0 \neq a_1, a_2$, $\langle b_0, b_1\rangle \neq 0$.

Under the above conditions and the rank-1 condition, the following theorem guarantees the existence of local isometries to realize the desired structure.

Theorem 2: *Assume that the optimal maximizer given in Eq. (14) satisfies conditions (A1) and (A2) and that the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (13). 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 from $\mathcal{H}_A$ to $\mathcal{H}'_A$ and V_B from $\mathcal{H}_B$ to $\mathcal{H}'_B$ such that*

$$V_A \otimes V_B|\psi\rangle = |\psi'\rangle, \tag{16}$$

$$V_A \otimes V_B|v_i\rangle = |v'_i\rangle, \tag{17}$$

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

Proof. See Appendix E 1. ■

Now we consider the general case. In addition to (A1) and (A2), we assume the following conditions.

(A3) Ideal systems $\mathcal{H}_A$ and $\mathcal{H}_B$ are two dimensional.
(A4) Each system has only two measurements. That is, the set $\bar{\mathcal{I}}_A$ ($\bar{\mathcal{I}}_B$) of all indices of the space $\mathcal{H}_A$ ($\mathcal{H}_B$) is composed of four elements. For any element $i_A \in \bar{\mathcal{I}}_A$ ($i_B \in \bar{\mathcal{I}}_B$), there exists an element $i'_A \in \bar{\mathcal{I}}_A$ ($i'_B \in \bar{\mathcal{I}}_B$) such that $\langle a_{i_A}|a_{i'_A}\rangle = 0$ ($\langle b_{i_B}|b_{i'_B}\rangle = 0$).

When conditions (A3) and (A4) hold, $\bar{\mathcal{I}}_A$ ($\bar{\mathcal{I}}_B$) is written as $\mathcal{B}_{A,0} \cup \mathcal{B}_{A,1}$ ($\mathcal{B}_{B,0} \cup \mathcal{B}_{B,1}$), where $\mathcal{B}_{A,j} = \{(0,j),(1,j)\}$ [$\mathcal{B}_{B,j} = \{(0,j),(1,j)\}$] 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 $\Pi_i = \Pi^A_{i_A} \otimes \Pi^B_{i_B}$.

(C1) When $i_A, i'_A \in \bar{\mathcal{I}}_A$ ($i_B, i'_B \in \bar{\mathcal{I}}_B$) satisfy $\langle a_{i_A}|a_{i'_A}\rangle = 0$ ($\langle b_{i_B}|b_{i'_B}\rangle = 0$), we have $\Pi^A_{i_A} + \Pi^A_{i'_A} = I$ ($\Pi^B_{i_B} + \Pi^B_{i'_B} = I$).

Then, we have the following extension of Theorem 2 without the rank-1 condition under the above additional conditions.

Theorem 3: *Assume that the optimal maximizer given in Eq. (14) satisfies conditions (A1)–(A4), the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (13), and that 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*

$$V_A \otimes V_B|\psi\rangle \otimes |\mathrm{junk}\rangle = |\psi'\rangle, \tag{18}$$

$$V_A \otimes V_B|v_i\rangle \otimes |\mathrm{junk}\rangle = |v'_i\rangle, \tag{19}$$

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

Proof. See Appendix E 1 a. ■

2. Tripartite 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 $i = (i_A, i_B, i_C) \in \mathcal{I}$,

$$v_i = a_{i_A} \otimes b_{i_B} \otimes c_{i_C}, \tag{20}$$

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 $\Pi^A_{i_A}$, $\Pi^B_{i_B}$, $\Pi^C_{i_C}$ on $\mathcal{H}'_A$, $\mathcal{H}'_B$, and $\mathcal{H}'_C$. Then, we define the projection $\Pi_i := \Pi^A_{i_A} \otimes \Pi^B_{i_B} \otimes \Pi^B_{i_C}$.

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

We consider the case in which the ranks of the projections $\Pi^A_{i_A}$, $\Pi^B_{i_B}$, and $\Pi^C_{i_C}$ are one. We introduce the following conditions.

Definition 5: Three distinct elements $i, j, k \in \mathcal{I}$ are called *linked* when the following two conditions hold.

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

(C2) Vectors v_i, v_j share 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 $i_C \neq j_C$. Vectors v_i, v_k share a $t_{i,k}$th common element for $t_{i,k} \in \{A, B, C\} \setminus \{t_{i,j}\}$. Vectors v_j, 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 the vectors of $\mathbb{C}^{d_A}$ are called *connected* when there exist three linked elements $i, j, k \in \mathcal{I}$ such that the first components of $i, j, k \in \mathcal{I}$ are x_A, x_A'.

For i_B, i_C, we use the notation

$$\psi_{(i_B,i_C)} := b_{i_B} \otimes c_{i_C}. \tag{21}$$

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

(A5) The vectors $\{v_i\}_{i\in\mathcal{I}_0}$ span the vector space $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$.

(A6) There exists a subset $\mathcal{I}_A$ of indices 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 indices 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 $\{\psi_{i_{BC}}\}_{i_{BC}\in\mathcal{I}_{BC,i_A}}$ spans the space $\mathcal{H}_B \otimes \mathcal{H}_C$ and $\mathcal{I}_0 = \bigcup_{i_A\in\mathcal{I}_A}(\{i_A\} \times \mathcal{I}_{BC,i_A})$. We consider the graph G_A with the set $\mathcal{I}_A$ of vertices such that the edges are given as the pair of all connected elements in $\mathcal{I}_A$ in accordance with Definition 5. The graph G_A is not divided into two disconnected parts.

(A7) The vectors $\{b_{i_B} \otimes c_{i_C}\}_{(i_B,i_C)\in\bigcup_{i_A\in\mathcal{I}_A}\mathcal{I}_{BC,i_A}}$ satisfy condition (A2) by substituting c_{i_C} into a_{i_A}. That is, there exist a subset $\mathcal{I}_B$ of the second indices and subsets $\mathcal{I}_{C,i_B}$ of the third indices such that they satisfy conditions (B1)–(B4). We denote the graph defined in this condition by G_B.

Under the above conditions and the rank-1 condition, the following theorem guarantees the existence of local isometries to realize the desired structure in the tripartite case.

Theorem 4: *Assume that the optimal maximizer given in Eq. (20) satisfies conditions (A5)–(A7) and that the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (13). In addition, the ranks of the projections $\Pi^A_{i_A}$, $\Pi^B_{i_B}$, and $\Pi^C_{i_C}$ are assumed to be one. Then there exist isometries V_A from $\mathcal{H}_A$ to $\mathcal{H}_A'$, V_B from $\mathcal{H}_B$ to $\mathcal{H}_B'$, and V_C from $\mathcal{H}_C$ to $\mathcal{H}_C'$ such that*

$$V_A \otimes V_B \otimes V_C|\psi\rangle = |\psi'\rangle, \tag{22}$$

$$V_A \otimes V_B \otimes V_C|v_i\rangle = |v_i'\rangle, \tag{23}$$

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

Proof. See Appendix E 2 a. ∎

Now we consider the general case. We define $|v_i'\rangle := \eta_i^{-1}\Pi^A_{i_A} \otimes \Pi^B_{i_B} \otimes \Pi^C_{i_C}|\psi'\rangle$. Let $\bar{\mathcal{I}}_A, \bar{\mathcal{I}}_B, \bar{\mathcal{I}}_C$ be the sets of indices of the spaces $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C$.

We introduce other conditions for the optimal maximizer given in Eq. (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 $\bar{\mathcal{I}}_A$, $\bar{\mathcal{I}}_B$, and $\bar{\mathcal{I}}_C$ are composed of four elements. For any element $i_A \in \bar{\mathcal{I}}_A$ ($i_B \in \bar{\mathcal{I}}_B$, $i_C \in \bar{\mathcal{I}}_C$), there exists an element $i_A' \in \bar{\mathcal{I}}_A$ ($i_B' \in \bar{\mathcal{I}}_B$, $i_C' \in \bar{\mathcal{I}}_C$) 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, $\bar{\mathcal{I}}_A$ ($\bar{\mathcal{I}}_B$, $\bar{\mathcal{I}}_C$) 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 $\mathcal{B}_{A,j} = \{(0,j), (1,j)\}$ [$\mathcal{B}_{B,j} = \{(0,j), (1,j)\}, \mathcal{B}_{C,j} = \{(0,j), (1,j)\}$] 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 $i_A, i_A' \in \bar{\mathcal{I}}_A$ ($i_B, i_B' \in \bar{\mathcal{I}}_B$, $i_C, i_C' \in \bar{\mathcal{I}}_C$) 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 $\Pi^A_{i_A} + \Pi^A_{i_A'} = I$ ($\Pi^B_{i_B} + \Pi^B_{i_B'} = I$, $\Pi^C_{i_C} + \Pi^C_{i_C'} = I$).

Then, we have the following extension of Theorem 4 without the rank-1 condition under the above additional conditions.

Theorem 5: *Assume that the optimal maximizer given in Eq. (20) satisfies conditions (A5)–(A9) and that the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in 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

$$V_A \otimes V_B \otimes V_C|\psi\rangle \otimes |\text{junk}\rangle = |\psi'\rangle, \tag{24}$$

$$V_A \otimes V_B \otimes V_C|v_i\rangle \otimes |\text{junk}\rangle = |v_i'\rangle, \tag{25}$$

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. See Appendix E 2 b. ■

IV. TEST CASES

Here, we apply our techniques to the CHSH, chained, Mermin, and AS Bell inequalities; see Table I.

A. CHSH self-testing

Self-testing is known to hold for the maximum quantum violation of the CHSH inequality [5]. Here, we study the CHSH inequality in the graph of exclusivity framework [39].

Recall that the graph of exclusivity corresponding to the Bell witness given by Eq. (4) is given by the $C_{i_8}(1,4)$ graph (see Fig. 1). We claim that the optimal solution to dual (10) for $C_{i_8}(1,4)$ is given by

$$Z_{\text{CHSH}} = \left(\begin{array}{c|cccccccc}
2+\sqrt{2} & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ \hline
-1 & 1 & h & 0 & 0 & k & 0 & 0 & h \\
-1 & h & 1 & h & 0 & 0 & k & 0 & 0 \\
-1 & 0 & h & 1 & h & 0 & 0 & k & 0 \\
-1 & 0 & 0 & h & 1 & h & 0 & 0 & k \\
-1 & k & 0 & 0 & h & 1 & h & 0 & 0 \\
-1 & 0 & k & 0 & 0 & h & 1 & h & 0 \\
-1 & 0 & 0 & k & 0 & 0 & h & 1 & h \\
-1 & h & 0 & 0 & k & 0 & 0 & h & 1
\end{array}\right), \tag{26}$$

where $k = 3 - 2\sqrt{2}$ and $h = 2 - \sqrt{2}$. The Lovász theta SDP has zero duality gap, that is, the primal optimal solution and optimal dual solution yields the same program value. It can be easily verified that Eq. (26) is a feasible solution to Eq. (10) for the graph $C_{i_8}(1,4)$. 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_{CHSH} is nondegenerate. This requires us to show that $M = 0$ is the only symmetric 9×9 matrix satisfying Eqs. (11) and (12) corresponding to the Lovász theta SDP. That is, the linear system

$$M_{00} = 0, \qquad M_{0i} = M_{ii}, \qquad M_{ij} = 0 \quad \text{for all } i \sim j, \qquad MZ^* = 0 \tag{27}$$

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 form

$$M = \left(\begin{array}{c|cccccccc}
0 & m_1 & m_2 & m_3 & m_4 & m_5 & m_6 & m_7 & m_8 \\ \hline
m_1 & m_1 & 0 & m_9 & m_{15} & 0 & m_{20} & m_{23} & 0 \\
m_2 & 0 & m_2 & 0 & m_{10} & m_{16} & 0 & m_{21} & m_{24} \\
m_3 & m_9 & 0 & m_3 & 0 & m_{11} & m_{17} & 0 & m_{22} \\
m_4 & m_{15} & m_{10} & 0 & m_4 & 0 & m_{12} & m_{18} & 0 \\
m_5 & 0 & m_{16} & m_{11} & 0 & m_5 & 0 & x_{13} & m_{19} \\
m_6 & m_{20} & 0 & m_{17} & m_{12} & 0 & m_6 & 0 & m_{14} \\
m_7 & m_{23} & m_{21} & 0 & m_{18} & m_{13} & 0 & m_7 & 0 \\
m_8 & 0 & m_{24} & m_{22} & 0 & m_{19} & m_{14} & 0 & m_8
\end{array}\right). \tag{28}$$

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

The optimal solution for primal (2) is given by

TABLE I. Summary of test cases. This table summarizes what theorem guarantees the self-testing for each Bell inequality. Some of our results assume the rank-1 condition, i.e., the projection operator is assumed to be rank 1. The column "Rank 1" shows the requirement for this condition.

Inequality	Approach	Rank 1
CHSH	Theorem 3	No
Mermin	Theorem 5	No
Chained Bell inequality	Theorem 2	Yes
AS	Theorem 2	Yes

$$P_{\mathrm{CHSH}} = \left(\begin{array}{c|cccccccc} 1 & \chi & \chi & \chi & \chi & \chi & \chi & \chi & \chi \\ \hline \chi & \chi & 0 & \frac{1}{2}\chi & \xi & 0 & \xi & \frac{1}{2}\chi & 0 \\ \chi & 0 & \chi & 0 & \frac{1}{2}\chi & \xi & 0 & \xi & \frac{1}{2}\chi \\ \chi & \frac{1}{2}\chi & 0 & \chi & 0 & \frac{1}{2}\chi & \xi & 0 & \xi \\ \chi & \xi & \frac{1}{2}\chi & 0 & \chi & 0 & \frac{1}{2}\chi & \xi & 0 \\ \chi & 0 & \xi & \frac{1}{2}\chi & 0 & \chi & 0 & \frac{1}{2}\chi & \xi \\ \chi & \xi & 0 & \xi & \frac{1}{2}\chi & 0 & \chi & 0 & \frac{1}{2}\chi \\ \chi & \frac{1}{2}\chi & \xi & 0 & \xi & \frac{1}{2}\chi & 0 & \chi & 0 \\ \chi & 0 & \frac{1}{2}\chi & \xi & 0 & \xi & \frac{1}{2}\chi & 0 & \chi \end{array}\right), \tag{29}$$

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

$$|v_1\rangle = |A_{1,0}\rangle \otimes |B_{1,1}\rangle, \tag{30a}$$
$$|v_2\rangle = |A_{0,0}\rangle \otimes |B_{1,0}\rangle, \tag{30b}$$
$$|v_3\rangle = |A_{0,1}\rangle \otimes |B_{0,1}\rangle, \tag{30c}$$
$$|v_4\rangle = |A_{1,0}\rangle \otimes |B_{0,0}\rangle, \tag{30d}$$
$$|v_5\rangle = |A_{1,1}\rangle \otimes |B_{1,0}\rangle, \tag{30e}$$
$$|v_6\rangle = |A_{0,1}\rangle \otimes |B_{1,1}\rangle, \tag{30f}$$
$$|v_7\rangle = |A_{0,0}\rangle \otimes |B_{0,0}\rangle, \tag{30g}$$
$$|v_8\rangle = |A_{1,1}\rangle \otimes |B_{0,1}\rangle, \tag{30h}$$

where the kets corresponding to the local measurements are given by

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

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

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

$$a_0 = |A_{0,0}\rangle, \qquad a_1 = a_2 = |A_{0,1}\rangle, \tag{31}$$
$$b_0 = |B_{0,0}\rangle, \qquad b_1 = |B_{1,0}\rangle. \tag{32}$$

Moreover, the local measurements for the CHSH case satisfy conditions (A3), (A4), and (C1) as well. Thus, the CHSH case satisfies all the conditions for Theorem 3, which implies that 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

$$V_A \otimes V_B|\psi\rangle \otimes |\mathrm{junk}\rangle = |\psi'\rangle, \tag{33}$$

$$V_A \otimes V_B|v_i\rangle \otimes |\mathrm{junk}\rangle = |v'_i\rangle, \tag{34}$$

for $i \in \mathcal{I}$, where $|\mathrm{junk}\rangle$ 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 [45]. As detailed in Appendix C, the Bell witness of this inequality includes 16 events. Their graph of exclusivity, denoted G_M, is shown in Fig. 2.

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

$$P_{\mathrm{Mermin}} = \begin{bmatrix} 1 & ae_{16}^T \\ ae_{16} & aI_{16} + bE_{\overline{G_M}} \end{bmatrix} \in \mathbb{R}^{(17\times 17)}, \tag{35}$$

where $a = 0.25$, $b = 0.125$, e_{16} is the all one column vector of size 16, $E_{\overline{G_M}}$ 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_{Mermin} is trivially similar to the CHSH case. The quantum state and measurement settings can be obtained via Gram decomposition of P_{Mermin}. A quantum realization is achieved with

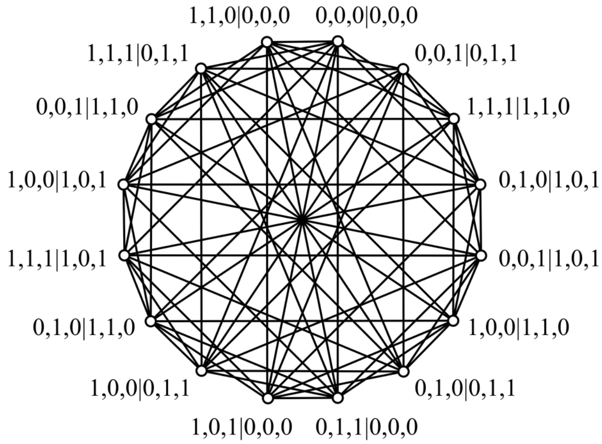

FIG. 2. Graph of exclusivity of the 16 events in the Bell witness (C5) of the Mermin inequality. Here, Z and X are denoted 0 and 1, respectively, while -1 and 1 are denoted 0 and 1, respectively. We refer to this graph as G_M. It is the complement of the Shrikhande graph [69].

the three-qubit GHZ state $|u_0\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ and the projective measurements

$$\begin{aligned}
|u_1\rangle &= |Z\rangle \otimes |P\rangle \otimes |P\rangle,\\
|u_2\rangle &= |O\rangle \otimes |M\rangle \otimes |P\rangle,\\
|u_3\rangle &= |O\rangle \otimes |P\rangle \otimes |M\rangle,\\
|u_4\rangle &= |Z\rangle \otimes |M\rangle \otimes |M\rangle,\\
|u_5\rangle &= |P\rangle \otimes |Z\rangle \otimes |P\rangle,\\
|u_6\rangle &= |M\rangle \otimes |O\rangle \otimes |P\rangle,\\
|u_7\rangle &= |M\rangle \otimes |Z\rangle \otimes |M\rangle,\\
|u_8\rangle &= |P\rangle \otimes |O\rangle \otimes |M\rangle,\\
|u_9\rangle &= |P\rangle \otimes |P\rangle \otimes |Z\rangle,\\
|u_{10}\rangle &= |M\rangle \otimes |M\rangle \otimes |Z\rangle,\\
|u_{11}\rangle &= |M\rangle \otimes |P\rangle \otimes |O\rangle,\\
|u_{12}\rangle &= |P\rangle \otimes |M\rangle \otimes |O\rangle,\\
|u_{13}\rangle &= |O\rangle \otimes |O\rangle \otimes |O\rangle,\\
|u_{14}\rangle &= |Z\rangle \otimes |Z\rangle \otimes |O\rangle,\\
|u_{15}\rangle &= |Z\rangle \otimes |O\rangle \otimes |Z\rangle,\\
|u_{16}\rangle &= |O\rangle \otimes |Z\rangle \otimes |Z\rangle,
\end{aligned}$$

where $|Z\rangle = |0\rangle$, $|O\rangle = |1\rangle$, $|P\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, and $|M\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$. This quantum realization achieves the quantum bound of the Bell witness [given by Eq. (C5) in Appendix C], i.e., 4, which is equal to the Lovász theta number of G_M (Fig. 2). 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)–(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 $\mathcal{I}_A := \{O, P\}$. We then have

$$\mathcal{I}_{BC,O} = \{(O,O),(Z,Z),(M,P),(P,M)\}, \tag{36}$$

$$\mathcal{I}_{BC,P} = \{(Z,P),(P,Z),(O,M),(M,O)\}. \tag{37}$$

Two elements $O, P \in \mathcal{I}_A$ are connected in the sense given at the end of Definition 5 by choosing $\{i,j,k\} = \{(P,Z,P),(O,Z,Z),(O,M,P)\}$. Based on Eqs. (36) and (37), we choose the subsets $\mathcal{I}_B$, $\mathcal{I}_{C,Z}$, and $\mathcal{I}_{C,P}$ as

$$\mathcal{I}_B := \{Z,P\}, \qquad \mathcal{I}_{C,Z} := \{Z,P\}, \qquad \mathcal{I}_{C,P} := \{Z,M\}. \tag{38}$$

The subsets $\mathcal{I}_B$, $\mathcal{I}_{C,Z}$, and $\mathcal{I}_{C,P}$ satisfy conditions (B1)–(B4). The Mermin case satisfies conditions (A8) and (A9) in addition to conditions (A5)–(A7). In short, it satisfies all requirements of Theorem 5. Thus, given the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ that realize the optimal solution in 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

$$V_A \otimes V_B \otimes V_C|\psi\rangle \otimes |\text{junk}\rangle = |\psi'\rangle, \tag{39}$$

$$V_A \otimes V_B \otimes V_C|v_i\rangle \otimes |\text{junk}\rangle = |v'_i\rangle, \tag{40}$$

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

Since P_{Mermin} is a Gram matrix of vectors $|u_0\rangle, |u_1\rangle, \ldots, |u_{16}\rangle$, the rank of P_{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_{Mermin} is 7. Thus, a seven-dimensional configuration can achieve the maximal violation of the Mermin inequality. We append a seven-dimensional configuration corresponding to P_{Mermin} in Appendix D. In the tripartite Bell scenario, one obtains maximal violation of the Mermin inequality using three qubits and thus a Hilbert space of dimension eight. This is purely because the seven-dimensional state cannot be realized as a tensor product of three two-dimensional subsystems. Moreover, as one expects, 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 7.

The graph G_M is the complement of the Shrikhande graph [69]. Since the Shrikhande graph is vertex transitive, it implies that G_M is also vertex transitive. We observe that there is a unique behavior in $Q_{\text{STAB}}(G_M)$ (see Definition 16 in Appendix A) that achieves $\alpha^\star(G_M)$. Moreover, by vertex transitivity in the theta body, we also observe that there is a unique behavior that achieves $\vartheta(G_M)$.

C. Self-testing chained Bell inequalities

The chained Bell inequalities [41,42] 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

$$\begin{aligned} I_N^{\text{Bell}} &= \langle A_1B_2\rangle + \langle A_5B_4\rangle + \cdots + \langle A_3B_2\rangle + \langle A_3B_4\rangle \\ &\quad + \langle A_{2N-1}B_{2N}\rangle - \langle A_1B_{2N}\rangle \\ &\leq_{\text{LHV}} 2N-2. \end{aligned} \tag{41}$$

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 $\langle A_iB_j\rangle$ denote the expectation value of the product of outcomes for A_i and B_j. The maximum quantum value of I_N^{Bell} is $2N\cos(\pi/2N)$.

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

$$\langle A_iB_j\rangle = 2P(1,1|i,j) + 2P(-1,-1|i,j) - 1, \tag{42}$$

$$-\langle A_iB_j\rangle = 2P(1,-1|i,j) + 2P(-1,1|i,j) - 1. \tag{43}$$

Using Eqs. (42) and (43), we can re-express the inequality in Eq. (41) as

$$\begin{aligned} I_N^{\text{CSW}} &= P(1,1|1,2) + P(-1,-1|1,2) + P(1,1|3,2) \\ &\quad + P(-1,-1|3,2) + \cdots + P(1,1|2N-1,2N) \\ &\quad + P(-1,-1|2N-1,2N) + P(1,-1|1,2N) \\ &\quad + P(-1,1|1,2N) \\ &\leq_{\text{LHV}} N-1, \end{aligned} \tag{44}$$

where CSW means Cabello-Severini-Winter. The graph of exclusivity for the events in I_N^{CSW} is $\text{Ci}_{4N}(1,2N)$ and is isomorphic to the Möbius ladder graph of order $4N$. The independence number of $\text{Ci}_{4N}(1,2N)$ is $2N-1$. The Lovász theta number, however, remains unknown and has been conjectured [67,70] to be equal to

$$\vartheta(\text{Ci}_{4N}(1,2N)) = N\left[1+\cos\left(\frac{\pi}{2N}\right)\right]. \tag{45}$$

D. Proof of the conjecture of Araújo *et al.*

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

$$Z_N^\star = \begin{bmatrix} N/l & -e_{4N}^T \\ -e_{4N} & lA_{C_{4N}} + \begin{bmatrix} I_{2N} & f\, I_{2N} \\ f\, I_{2N} & I_{2N} \end{bmatrix} \end{bmatrix} \times \in \mathbb{R}^{(4N+1)\times(4N+1)}, \tag{46}$$

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

Lemma 2: *It holds that* $Z_N^\star \succcurlyeq 0$.

Proof. Taking the Schur complement of $Z_N^\star$ with respect to its top left entry, we have

$$Z_N^\star \succcurlyeq 0 \quad \Longleftrightarrow \quad M_N - \frac{l}{N}e_{4N}e_{4N}^T \succcurlyeq 0, \tag{47}$$

where

$$M_N = lA_{C_{4N}} + \begin{bmatrix} I_{2N} & f\, I_{2N} \\ f\, I_{2N} & I_{2N} \end{bmatrix}.$$

To prove that $Z_N^\star$ is positive semidefinite, it remains to show that the eigenvalues of $M_N - (l/N)e_{4N}e_{4N}^T$ are non-negative. Note that e_{4N} is a common eigenvector of M_N and $e_{4N}e_{4N}^T$ 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 characterized. ■

Fact 1: *The eigenvalues of the circulant matrix*

$$C = \begin{bmatrix} c_0 & c_{n-1} & \dots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \dots & c_1 & c_0 \end{bmatrix} \tag{48}$$

are given by

$$\begin{aligned} \lambda_j &= c_0 + c_{n-1}\omega^j + c_{n-2}\omega^{2j} + \cdots + c_1\omega^{(n-1)j}, \\ j &= 0,1,\dots,n-1, \end{aligned} \tag{49}$$

where $\omega = \exp(2\pi i/n)$ *is the* nth *root of unity.*

Note that matrix M_N is a circulant matrix with $n=4N$, $c_0=1, c_1=l, c_{2N}=f, c_{n-1}=l$, and $c_i=0$ for $i\notin\{0,1,2N,n-1\}$. Therefore, its eigenvalues are given by

$\lambda_j = 1 + l(\omega^j + \omega^{(n-1)j}) + f\omega^{2Nj}$ for $j = 0, 1, \ldots, n-1$. Simplifying this, we obtain

$$\lambda_j = \begin{cases} 1 - f + 2l\cos\frac{\pi j}{2N} & \text{if } j \text{ is odd,} \\ 1 + f + 2l\cos\frac{\pi j}{2N} & \text{if } j \text{ is even.} \end{cases} \quad (50)$$

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

$$\lambda_{2N} = 1 + f - 2l = 1 + \frac{1-k}{1+k} - \frac{2}{1+k} = 0. \quad (51)$$

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

$$\begin{aligned} \lambda_{2N-1} &= 1 - f + 2l\cos\left(\frac{(2N-1)\pi}{2N}\right) \\ &= 1 - f - 2l\cos\left(\frac{\pi}{2N}\right) \\ &= 1 - f - 2lk \\ &= 1 - \frac{1-k}{1+k} - \frac{2k}{1+k} \\ &= 0. \end{aligned} \quad (52)$$

Finally, note that the eigenvalue of M_N corresponding to the eigenvector e_{4N} is $1 + 2l + f$. Whereas $(l/N)e_{4N}e_{4N}^T$ is a rank-1 matrix with eigenvector e_{4N} with eigenvalue $(l/N) \times 4N = 4l$. Therefore, the eigenvalue of $M_N - (l/N)e_{4N}e_{4N}^T$ corresponding to the eigenvector e_{4N} is $1 + 2l + f - 4l = 1 + f - 2l = 1 + (1-k)/(1+k) - 2/(1+k) = 0$. The rest of the eigenvalues of $M_N - (l/N)e_{4N}e_{4N}^T$ 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 optimization program (10) for* $\mathrm{Ci}_{4N}(1, 2N)$ *is* $Z_N^\star$ *(Eq. (46)).*

Proof. We need to show that

1. Z_N^* is dual feasible for the program in Eq. (10).
2. $Z_N^\star$ corresponds to the dual optimal value.

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

Using the measurement settings for chained Bell inequalities in Ref. [67], one obtains the output of the primal SDP (2) for I_N^{CSW} equal to $N[1 + \cos(\pi/2N)]$. Strong duality for SDP (2) implies that $Z_N^\star$ corresponds to the dual optimal value. ■

The proof of the uniqueness of the primal optimal is similar to the proof corresponding to n-cycle graphs in Ref. [9]. Chained Bell inequalities satisfy conditions (A1) and (A2), and this can be checked by choosing the vectors in Eq. (15) as follows:

$$\begin{aligned} a_0 = |A_1 = 1\rangle, \quad a_1 = |A_3 = 1\rangle, \quad a_2 = |A_{2N-1} = -1\rangle, \\ b_0 = |B_2 = 1\rangle, \qquad b_1 = |B_{2N} = -1\rangle. \end{aligned} \quad (53)$$

Here, $|A_1 = 1\rangle$ expresses the eigenvector of A_1 with eigenvalue 1. This notation applies to other observables. The optimal maximizer given in Eq. (14) satisfies conditions (A1) and (A2) and the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (13). In addition, the ranks of the projections $\Pi_{i_A}^A$ and $\Pi_{i_B}^B$ are assumed to be one. Thus, due to Theorem 2, there exist isometries V_A from $\mathcal{H}_A$ to $\mathcal{H}_A'$ and V_B from $\mathcal{H}_B$ to $\mathcal{H}_B'$ such that

$$V_A \otimes V_B|\psi\rangle = |\psi'\rangle, \quad (54)$$

$$V_A \otimes V_B|v_i\rangle = |v_i'\rangle, \quad (55)$$

for $i \in \mathcal{I}$. This completes the proof of self-testability for the chained Bell inequalities for rank-1 projectors.

Since $Z_N^\star$ corresponds to the dual optimal value, we have $\vartheta(\mathrm{Ci}_{4N}(1, 2N)) = N[1 + \cos(\pi/2N)]$ as conjectured in Ref. [70].

E. AS self-testing

The AS Bell inequalities [53] 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

$$A_{s_n} = \sum_{i+j<n} \langle A_i B_j\rangle - \sum_{i+j=n} \min\{i-1, j-1\}\langle A_i B_j\rangle \overset{\text{LHV}}{\leq} \frac{n(n+2)}{4}. \quad (56)$$

By taking into account the facts that

$$\langle A_i B_j\rangle = 2[P(0,0|i,j) + P(1,1|i,j)] - 1, \quad (57)$$

$$-\langle A_i B_j\rangle = 2[P(0,1|i,j) + P(1,0|i,j)] - 1, \quad (58)$$

Eq. (56) can be rewritten as

$$\begin{aligned} A_{s_n}^c = &\sum_{i+j<n} [P(0,0|i,j) + P(1,1|i,j)] \\ &+ \sum_{i+j=n} \min\{i-1, j-1\}[P(0,1|i,j) + P(1,0|i,j)] \\ &\overset{\text{LHV}}{\leq} \frac{n(n+1)}{2}. \end{aligned} \quad (59)$$

For example, for the case $n = 4$,

$$
\begin{aligned}
A^c_{s_4} = {} & P(0,0|0,0) + P(1,1|0,0) + P(0,0|0,1) \\
& + P(1,1|0,1) + P(0,0|0,2) + P(1,1|0,2) \\
& + P(0,0|0,3) + P(1,1|0,3) + P(0,0|1,0) \\
& + P(1,1|1,0) + P(0,0|1,1) + P(1,1|1,1) \\
& + P(0,0|1,2) + P(1,1|1,2) + P(0,0|1,3) \\
& + P(1,1|1,3) + P(0,0|2,0) + P(1,1|2,0) \\
& + P(0,0|2,1) + P(1,1|2,1) + 2[P(0,0|2,2) \\
& + P(1,1|2,2)] + P(0,0|3,0) + P(1,1|3,0) \\
& + P(0,0|3,1) + P(1,1|3,1). \qquad (60)
\end{aligned}
$$

The (vertex-weighted) graph of exclusivity of the 26 events in Eq. (60) is shown in Fig. 3 and has $\alpha(G,w) = 10$, $\vartheta(G,w) = 7 + 5\sqrt{6}/3$, and $\alpha^*(G,w) = 14$. Note that the vertex weight is 2 for events $[0,0|2,2]$ and $[1,1|2,2]$ and 1 otherwise. We have

$$
\begin{aligned}
|w_1\rangle &= |A_0\rangle \otimes |A_0\rangle, & |w_2\rangle &= |B_0\rangle \otimes |B_0\rangle, && (61a)\\
|w_3\rangle &= |A_0\rangle \otimes |A_1\rangle, & |w_4\rangle &= |B_0\rangle \otimes |B_1\rangle, && (61b)\\
|w_5\rangle &= |A_0\rangle \otimes |A_2\rangle, & |w_6\rangle &= |B_0\rangle \otimes |B_2\rangle, && (61c)\\
|w_7\rangle &= |A_0\rangle \otimes |A_3\rangle, & |w_8\rangle &= |B_0\rangle \otimes |B_3\rangle, && (61d)\\
|w_9\rangle &= |A_1\rangle \otimes |A_0\rangle, & |w_{10}\rangle &= |B_1\rangle \otimes |B_0\rangle, && (61e)\\
|w_{11}\rangle &= |A_1\rangle \otimes |A_1\rangle, & |w_{12}\rangle &= |B_1\rangle \otimes |B_1\rangle, && (61f)\\
|w_{13}\rangle &= |A_1\rangle \otimes |A_2\rangle, & |w_{14}\rangle &= |B_1\rangle \otimes |B_2\rangle, && (61g)\\
|w_{15}\rangle &= |A_1\rangle \otimes |A_3\rangle, & |w_{16}\rangle &= |B_1\rangle \otimes |B_3\rangle, && (61h)\\
|w_{17}\rangle &= |A_2\rangle \otimes |A_0\rangle, & |w_{18}\rangle &= |B_2\rangle \otimes |B_0\rangle, && (61i)\\
|w_{19}\rangle &= |A_2\rangle \otimes |A_1\rangle, & |w_{20}\rangle &= |B_2\rangle \otimes |B_1\rangle, && (61j)\\
|w_{21}\rangle &= |A_2\rangle \otimes |A_2\rangle, & |w_{22}\rangle &= |B_2\rangle \otimes |B_2\rangle, && (61k)\\
|w_{23}\rangle &= |A_3\rangle \otimes |A_0\rangle, & |w_{24}\rangle &= |B_3\rangle \otimes |B_0\rangle, && (61l)\\
|w_{25}\rangle &= |A_3\rangle \otimes |A_1\rangle, & |w_{26}\rangle &= |B_3\rangle \otimes |B_1\rangle. && (61m)
\end{aligned}
$$

The violation of the Bell inequality $A^c_{s_4}$ can achieve $\vartheta(G,w)$ by choosing as the initial state

$$|s\rangle = \cos t(|00\rangle - |11\rangle) + \sin t(|01\rangle - |10\rangle), \qquad (62)$$

and as local measurements

$$A_i = |m(\alpha_i)\rangle, \qquad B_i = |m(\pi/2 + \alpha_i)\rangle \qquad (63)$$

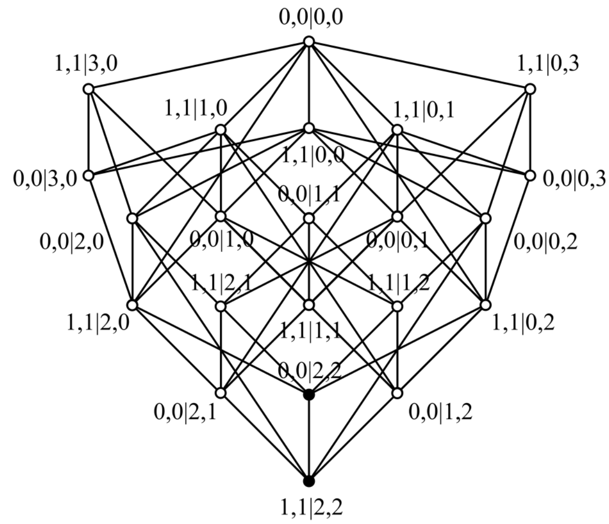

FIG. 3. Vertex-weighted graph of exclusivity for the events in the Bell inequality A_{s_4} in Eq. (60). There are 26 events. Black nodes represent vertices with weight 2 in Eq. (60) and white nodes represent vertices with weight 1.

with $i = 0,1,2,3$, $m(\alpha) = \cos\alpha|0\rangle + \sin\alpha|1\rangle$, and

$$\alpha_0 = 0, \qquad \alpha_1 = \arcsin\left(\frac{1}{\sqrt{6}}\right) \qquad (64a)$$

$$\alpha_2 = \frac{1}{2}\left(\pi - \arctan\left(\sqrt{\frac{5\sqrt{145}}{8} + \frac{77}{8}}\right)\right), \qquad (64b)$$

$$\alpha_3 = \frac{1}{2}\left(\pi - \arctan\left(48\sqrt{\frac{2}{275\sqrt{145} + 3317}}\right)\right), \qquad (64c)$$

$$t = \frac{1}{8}\left(\alpha_2 + 2\alpha_4 - \frac{\pi}{2}\right). \qquad (64d)$$

The primal optimal for the SDP corresponding to the quantum violation of $A^c_{s_4}$ can be obtained by the state and measurement directions given in Eqs. (62)–(64). Here, we omit its full expression, as it is straightforward, albeit 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 Eq. (15) as

$$
\begin{aligned}
a_0 &= |A_2 = 0\rangle, & a_1 = a_2 &= |A_3 = 0\rangle, \\
b_0 &= |B_0 = 0\rangle, & b_1 &= |B_1 = 0\rangle.
\end{aligned} \qquad (65)
$$

Here, $|A_1 = 1\rangle$ expresses the eigenvector of A_1 with eigenvalue 1. This notation is applied to other observables. The optimal maximizer given in Eq. (14) satisfies conditions (A1) and (A2) and the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (13). In addition, the ranks of the projections $\Pi^A_{i_A}$ and $\Pi^B_{i_B}$ are assumed to be one. Therefore, due to Theorem 2, there exist isometries V_A from $\mathcal{H}_A$ to $\mathcal{H}'_A$ and V_B from $\mathcal{H}_B$ to $\mathcal{H}'_B$ such that

$$V_A \otimes V_B|\psi\rangle = |\psi'\rangle, \tag{66}$$

$$V_A \otimes V_B|v_i\rangle = |v_i'\rangle, \tag{67}$$

for $i \in \mathcal{I}$. This completes the proof of self-testability for the $A^c_{s_4}$ Bell inequality for rank-1 projectors.

V. COMPARISON WITH EXISTING SEMIDEFINITE PROGRAMMING APPROACHES

The importance of semidefinite programming for studying the set of quantum correlations for Bell experiments was stimulated by Tsirelson's work [55] and developed in Refs. [36,56]. Most studies rely on the Navascués-Pironio-Acín (NPA) hierarchy of SDPs.

The first important observation is that the theta body of G defined before is not one of the levels of the NPA hierarchy [36]. See Appendix B for an overview of the NPA hierarchy. The NPA hierarchy includes the no-signaling and normalization conditions, which induce linear constraints in the corresponding SDPs. The aforementioned linear constraints are absent in the maximization over the theta body of G. Note that, e.g., the all-zero behavior $(0, 0, \ldots, 0, 0, 0)$ belongs to the theta body, but it is not in any of the levels of NPA hierarchy since it does not satisfy the normalization constraints.

The relevance of the theta body for the study of quantum correlations was pointed out in Ref. [39]. Graph-theoretic techniques to study sets of quantum correlations have also been used in Refs. [57,58]. Regarding self-testing, the techniques in Ref. [39] have been used to provide robust self-testing schemes in the framework of noncontextuality inequalities tested in experiments with sequential measurements on indivisible systems [9].

The second important observation is that, in contrast to existing methods of studying self-testing in Bell scenarios, which rely on the NPA hierarchy (e.g., Refs. [59–65]) and where semidefinite programming is used to get robustness curves, our work uses semidefinite programming to obtain rigorous analytical results. The only work that we are aware of that uses semidefinite programming to get Bell self-testing statements analytically is Ref. [66]. However, there the self-testing statements are only up to *global* isometries, while here we harness linear algebra arguments to provide self-testing statements up to *local* isometries. Moreover, our approach allows us to systematically obtain self-testing statements and allows us to establish connections with problems in discrete mathematics.

VI. ROBUSTNESS

Since our self-testing approach is based on SDP, the partial answer to the question regarding the robustness of our scheme is provided by the following lemma that was first used as a part of a proof in Ref. [9]. This lemma can be used to bound the distance between X^{opt}, the unique optimal solution of SDP (13), and X, which is any ϵ-suboptimal solution of the same SDP, i.e., $\sum_{i\in\mathcal{I}} w_i X_{ii} \geq \vartheta(\mathcal{G}_{\text{ex}}, w) - \epsilon$. The *Frobenius norm* is used as a distance measure here, which is defined as

$$\|A\|_F = \sqrt{\text{tr}(A^H A)}, \tag{68}$$

where A^H is the conjugate transpose of A.

Lemma 3 (Robustness)**:** *If a matrix X achieves an ϵ-suboptimal value in SDP (13) and X^{opt} is the unique solution then we can upper bound the Frobenius-norm distance between X^{opt} and X as*

$$\|X^{\text{opt}} - X\|_F \leq \mathcal{O}(\epsilon). \tag{69}$$

The proof of this lemma can be found in Appendix B of Ref. [9] under the section titled "Step 2." Equation (B4) of Ref. [9] therein is essentially the above lemma.

Note that this is not the complete answer to the robustness question as further work is required to translate the result at the level of measurement settings and states. Apart from analytical approaches, one can always use numerical methods such as SWAP [60] to analyze the robustness of our scheme.

VII. SUMMARY AND OPEN PROBLEMS

We have shown how, by combining ideas from graph theory and SDP, we can obtain a new perspective on the problem of self-testing quantum states and measurements in Bell scenarios. The motivation for our approach was the observation that the set of quantum correlations for a Bell scenario is difficult to characterize, while, using ideas from Ref. [39], one can provide an easy to characterize single SDP-based relaxation of this set. Then, 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.

There is a requirement that is inherent to the method: that the maximum quantum violation of the Bell inequality is equal to the Lovász theta number of the corresponding graph. Interestingly, this is frequently the case and the maximum quantum violation of many fundamental Bell and Bell-like inequalities satisfy this condition. An interesting open problem though is understanding whether there is a fundamental physical reason why this condition holds for some Bell inequalities but not for others. At first sight, the only reason is that, for some Bell inequalities, the constraints introduced by the Bell scenario (see Ref. [71, Secs. II G and IV G] for details) do not forbid the quantum set achieving the Lovász theta number of the corresponding G, while others do. In general, the simpler the Bell inequality is, the less likely it is that the constraints of the scenario prohibit reaching Lovász's theta number. However, this point may require further investigation.

Our results for bipartite and tripartite cases have been stated as Theorems 2, 3, 4, and 5. In addition, we have applied our techniques to quantum correlations maximally violating the CHSH [40], chained [41,42], three-party Mermin [45], and AS [53] Bell inequalities.

For the CHSH and tripartite Mermin Bell inequalities, we recovered self-testing statements for projectors of arbitrary rank. Interestingly, for the Mermin inequality, the rank of the primal optimal matrix is seven, indicating that the self-testing preparation dimension can be seven (rather than eight, which is the minimum quantum dimension to accommodate a tripartite quantum system).

For the chained and AS Bell inequalities, we proved a self-testing statement for local measurements represented by rank-1 projective measurements. To our knowledge, this is the first time that the AS inequality has been proven to allow for self-testing. However, an open problem is whether the assumption of rank-1 projectors can be removed. This is an interesting challenge for future work.

Arguably, the most unexpected result is the proof, using our approach to the chained Bell inequalities, of a conjecture [67,70] about the closed-form expression for the Lovász theta number for Möbius ladder graphs [72]. This illustrates, on the one hand, that the interplay of ideas from graph theory and quantum mechanics can be useful for solving problems in both areas. In addition, it vindicates the independent interest of our approach, as the standard one based on the NPA hierarchy would not have allowed for such a proof.

Self-testing of multipartite Bell inequalities is more interesting and challenging than that of bipartite and tripartite Bell inequalities. We believe that the self-testing statement pertaining could be recovered after additional work using the techniques developed in this study.

To conclude, the aim of this article has been to show that combining methods from graph theory and Bell nonlocality is useful to solving problems in both areas. In future developments it would be interesting to apply this approach to identify new quantum correlations allowing for self-testing and open problems in graph theory that may benefit from these methods, improve some of the proofs of self-testing by removing additional assumptions, and generalize the approach to include the effect of noise.

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APPENDIX A: GRAPH THEORY BASICS

A graph $G=(V,E)$ consists of a set of vertices V and edges E [73]. Two vertices are *adjacent* if they share an edge between them. The complement graph $\bar{G}$ has the same vertices as G, but its edge set is complement to set E. A *clique* of a graph is a set of pairwise adjacent vertices. The complement of a clique is a set of vertices that are pairwise nonadjacent. A natural generalization of a graph is a hypergraph with generalized edges connecting more than two vertices. These generalized edges are called hyperedges.

Definition 6 (**Cyclic graph**)**:** A graph with n vertices such that every ith vertex of the graph is connected to $[(i+1) \mod n]$th and $[(i-1) \mod n]$th vertices is called a cyclic graph and denoted C_n.

An elegant generalization of the concept of a cyclic graph is the concept of a circulant graph.

Definition 7 (**Circulant graph**)**:** Given a list $[L]$ of integers, a graph with n vertices where the ith vertex is connected to $[(i+l) \mod n]$th and $[(i-l) \mod n]$th vertices for all $l\in[L]$ is called a circulant graph and denoted $\mathrm{Ci}_n[L]$. We call $\mathrm{Ci}_n[1]$ a cyclic graph.

Definition 8 (**Orthonormal representation of a graph [74]**)**:** 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

$$\langle v_i|v_j\rangle=0 \quad \text{for all } i,j\notin E. \tag{A1}$$

We use the notation $\mathrm{OR}(G)$ to represent the orthonormal representation of G.

Definition 9 (Stable set)**:** A stable set is a set of vertices of a graph such that no two vertices that lie in it share an edge.

Definition 10 (Independence number)**:** The independence number of a graph is the cardinality of the largest stable set of the graph. It is denoted $\alpha(G)$.

Definition 11 (Convex hull)**:** The convex hull of a set A is the smallest convex set containing A.

Definition 12 (Incidence vector)**:** An incidence vector of a set $B\subset A$ is a vector $P\in\mathbb{R}_+^{|A|}$ such that, for every $i\in A$,

$$P_i=\begin{cases}1 & \text{if } i\in B,\\ 0 & \text{otherwise.}\end{cases} \tag{A2}$$

Definition 13 (Stable set polytope)**:** The convex hull of all the incidence vectors of stable sets of graph G is called a stable set polytope of the graph. It is denoted STAB(G).

Definition 14 (**Theta body**)**:** Let $\{|v\rangle_i\}$ correspond to the orthonormal representation of $\bar{G}$. Given a unit vector $|\phi\rangle = (1, 0, 0, \ldots, 0) \in \mathbb{R}^d$ with only first coordinate 1 and 0 elsewhere, the theta body of graph G is defined as

$$\Theta(G) = \{P \in \mathbb{R}^{|V|} : P_i = |\langle\psi|v_i\rangle|^2\}. \tag{A3}$$

Definition 15 (**Lovász theta number [74]**)**:** The Lovász theta number $\vartheta(G)$ of a graph G is defined as

$$\vartheta(G) = \max_{|\phi\rangle,\{|v_i\rangle\}} \sum_i |\langle\phi|v_i\rangle|^2,$$

where $|\phi\rangle$ is a unit vector and $\{|v_i\rangle\}$ is an orthonormal representation of graph G. Vector $|\phi\rangle$ is also known as the handle.

Definition 16 (**Fractional stable set polytope**)**:** The fractional stable set polytope is given by

$$Q_{\text{STAB}}(G) = \left\{P \in \mathbb{R}^{|V|_+} : \sum_{i\in C} P_i \le 1 \right. \\ \left. \text{for every clique } C \text{ of graph } G\right\}. \tag{A4}$$

Definition 17 (**Fractional packing number**)**:** The fractional packing of a graph G is the value of the linear program

$$\alpha^*(G) = \max\left\{\sum_{i=1}^n x_i : x \in Q_{\text{STAB}}(G)\right\}. \tag{A5}$$

Definition 18 (**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 $\text{rank}\, X = \dim \text{span}(v_1, v_2, \ldots, v_k)$. Decomposing Gram matrix X such that $X = AA^\dagger$ is called the Gram decomposition of X. The rows of A are related to v_i up to isometry.

Definition 19 (**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 from V to V such that $h(v_1) = v_2$.

Fact 2 (**Ref. [74]**)**:** *For a given graph G,* $\alpha(G) \le \vartheta(G) \le \alpha^*(G)$.

It is worthwhile to note that $\text{STAB}(G) \subseteq \Theta(G) \subseteq Q_{\text{STAB}}(G)$ [75]. An alternate formulation of the theta body of a graph $G = ([n], E)$ is given by

$$\Theta(G) = \{x \in \mathbb{R}^n_+ | \exists X \in \mathbb{S}^{1+n}_+, X_{00} = 1, X_{ii} = X_{0i}, \\ X_{ij} = 0 \text{ for all } ij \in E\}. \tag{A6}$$

Lemma 4 (**Ref. [76]**)**:** *We have* $x \in \Theta(G)$ *if and only if there exist unit vectors* $d, w_1, \ldots, w_n$ *such that*

$$x_i = \langle d, w_i\rangle^2 \quad \text{for all } i \in [n] \quad \text{and} \quad \langle w_i, w_j\rangle = 0 \\ \text{for } ij \in E. \tag{A7}$$

APPENDIX B: NPA HIERARCHY BASICS

In this section, we review the basics of the semidefinite programming hierarchy of Navascués, Pironio, and Acin, also referred to as the NPA hierarchy. This hierarchy provides a uniform family of semidefinite programs that converges to the commuting measurement value of any nonlocal game. This section has been adapted from Ref. [77]. For the details of NPA hierarchy, we refer the reader to Refs. [36,78]. Let us consider a Bell scenario where two spatially separated parties receive inputs $x, y = 1, 2, \ldots, m$ and provide outputs $a, b = 1, 2, \ldots, d$. The resulting correlation $P(a, b|x, y)$ is called quantum if there exist a bipartite quantum state ρ and local operators A^x_a and B^y_b such that

$$P(a, b|x, y) = \text{tr}(\rho A^x_a \otimes B^y_b).$$

We denote the set of resulting correlations by $\mathcal{Q}$. Without loss of generality, the state ρ and the measurement operators A^x_a and B^y_b can be taken as pure and projective, respectively. Consequently, the conditions for the correlation $P(a, b|x, y)$ to be quantum is recast as follows. The condition

$$P(a, b|x, y) \in \mathcal{Q}$$

holds if and only if there exist a pure bipartite quantum state ψ and local operators A^x_a and B^y_b such that the relations

$$P(a, b|x, y) = \langle\psi|A^x_a \otimes B^y_b|\psi\rangle, \\ A^x_a A^x_{a'} = A^x_a \delta_{a,a'}, \qquad B^y_b B^y_{b'} = B^y_b \delta_{b,b'}$$

hold for any elements x, a, a', y, b, b'. Let us define the set $\mathcal{S}_k$ as consisting of the identity operator and all products of operators A^x_a and B^y_b up to degree k. For example, we have

$$\mathcal{S}_1 = \{\mathbb{I}\} \bigcup_{a,x} \{A^x_a\} \bigcup_{b,y} \{B^y_b\}$$

and

$$\mathcal{S}_{k+1} = \mathcal{S}_k \bigcup_{i,j} \{S^{(i)}_k S^{(j)}_1\}.$$

Here, $S_k^{(i)}$ is the ith element of $\mathcal{S}_k$. Using the elements of $\mathcal{S}_k$, we define a moment matrix Γ_k of order k, with elements

$$\Gamma_k^{(i,j)} = \langle\psi|(S_k^{(i)})^\dagger S_k^{(j)}|\psi\rangle. \tag{B1}$$

The moment matrix Γ_k must satisfy three different kinds of property.

1. *Linear constraints.*—These constraints arise from normalization of the measurement operators, commutation of Alice's and Bob's operators, and their local orthogonality properties. These constraints can be written as
$$\mathrm{Tr}[\Gamma_k G_l] = 0$$
by using some fixed suitable matrices G_l with $l \in \mathcal{G}_k$. That is, the set $\{G_l\}_{l\in\mathcal{G}_k}$ of linear constraints depends on k.
2. *Observable probability property.*—The moment matrix Γ_k contains some elements that correspond to observable probabilities. For example, a correlation $P(a,b|x,y) = \langle\psi|A_a^x B_b^y|\psi\rangle$ is recovered from Γ_k as follows. Since A_a^x and B_b^y are elements of $\mathcal{S}_1 \subset \mathcal{S}_{k+1}$, we choose $i(a,x)$ and $j(b,y)$ as $A_a^x = S_1^{i(a,x)}$ and $B_b^y = S_1^{j(b,y)}$. Then, a correlation is recovered as the observable probability; $P(a,b|x,y) = \Gamma_k^{i(a,x),j(b,y)}$.
3. *Positive semidefinite condition.*—We have $\Gamma_k^\dagger = \Gamma_k$ and $\Gamma_k \succcurlyeq 0$.

Suppose that we want to determine whether a correlation $P(a,b|x,y)$ is quantum, is highly nontrivial. The NPA hierarchy provides an outer relaxation of the quantum set and thus provides a way to tackle a relaxed version of the aforementioned membership problem for the correlation $P(a,b|x,y)$. The NPA hierarchy at level k for a correlation $P(a,b|x,y)$ is given by

$$\text{Find } \Gamma_k \tag{B2}$$

such that

$$\begin{gathered}\Gamma_k \succcurlyeq 0, \qquad \Gamma_k^\dagger = \Gamma_k, \qquad \Gamma_k^{(0,0)} = 1,\\ \mathrm{Tr}[\Gamma_k G_l] = 0 \quad \text{for all } l \in \mathcal{G}_{\|},\\ \Gamma_k^{i(a,x),j(b,y)} = P(a,b|x,y) \quad \text{for all } a,b,x,y.\end{gathered}$$

Let us refer to the set of correlations $P(a,b|x,y)$ that have a solution Γ_k that satisfies the above feasibility problem (B2) at the kth level as $\mathcal{Q}_k$. We get a sequence of SDPs, each of which provides a relaxation to the membership problem, i.e., the problem of deciding whether $P \in \mathcal{Q}$. Since the matrix given in Eq. (B1) satisfies the condition of $\mathcal{Q}_k$, the relation $\mathcal{Q} \subseteq \mathcal{Q}_k$ holds. Also, the relation $\mathcal{Q}_{k+1} \subseteq \mathcal{Q}_k$ holds because we have the inclusion relation $\{G_l\}_{l\in\mathcal{G}_k} \subset \{G_l\}_{l\in\mathcal{G}_{k+1}}$ for linear constraints by considering Γ_k as a submatrix of Γ_{k+1}. Even though the membership problem is hard, the relaxations are SDPs and hence easy to solve. Although the membership problem of $\mathcal{Q}_k$ is a relaxation of the membership problem of $\mathcal{Q}$, we can get a tighter approximation of $\mathcal{Q}$ by increasing k.

APPENDIX C: MERMIN INEQUALITY

Mermin's Bell inequality [45] refers to an n-partite Bell scenario (with $n \geq 3$ odd; there is also a version for n even [46], but we do not consider it here). The interest of this Bell inequality is based on the fact that the Bell operator

$$S_n = \frac{1}{2i}\left[\bigotimes_{j=1}^{n}(\sigma_x^{(j)} + i\sigma_z^{(j)}) - \bigotimes_{j=1}^{n}(\sigma_x^{(j)} - i\sigma_z^{(j)})\right], \tag{C1}$$

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

$$\langle S_n\rangle \overset{\text{LHV, NCHV}}{\leq} 2^{(n-1)/2}. \tag{C2}$$

For example,

$$\begin{aligned}S_3 = {}& \sigma_z^{(1)}\otimes\sigma_x^{(2)}\otimes\sigma_x^{(3)} + \sigma_x^{(1)}\otimes\sigma_z^{(2)}\otimes\sigma_x^{(3)}\\ &+ \sigma_x^{(1)}\otimes\sigma_x^{(2)}\otimes\sigma_z^{(3)} - \sigma_z^{(1)}\otimes\sigma_z^{(2)}\otimes\sigma_z^{(3)}.\end{aligned} \tag{C3}$$

Therefore, we can write (using obvious notation),

$$\langle S_3\rangle = \langle ZXX\rangle + \langle XZX\rangle + \langle XXZ\rangle - \langle ZZZ\rangle. \tag{C4}$$

Then, by taking into account the facts that

$$\begin{aligned}\langle ZXX\rangle = {}& P(Z = X = X = 1) + P(Z = X = -X = -1)\\ &+ P(Z = -X = X = -1) + P(-Z = X = X\\ &= -1) - P(Z = X = X = -1) - P(Z = X =\\ &-X = 1) - P(Z = -X = X = 1) - P(-Z = X\\ &= X = 1) = 2[P(Z = X = X = 1)\\ &+ P(Z = X = -X = -1) + P(Z = -X\\ &= X = -1) + P(-Z = X = X = -1)] - 1,\end{aligned}$$

$$
\begin{aligned}
\langle XZX\rangle &= P(X=Z=X=1)+P(X=Z=-X=-1)+P(X=-Z=X=-1)\\
&\quad +P(-X=Z=X=-1)-P(X=Z=X=-1)-P(X=Z=-X=1)\\
&\quad -P(X=-Z=X=1)-P(-X=Z=X=1)\\
&=2[P(X=Z=X=1)+P(X=Z=-X=-1)+P(X=-Z=X=-1)\\
&\quad +P(-X=Z=X=-1)]-1,\\
\langle XXZ\rangle &= P(X=X=Z=1)+P(X=X=-Z=-1)+P(X=-X=Z=-1)\\
&\quad +P(-X=X=Z=-1)-P(X=X=Z=-1)-P(X=X=-Z=1)\\
&\quad -P(X=-X=Z=1)-P(-X=X=Z=1)\\
&=2[P(X=X=Z=1)+P(X=X=-Z=-1)+P(X=-X=Z=-1)\\
&\quad +P(-X=X=Z=-1)]-1,\\
-\langle ZZZ\rangle &= P(Z=Z=Z=-1)+P(Z=Z=-Z=1)+P(Z=-Z=Z=1)\\
&\quad +P(-Z=Z=Z=1)-P(Z=Z=Z=1)-P(Z=Z=-Z=-1)\\
&\quad -P(Z=-Z=Z=-1)-P(-Z=Z=Z=-1)\\
&=2[P(Z=Z=Z=-1)+P(Z=Z=-Z=1)+P(Z=-Z=Z=1)\\
&\quad +P(-Z=Z=Z=1)]-1,
\end{aligned}
$$

we can rewrite $\langle S_3\rangle$ as a sum of the probabilities of 16 events. That is,

$$
\begin{aligned}
\langle S_3\rangle = 2[&P(Z=X=X=1)+P(Z=X=-X=-1)+P(Z=-X=X=-1)\\
&+P(-Z=X=X=-1)+P(X=Z=X=1)+P(X=Z=-X=-1)\\
&+P(X=-Z=X=-1)+P(-X=Z=X=-1)+P(X=X=Z=1)\\
&+P(X=X=-Z=-1)+P(X=-X=Z=-1)+P(-X=X=Z=-1)\\
&+P(Z=Z=Z=-1)+P(Z=Z=-Z=1)+P(Z=-Z=Z=1)\\
&+P(-Z=Z=Z=1)]-4.
\end{aligned}
\tag{C5}
$$

The graph of exclusivity of these 16 events is the complement of the Shrikhande graph [69]. This graph, shown in Fig. 2, has $\alpha=3$ and $\vartheta=\alpha^*=4$. Similarly, one can obtain the graph corresponding to any $\langle S_n\rangle$.

APPENDIX D: SEVEN-DIMENSIONAL CONFIGURATION FOR THE MERMIN CASE

We have numerically obtained (rounded up to three digits after the decimal) the following seven-dimensional configuration achieving the Lováz theta number of the graph in Fig. 2:

$$
\begin{aligned}
|u_0\rangle &= (1,0,0,0,0,0,0)^T,\\
|u_1\rangle &= (0.25,-0.113,-0.241,0.284,0.088,0.166,-0.029)^T,\\
|u_2\rangle &= (0.25,-0.110,-0.251,-0.120,0.247,-0.021,-0.191)^T,\\
|u_3\rangle &= (0.25,-0.292,0.079,0.151,0.075,-0.051,-0.255)^T,\\
|u_4\rangle &= (0.25,0.182,-0.087,0.003,0.311,0.215,0.059)^T,\\
|u_5\rangle &= (0.25,-0.226,0.069,0.104,-0.227,0.262,-0.021)^T,\\
|u_6\rangle &= (0.25,0.223,-0.059,0.300,0.068,-0.075,0.184,)^T,
\end{aligned}
$$

$$|u_7\rangle = (0.25, -0.004, -0.232, 0.130, -0.298, 0.001, 0.167)^T,$$
$$|u_8\rangle = (0.25, -0.247, 0.049, -0.152, 0.140, -0.278, 0.059)^T,$$
$$|u_9\rangle = (0.25, 0.25, -0.059, -0.25, 0.019, 0.09, -0.22)^T,$$
$$|u_{10}\rangle = (0.25, 0, -0.24, -0.27, -0.139, -0.186, 0.004)^T,$$
$$|u_{11}\rangle = (0.25, 0.069, 0.27, 0.019, -0.15, 0.062, -0.285)^T,$$
$$|u_{12}\rangle = (0.25, 0.044, 0.261, 0.167, 0.054, -0.29, -0.04)^T,$$
$$|u_{13}\rangle = (0.25, 0.069, 0.22, -0.178, -0.004, 0.31, 0.067)^T,$$
$$|u_{14}\rangle = (0.25, 0.045, 0.21, -0.030, 0.204, -0.04, 0.31)^T,$$
$$|u_{15}\rangle = (0.25, -0.18, 0.039, -0.20, -0.16, 0.035, 0.293)^T,$$
$$|u_{16}\rangle = (0.25, 0.29, -0.03, 0.046, -0.225, -0.199, -0.097)^T.$$

APPENDIX E: PROOFS OF SELF-TESTING

We consider two types of sets of indices $\mathcal{I}$ and $\mathcal{I}_0 = \mathcal{I} \cup \{0\}$. We consider the matrix $X_{ij} := \langle\psi|\Pi_j \Pi_i|\psi\rangle$, where Π_i is a projection and Π_0 is the identity operator. We set $n := |\mathcal{I}|$. Then, we assume that the following SDP has a unique solution:

$$\vartheta(\mathcal{G}_{\rm ex}, w) = \max \sum_{i\in\mathcal{I}} w_i X_{ii} \tag{E1a}$$

$$\text{such that} \quad X_{ii} = X_{0i} \quad \text{for all } i \in [n], \tag{E1b}$$

$$X_{ij} = 0 \quad \text{for all } i \sim j, \tag{E1c}$$

$$X_{00} = 1, \quad X \in \mathbb{S}_+^{1+n}. \tag{E1d}$$

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 $i = (i_A, i_B) \in \mathcal{I}$,

$$v_i = a_{i_A} \otimes b_{i_B}, \tag{E2}$$

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 $\eta_i > 0$.

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

In the following, we discuss how state $|\psi'\rangle$ is locally converted to $|\psi\rangle$ when the vectors $\Pi_i|\psi'\rangle$ realize the optimal solution in SDP (E1). We define $|v'_i\rangle := \eta_i^{-1}\Pi_i|\psi'\rangle$.

First, we consider the case that the ranks of the projections $\Pi^A_{i_A}$ and $\Pi^B_{i_B}$ are one. Now, we consider conditions (A1), (A2), (B1)–(B4), which are introduced in the main text. To understand these conditions, we list several examples.

Example 1: The CHSH inequality satisfies conditions (A1) and (A2), which can be checked by choosing the vectors in Eq. (15) as

$$\begin{aligned} a_0 &= |A_{0,0}\rangle, \qquad a_1 = a_2 = |A_{0,1}\rangle, \\ b_0 &= |B_{0,0}\rangle, \qquad b_1 = |B_{1,0}\rangle. \end{aligned} \tag{E3}$$

For the canonical realization corresponding to the CHSH inequality, see Eqs. (30).

Example 2: The chained Bell inequalities satisfy conditions (A1) and (A2), which can be checked by choosing the vectors in Eq. (15) as

$$a_0 = |A_1 = 1\rangle, \quad a_1 = |A_3 = 1\rangle, \quad a_2 = |A_{2N-1} = -1\rangle, \tag{E4}$$

$$b_0 = |B_2 = 1\rangle, \quad b_1 = |B_{2N} = -1\rangle.$$

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: AS self-testing satisfies conditions (A1) and (A2), which can be checked by choosing the vectors in Eq. (15) as

$$\begin{aligned} a_0 = |A_2 = 0\rangle, \qquad a_1 = a_2 = |A_3 = 0\rangle, \\ b_0 = |B_0 = 0\rangle, \qquad b_1 = |B_1 = 0\rangle. \end{aligned} \tag{E5}$$

For the canonical realization corresponding to the AS inequalities, see Eqs. (61).

Proof of Theorem 2. Since the vectors $\Pi_i|\psi'\rangle$ realize the optimal solution in SDP (E1), there exists an isometry V from $\mathcal{H}_A \otimes \mathcal{H}_B$ to $\mathcal{H}'_A \otimes \mathcal{H}'_B$ such that

$$V\Pi_i|\psi\rangle = \Pi_i|\psi'\rangle \quad \text{for } i \in \mathcal{I}. \tag{E6}$$

We define $\Pi_i|\psi'\rangle = \eta_i|a'_{i_A} \otimes b'_{i_B}\rangle$.

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 that

$$\begin{aligned} \langle a_{i_A}, a_{i'_A}\rangle &= \langle a_{i_A} \otimes b_{i_B}, a_{i'_A} \otimes b_{i_B}\rangle \\ &= \langle a'_{i_A} \otimes b'_{i_B}, a'_{i'_A} \otimes b'_{i_B}\rangle \\ &= \langle a'_{i_A}, a'_{i'_A}\rangle. \end{aligned} \tag{E7}$$

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

$$V_{A,i_B}|a_{i_A}\rangle = |a'_{i_A}\rangle \quad \text{for } i_A \in \mathcal{I}_{A,i_B}. \tag{E8}$$

We choose two connected elements $i_B, i'_B \in \mathcal{I}_B$. For $i_A \in \mathcal{I}_{A,i_B} \cap \mathcal{I}_{A,i'_B}$, Eq. (E6) implies that

$$\begin{aligned} \langle b_{i_B}, b_{i'_B}\rangle &= \langle a_{i_A} \otimes b_{i_B}, a_{i_A} \otimes b_{i'_B}\rangle \\ &= \langle a'_{i_A} \otimes b'_{i_B}, a'_{i_A} \otimes b'_{i'_B}\rangle \\ &= \langle b'_{i_B}, b'_{i'_B}\rangle. \end{aligned} \tag{E9}$$

Hence, for $i_A \in \mathcal{I}_{A,i_B}$ and $i'_A \in \mathcal{I}_{A,i'_B}$, Eq. (E6) implies that

$$\begin{aligned} \langle a_{i_A}, a_{i'_A}\rangle\langle b_{i_B}, b_{i'_B}\rangle &= \langle a_{i_A} \otimes b_{i_B}, a_{i'_A} \otimes b_{i'_B}\rangle \\ &= \langle a'_{i_A} \otimes b'_{i_B}, a'_{i'_A} \otimes b'_{i'_B}\rangle \\ &= \langle a'_{i_A}, a'_{i'_A}\rangle\langle b'_{i_B}, b'_{i'_B}\rangle. \end{aligned} \tag{E10}$$

Since condition (B4-1) guarantees $\langle b_{i_B}, b_{i'_B}\rangle \neq 0$, the combination of Eqs. (E9) and (E10) implies that

$$\langle a_{i_A}, a_{i'_A}\rangle = \langle a'_{i_A}, a'_{i'_A}\rangle. \tag{E11}$$

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

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

$$\langle a_{i_A}, a_{i'_A}\rangle \neq 0. \tag{E12}$$

Condition (A1) implies that

$$\begin{aligned} \langle a_{i_A}, a_{i'_A}\rangle\langle b_{i_B}, b_{i'_B}\rangle &= \langle a_{i_A} \otimes b_{i_B}, a_{i'_A} \otimes b_{i'_B}\rangle \\ &= \langle a'_{i_A} \otimes b'_{i_B}, a'_{i'_A} \otimes b'_{i'_B}\rangle \\ &= \langle a'_{i_A}, a'_{i'_A}\rangle\langle b'_{i_B}, b'_{i'_B}\rangle \\ &= \langle V_A a_{i_A}, V_A a_{i'_A}\rangle\langle b'_{i_B}, b'_{i'_B}\rangle \\ &= \langle a_{i_A}, a_{i'_A}\rangle\langle b'_{i_B}, b'_{i'_B}\rangle. \end{aligned} \tag{E13}$$

The combination of Eqs. (E12) and (E13) implies that

$$\langle b_{i_B}, b_{i'_B}\rangle = \langle b'_{i_B}, b'_{i'_B}\rangle. \tag{E14}$$

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

$$V_B|b_{i_B}\rangle = |b'_{i_B}\rangle \quad \text{for } i_B \in \mathcal{I}_B. \tag{E15}$$

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 $V = V_A \otimes V_B$. ■

a. General case

We consider the general case. In addition to conditions (A1) and (A2), we consider conditions (A3) and (A4). To show Theorem 3, we prepare the following lemma.

Lemma 5: *Assume that the vectors $(\Pi_i|\psi'\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (E1). Assume that a projection Π is commutative with Π_i for any $i \in \mathcal{I}$. Also, assume that $\Pi\psi' \neq 0$. Let $\psi'(\Pi)$ be the normalized vector of $\Pi\psi'$. Then the vectors $\Pi_i|\psi'(\Pi)\rangle$ realize the optimal solution in SDP (E1).*

Proof. We have

$$\sum_i \langle\psi'|\Pi_i|\psi'\rangle = \sum_i \langle\Pi\psi'|\Pi_i|\Pi\psi'\rangle + \sum_i \langle(I-\Pi)\psi'|\Pi_i|(I-\Pi)\psi'\rangle = \|\Pi\psi'\|^2 \sum_i \langle\psi'(\Pi)|\Pi_i|\psi'(\Pi)\rangle + \|(I-\Pi)\psi'\|^2 \sum_i \langle\psi'(I-\Pi)|\Pi_i|\psi'(I-\Pi)\rangle. \tag{E16}$$

Since the vectors $(\Pi_i|\psi'(\Pi)\rangle)_{i\in\mathcal{I}}$ and the vectors $(\Pi_i|\psi'(I-\Pi)\rangle)_{i\in\mathcal{I}}$ satisfy the condition of SDP (E1), Eq. (E16) shows that either the vectors $(\Pi_i|\psi'(\Pi)\rangle)_{i\in\mathcal{I}}$ or the vectors $(\Pi_i|\psi'(I-\Pi)\rangle)_{i\in\mathcal{I}}$ realize the optimal solution in SDP (E1). Hence, the remaining $(\Pi_i|\psi'(\Pi)\rangle)_{i\in\mathcal{I}}$ vectors or $(\Pi_i|\psi'(I-\Pi)\rangle)_{i\in\mathcal{I}}$ vectors also realize the optimal solution in SDP (E1). ■

Considering the contraposition of Lemma 5, we have the following lemma.

Lemma 6: *Assume that the vectors $\Pi_i|\psi'\rangle$ realize the optimal solution in SDP (E1). Assume that a projection Π is commutative with Π_i for any $i\in\mathcal{I}$. Also, there exists an element $j\in\mathcal{I}$ such that $\Pi\Pi_j=0$. Then $\Pi\psi'=0$.*

Proof of Theorem 3. Step 1. Let $P_{A,(0,0),(0,1)}$ be the projection to the eigenspace of $\Pi^A_{(0,0)}\Pi^A_{(0,1)}\Pi^A_{(0,0)}$ with one eigenvalue. Let $P_{A,(0,0),(1,1)}$ be the projection to the eigenspace of $\Pi^A_{(0,0)}\Pi^A_{(0,1)}\Pi^A_{(0,0)}$ with zero eigenvalue. Let $\{e^A_{j_A}\}$ be the orthogonal basis corresponding to the orthogonal eigenvectors of $\Pi^A_{(0,0)}\Pi^A_{(0,1)}\Pi^A_{(0,0)}$ with other eigenvalues. We define $f^A_{j_A}$ as the normalized vector of $\Pi^A_{(0,1)}e^A_{j_A}$. For $j_A\neq j'_A$, $f^A_{j_A}$ is orthogonal to $f^A_{j'_A}$ due to the choice of $\{e^A_{j_A}\}$. We define $g^A_{j_A}$ as the normalized vector of $f^A_{j_A}-\langle e^A_{j_A},f^A_{j_A}\rangle e^A_{j_A}$. Vector $g^A_{j_A}$ belongs to $\mathcal{H}^A_{(1,0)}$. For $j_A\neq j'_A$, $g^A_{j_A}$ is orthogonal to $g^A_{j'_A}$ because $e^A_{j_A}$ and $f^A_{j_A}$ are orthogonal to $e^A_{j'_A}$ and $f^A_{j'_A}$, respectively. We define the projection $\bar{\Pi}^A_{j_A}:=|e^A_{j_A}\rangle\langle e^A_{j_A}|+|g^A_{j_A}\rangle\langle g^A_{j_A}|$. For $j_A\neq j'_A$, we have $\bar{\Pi}^A_{j_A}\bar{\Pi}^A_{j'_A}=0$. Projection $\bar{\Pi}^A_{j_A}$ is commutative with $\Pi^A_{(0,0)}$, $\Pi^A_{(1,0)}$, $\Pi^A_{(0,1)}$, and $\Pi^A_{(1,1)}$. We define $\Pi^A:=\sum_{j_A}\bar{\Pi}^A_{j_A}$. Also, projections Π^A, $P_{A,(0,0),(0,1)}$, and $P_{A,(0,0),(1,1)}$ are commutative with $\Pi^A_{(0,0)}$, $\Pi^A_{(1,0)}$, $\Pi^A_{(0,1)}$, and $\Pi^A_{(1,1)}$. Since $(I-\Pi^A-P_{A,(0,0),(0,1)}-P_{A,(0,0),(1,1)})\Pi^A_{(0,0)}=0$, $P_{A,(0,0),(0,1)}\Pi^A_{(1,1)}=0$, and $P_{A,(0,0),(1,1)}\Pi^A_{(0,1)}=0$, Lemma 6 implies that $(I-\Pi^A-P_{A,(0,0),(0,1)}-P_{A,(0,0),(1,1)})\psi'=0$, $P_{A,(0,0),(0,1)}\psi'=0$, and $P_{A,(0,0),(1,1)}\psi'=0$. Hence, we have $\Pi^A\psi'=\psi'$.

In the same way, we define the projections $\bar{\Pi}^B_{j_B}$ and $\bar{\Pi}^B$. We define the projection $\bar{\Pi}_{(j_A,j_B)}:=\bar{\Pi}^A_{j_A}\bar{\Pi}^B_{j_B}$. Projection $\bar{\Pi}_{(j_A,j_B)}$ is commutative with Π_i for $i\in\mathcal{I}$. When $\bar{\Pi}_{(j_A,j_B)}\psi'\neq 0$, we define $\psi_{(j_A,j_B)}:=\alpha_{(j_A,j_B)}\bar{\Pi}_{(j_A,j_B)}\psi'$, where $\alpha_{(j_A,j_B)}:=\|\bar{\Pi}_{(j_A,j_B)}\psi'\|^{-1}$.

Step 2. Because of Lemma 5, the vectors $\Pi_i\psi_{(j_A,j_B)}=\Pi_i\bar{\Pi}_{(j_A,j_B)}\psi_{(j_A,j_B)}$ realize the optimal solution in SDP (E1). Also, $\Pi_i\bar{\Pi}_{(j_A,j_B)}$ is rank 1. Hence, we can apply Theorem 2 to the vectors $\Pi_i\bar{\Pi}_{(j_A,j_B)}\psi_{(j_A,j_B)}$. Thus, there exist isometries $V_{A,(j_A,j_B)}$ from $\mathcal{H}_A$ to $\operatorname{Im}\Pi^A_{j_A}$ and $V_{B,(j_A,j_B)}$ from $\mathcal{H}_B$ to $\operatorname{Im}\Pi^B_{j_B}$ such that

$$\begin{aligned}V_{A,(j_A,j_B)}\otimes V_{B,(j_A,j_B)}\psi &= \psi_{(j_A,j_B)}\eta_i(V_{A,(j_A,j_B)}a_{i_A})\otimes(V_{B,(j_A,j_B)}b_{i_B})\\ &= V_{A,(j_A,j_B)}\otimes V_{B,(j_A,j_B)}(\eta_i a_{i_A}\otimes b_{i_B})\\ &= \Pi_i\bar{\Pi}_{(j_A,j_B)}\psi_{(j_A,j_B)}\\ &= \Pi^A_{i_A}\bar{\Pi}^A_{j_A}\otimes\Pi^B_{i_B}\bar{\Pi}^B_{j_B}\psi_{(j_A,j_B)}.\end{aligned}$$

As shown in step 3 below, for $j_B\neq j'_B$, we have $V_{A,(j_A,j_B)}=\beta_{j_A,j_B,j'_B}V_{A,(j_A,j'_B)}$ with a constant β_{j_A,j_B,j'_B} when $\Pi_{(j_A,j_B)}\psi'\neq 0$ and $\Pi_{(j_A,j'_B)}\psi'\neq 0$. That is,

$$V_{A,(j_A,j_B)}\otimes V_{B,(j_A,j'_B)}\psi=\beta_{j_A,j_B,j'_B}\psi_{(j_A,j'_B)}. \tag{E17}$$

Then, for j_A, we choose an element j_B such that $\Pi_{(j_A,j_B)}\psi'\neq 0$. Then, we define $V_{A,j_A}:=V_{A,(j_A,j_B)}$. Thus, for elements j'_A and j'_B, there exists a constant $\beta_{j'_A,j'_B}$ such that

$$\begin{aligned}V_{A,j'_A}\otimes V_{B,j'_B}\psi &= \beta_{j'_A,j'_B}\psi_{(j'_A,j'_B)}\\ &= \beta_{j'_A,j'_B}\alpha_{(j'_A,j'_B)}\bar{\Pi}_{(j'_A,j'_B)}\psi'\\ &= \beta_{j'_A,j'_B}\alpha_{(j'_A,j'_B)}\bar{\Pi}^A_{j'_A}\bar{\Pi}^B_{j'_B}\psi'.\end{aligned}$$

Hence, we have

$$\beta^{-1}_{j'_A,j'_B}\alpha^{-1}_{(j'_A,j'_B)}V_{A,j'_A}\otimes V_{B,j'_B}\psi=\bar{\Pi}^A_{j'_A}\bar{\Pi}^B_{j'_B}\psi'. \tag{E18}$$

We define the spaces $\mathcal{K}_A$ and $\mathcal{K}_B$ spanned by $\{|j_A\rangle\}$ and $\{|j_B\rangle\}$, respectively. We define the junk state on $\mathcal{K}_A\otimes\mathcal{K}_B$ as

$$|\mathrm{junk}\rangle:=\sum_{j_A,j_B}\beta^{-1}_{j_A,j_B}\alpha^{-1}_{(j_A,j_B)}|j_A,j_B\rangle. \tag{E19}$$

We define the 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 $\mathcal{H}'_B$ as

$$V_A:=\sum_{j_A}V_{A,j_A}\langle j_A|,\qquad V_B:=\sum_{j_B}V_{B,j_B}\langle j_B|. \tag{E20}$$

The isometries V_A and V_B satisfy conditions (18) and (19).

Step 3. We show the following fact: for $j_B \neq j_B'$, we have $V_{A,(j_A,j_B)} = \beta_{j_A,j_B,j_B'} V_{A,(j_A,j_B')}$ with a constant $\beta_{j_A,j_B,j_B'}$ when $\Pi_{(j_A,j_B)}\psi' \neq 0$ and $\Pi_{(j_A,j_B')}\psi' \neq 0$.

We define $a_{i_A,j_A,j_B} := V_{A,(j_A,j_B)} a_{i_A}$. Then, we have

$$\Pi_i \bar{\Pi}_{(j_A,j_B')}\psi_{(j_A,j_B')} = \Pi^A_{i_A}\bar{\Pi}^A_{j_A} \otimes \Pi^B_{i_B}\bar{\Pi}^B_{j_B'}\psi_{(j_A,j_B')}. \tag{E21}$$

The above vector is a constant times $\eta_i a_{i_A,j_A,j_B} \otimes b_{i_B,j_A,j_B'}$. Also, the vectors $(\eta_i a_{i_A,j_A,j_B} \otimes b_{i_B,j_A,j_B'})_i$ and $(\Pi_i \bar{\Pi}_{(j_A,j_B')}\psi_{(j_A,j_B')})_i$ are the unique optimal solution in SDP (E1). Hence, there exists a constant $\beta_{j_A,j_B,j_B'}$ such that $\eta_i a_{i_A,j_A,j_B} \otimes b_{i_B,j_A,j_B'} = \beta_{j_A,j_B,j_B'} \Pi_i \bar{\Pi}_{(j_A,j_B')}\psi_{(j_A,j_B')}$, which is the desired statement. ∎

2. Tripartite 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 $i = (i_A, i_B, i_C) \in \mathcal{I}$,

$$v_i = a_{i_A} \otimes b_{i_B} \otimes c_{i_C}, \tag{E22}$$

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 $\Pi^A_{i_A}$, $\Pi^B_{i_B}$, $\Pi^C_{i_C}$ on $\mathcal{H}_A'$, $\mathcal{H}_B'$, and $\mathcal{H}_C'$. Then, we define the projection $\Pi_i := \Pi^A_{i_A} \otimes \Pi^B_{i_B} \otimes \Pi^B_{i_C}$.

In the following, we discuss how state $|\psi'\rangle$ is locally converted to $|\psi\rangle$ when the vectors $\Pi_i|\psi'\rangle$ realize the optimal solution in SDP (E1). We define $|v_i'\rangle := \eta_i^{-1}\Pi_i|\psi'\rangle$.

a. Rank-1 case

We consider the case in which the ranks of projections $\Pi^A_{i_A}$, $\Pi^B_{i_B}$, and $\Pi^C_{i_C}$ are one. We focus on conditions (C1), (C2), (A5)–(A7). The following is an example for conditions (A5)–(A7).

Example 4: We can check that Mermin self-testing satisfies conditions (A5)–(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

$$\mathcal{I}_{BC,O} = \{(O,O),(Z,Z),(M,P),(P,M)\}, \tag{E23}$$

$$\mathcal{I}_{BC,P} = \{(Z,P),(P,Z),(O,M),(M,O)\}. \tag{E24}$$

Two elements $O, P \in \mathcal{I}_A$ are connected in the sense given at the end of Definition 5 by choosing $\{i,j,k\} = \{(P,Z,P),(O,Z,Z),(O,M,P)\}$. Based on Eqs. (E23) and (E24), we choose subsets $\mathcal{I}_B$, $\mathcal{I}_{C,Z}$, and $\mathcal{I}_{C,P}$ as

$$\mathcal{I}_B := \{Z,P\}, \qquad \mathcal{I}_{C,Z} := \{Z,P\}, \qquad \mathcal{I}_{C,P} := \{Z,M\}. \tag{E25}$$

Subsets $\mathcal{I}_B$, $\mathcal{I}_{C,Z}$, and $\mathcal{I}_{C,P}$ satisfy conditions (B1)–(B4).

To show Theorem 4, we prepare the following lemma.

Lemma 7: *Assume that $i,j,k \in \mathcal{I}_0$ are connected by one edge, i.e., they satisfy conditions (C1) and (C2). We choose $x_A, x_A', x_B, x_B', x_C, x_C'$ in the way as condition (C2). We consider three normalized vectors v_i', v_j', v_k', where*

$$v_l' = a_{l_A} \otimes b_{l_B} \otimes c_{l_C} \tag{E26}$$

for $l = i,j,k$. We assume that $\langle v_l, v_l\rangle = \langle v_l', v_l'\rangle$ for $l, l' = i,j,k$. Then we have

$$\langle a_{x_A}, a_{x_A'}\rangle = \langle a'_{x_A}, a'_{x_A'}\rangle, \tag{E27}$$

$$\langle b_{x_B}, b_{x_B'}\rangle = \langle b'_{x_B}, b'_{x_B'}\rangle, \tag{E28}$$

$$\langle c_{x_C}, c_{x_C'}\rangle = \langle c'_{x_C}, c'_{x_C'}\rangle, \tag{E29}$$

or

$$\langle a_{x_A}, a_{x_A'}\rangle = -\langle a'_{x_A}, a'_{x_A'}\rangle, \tag{E30}$$

$$\langle b_{x_B}, b_{x_B'}\rangle = -\langle b'_{x_B}, b'_{x_B'}\rangle, \tag{E31}$$

$$\langle c_{x_C}, c_{x_C'}\rangle = -\langle c'_{x_C}, c'_{x_C'}\rangle. \tag{E32}$$

Proof. For simplicity, without loss of generality, we assume that

$$i = (x_A', x_B, x_C), \qquad j = (x_A, x_B', x_C), \qquad k = (x_A, x_B, x_C'). \tag{E33}$$

Since

$$\langle v_i, v_j\rangle = \langle v_i', v_j'\rangle, \qquad \langle v_i, v_k\rangle = \langle v_i', v_k'\rangle, \qquad \langle v_k, v_j\rangle = \langle v_k', v_j'\rangle,$$

we have

$$\langle a_{x_A}, a_{x_A'}\rangle\langle b_{x_B}, b_{x_B'}\rangle = \langle a'_{x_A}, a'_{x_A'}\rangle\langle b'_{x_B}, b'_{x_B'}\rangle, \tag{E34}$$

$$\langle a_{x_A}, a_{x_A'}\rangle\langle c_{x_C}, c_{x_C'}\rangle = \langle a'_{x_A}, a'_{x_A'}\rangle\langle c'_{x_C}, c'_{x_C'}\rangle, \tag{E35}$$

$$\langle b_{x_B}, b_{x_B'}\rangle\langle c_{x_C}, c_{x_C'}\rangle = \langle b'_{x_B}, b'_{x_B'}\rangle\langle c'_{x_C}, c'_{x_C'}\rangle. \tag{E36}$$

Hence,

$$\begin{aligned}
\langle a_{x_A}, a_{x_A'}\rangle^2 &= (\langle a_{x_A}, a_{x_A'}\rangle\langle b_{x_B}, b_{x_B'}\rangle)(\langle a_{x_A}, a_{x_A'}\rangle\langle c_{x_C}, c_{x_C'}\rangle) \\
&\quad\times (\langle b_{x_B}, b_{x_B'}\rangle\langle c_{x_C}, c_{x_C'}\rangle)^{-1} \\
&= (\langle a'_{x_A}, a'_{x_A'}\rangle\langle b'_{x_B}, b'_{x_B'}\rangle)(\langle a'_{x_A}, a'_{x_A'}\rangle\langle c'_{x_C}, c'_{x_C'}\rangle) \\
&\quad\times (\langle b'_{x_B}, b'_{x_B'}\rangle\langle c'_{x_C}, c'_{x_C'}\rangle)^{-1} \\
&= \langle a'_{x_A}, a'_{x_A'}\rangle^2,
\end{aligned}$$

which implies Eq. (E27) or (E30). When Eq. (E27) holds, we have Eqs. (E28) and (E29). When Eq. (E30) holds, we have Eqs. (E31) and (E32). ∎

Proof of Theorem 4. Step 1. We fix an arbitrary element $i_A \in \mathcal{I}_A$. For $i_{BC}, i'_{BC} \in \mathcal{I}_{BC,i_A}$, condition (A5) implies that

$$\begin{aligned}\langle \psi_{i_{BC}}, \psi_{i'_{BC}}\rangle &= \langle a_{i_A} \otimes \psi_{i_{BC}}, a_{i_A} \otimes \psi_{i'_{BC}}\rangle \\ &= \langle a'_{i_A} \otimes \psi'_{i_{BC}}, a'_{i_A} \otimes \psi'_{i'_{BC}}\rangle \\ &= \langle \psi'_{i_{BC}}, \psi'_{i'_{BC}}\rangle. \end{aligned} \tag{E37}$$

Hence, there exists an isometry V_{BC,i_A} from $\mathcal{H}_B \otimes \mathcal{H}_C$ to $\mathcal{H}'_B \otimes \mathcal{H}'_C$ such that

$$V_{BC,i_A}\psi_{i_{BC}} = \psi'_{i_{BC}} \quad \text{for } i_{BC} \in \mathcal{I}_{BC,i_A}. \tag{E38}$$

Step 2. We choose a subgraph $G_{A,0} \subset G_A$ to satisfy the following three conditions. (a) The vertices of $G_{A,0}$ is $\mathcal{I}_A$, (b) the subgraph $G_{A,0}$ has no cycle, and (c) the subgraph $G_{A,0}$ cannot be divided into two parts.

We fix the origin $i_{A,0} \in \mathcal{I}_A$. For any element $i_A \in \mathcal{I}_A$, 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 $i_{A,0} - i_{A,1} - \cdots - i_{A,n} = i_A$. We define $\alpha(i_A)$ as

$$\alpha(i_A) := \prod_{m=1}^{n} \frac{\langle a_{i_{A,m-1}}, a_{i_{A,m}}\rangle}{\langle a'_{i_{A,m-1}}, a'_{i_{A,m}}\rangle}. \tag{E39}$$

Lemma 7 guarantees that $\alpha(i_A)$ takes value 1 or -1. Because of the above definition and the uniqueness of the above path, we find that

$$\alpha(i_{A,l}) := \prod_{m=1}^{l} \frac{\langle a_{i_{A,m-1}}, a_{i_{A,m}}\rangle}{\langle a'_{i_{A,m-1}}, a'_{i_{A,m}}\rangle}. \tag{E40}$$

For $i_{BC} \in \mathcal{I}_{BC,i_{A,l}}$ and $i'_{BC} \in \mathcal{I}_{BC,i_{A,l+1}}$, we find that

$$\begin{aligned}\langle a_{i_{A,l}}, a_{i_{A,l+1}}\rangle\langle \psi_{i_{BC}}, \psi_{i'_{BC}}\rangle &= \langle a_{i_{A,l}} \otimes \psi_{i_{BC}}, a_{i_{A,l+1}} \otimes \psi_{i'_{BC}}\rangle \\ &= \langle a'_{i_{A,l}} \otimes \psi'_{i_{BC}}, a'_{i_{A,l+1}} \otimes \psi'_{i'_{BC}}\rangle \\ &= \langle a'_{i_{A,l}}, a'_{i_{A,l+1}}\rangle\langle \psi'_{i_{BC}}, \psi'_{i'_{BC}}\rangle \\ &= \alpha(i_{A,l})\alpha(i_{A,l+1})\langle a_{i_{A,l}}, a_{i_{A,l+1}}\rangle \\ &\quad \times \langle V_{BC,i_{A,l}}\psi_{i_{BC}}, V_{BC,i_{A,l+1}}\psi_{i'_{BC}}\rangle \\ &= \alpha(i_{A,l})\alpha(i_{A,l+1})\langle a_{i_{A,l}}, a_{i_{A,l+1}}\rangle \\ &\quad \times \langle \psi_{i_{BC}}, V^\dagger_{BC,i_{A,l}}V_{BC,i_{A,l+1}}\psi_{i'_{BC}}\rangle. \end{aligned} \tag{E41}$$

Since $\langle a_{i_{A,l}}, a_{i_{A,l+1}}\rangle \neq 0$ and the sets $\{\psi_{i_{BC}}\}_{i_{BC}\in\mathcal{I}_{BC,i_{A,l}}}$ and $\{\psi_{i'_{BC}}\}_{i'_{BC}\in\mathcal{I}_{BC,i_{A,l+1}}}$ span the space $\mathbb{C}^{d_B d_C}$, we find that $\alpha(i_{A,l})\alpha(i_{A,l+1})V^\dagger_{BC,i_{A,l}}V_{BC,i_{A,l+1}}$ is identity. Then, we find that

$$V_{BC} := V_{BC,i_{A,0}} = \alpha(i_{A,l})V_{BC,i_{A,l}}. \tag{E42}$$

That is, we have

$$V_{BC} = \alpha(i_A)V_{BC,i_A}. \tag{E43}$$

Also, we define the isometry V_A from $\mathcal{H}_A$ to $\mathcal{H}'_A$ such that

$$V_A a_{i_A} = \alpha(i_A)a'_{i_A} \quad \text{for } i_A \in \mathcal{I}_A. \tag{E44}$$

Therefore, for $(i_A, i_{BC}) \in \bigcup_{i_A\in\mathcal{I}_A}(\{i_A\} \times \mathcal{I}_{BC,i_A})$, we have

$$Va_{i_A} \otimes \psi_{i_{BC}} = a'_{i_A} \otimes \psi'_{i_{BC}} = (V_A \otimes V_{BC})a_{i_A} \otimes \psi_{i_{BC}}. \tag{E45}$$

Since the set $\{a_{i_A}\}_{i_A\in\mathcal{I}_A}$ spans the space $\mathbb{C}^{d_A}$, we have

$$V = V_A \otimes V_{BC}. \tag{E46}$$

Step 3. For $i_B \in \mathcal{I}_B$ and $i_C \in \mathcal{I}_{C,i_B}$, we choose i_A such that $(i_B, i_C) \in \mathcal{I}_{BC,i_A}$. Then, we define $\beta(i_B, i_C) := \alpha(i_A)$. We fix an arbitrary element $i_B \in \mathcal{I}_B$. For $i_C, i'_C \in \mathcal{I}_{C,i_B}$, relation (E43) implies that

$$\begin{aligned}\langle c_{i_C}, c_{i'_C}\rangle &= \langle b_{i_B} \otimes c_{i_C}, b_{i_B} \otimes c_{i'_C}\rangle \\ &= \beta(i_B, i_C)\beta(i_B, i'_C)\langle b'_{i_B} \otimes c'_{i_C}, b'_{i_B} \otimes c'_{i'_C}\rangle \\ &= \beta(i_B, i_C)\beta(i_B, i'_C)\langle c'_{i_C}, c'_{i'_C}\rangle. \end{aligned} \tag{E47}$$

Hence, there exists an isometry V_{C,i_B} from $\mathcal{H}_C$ to $\mathcal{H}'_C$ such that

$$V_{C,i_B}c_{i_C} = \beta(i_B, i_C)c'_{i_C} \quad \text{for } i_C \in \mathcal{I}_{C,i_B}. \tag{E48}$$

Step 4. We choose a subgraph $G_{B,0} \subset G_B$ to satisfy the following three conditions. (a) The vertices of $G_{B,0}$ is $\mathcal{I}_B$, (b) $G_{B,0}$ has no cycle, and (c) $G_{B,0}$ 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 $i_{B,0} - i_{B,1} - \cdots - i_{B,n'} = i_B$. We choose a nonzero element $i_{C,l} \in \mathcal{I}_{C,i_{B,l-1}} \cap \mathcal{I}_{C,i_{B,l}}$. 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 $\gamma(i_B)$ as

$$\gamma(i_B) := \prod_{l=1}^{n'} \beta(i_{B,l-1}, i_{C,l})\beta(i_{B,l}, i_{C,l}). \tag{E49}$$

Then, we have

$$\begin{aligned}\langle b_{i_{B,l-1}}, b_{i_{B,l}}\rangle &= \langle b_{i_{B,l-1}} \otimes c_{i_{C,l}}, b_{i_{B,l}} \otimes c_{i_{C,l}}\rangle \\ &= \beta(i_{B,l-1}, i_{C,l})\beta(i_{B,l}, i_{C,l})\langle b'_{i_{B,l-1}} \otimes c'_{i_{C,l}}, b'_{i_{B,l}} \otimes c'_{i_{C,l}}\rangle \\ &= \beta(i_{B,l-1}, i_{C,l})\beta(i_{B,l}, i_{C,l})\langle b'_{i_{B,l-1}}, b'_{i_{B,l}}\rangle \\ &= \gamma(i_{B,l-1})\gamma(i_{B,l})\langle b'_{i_{B,l-1}}, b'_{i_{B,l}}\rangle.\end{aligned} \tag{E50}$$

For $i_C \in \mathcal{I}_{C,i_{B,l}}$ and $i'_C \in \mathcal{I}_{C,i_{B,l+1}}$, we find that

$$\begin{aligned}\langle b_{i_{B,l}}, b_{i_{B,l+1}}\rangle\langle c_{i_C}, c_{i'_C}\rangle &= \langle b_{i_{B,l}} \otimes c_{i_C}, b_{i_{B,l+1}} \otimes c_{i'_C}\rangle \\ &= \beta(i_{B,l}, i_C)\beta(i_{B,l+1}, i'_C)\langle b'_{i_{B,l}} \otimes c'_{i_C}, b'_{i_{B,l+1}} \otimes c'_{i'_C}\rangle \\ &= \langle b'_{i_{B,l}}, b'_{i_{B,l+1}}\rangle\beta(i_{B,l}, i_C)\beta(i_{B,l+1}, i'_C)\langle c'_{i_C}, c'_{i'_C}\rangle \\ &= \gamma(i_{B,l})\gamma(i_{B,l+1})\langle b_{i_{B,l}}, b_{i_{B,l+1}}\rangle\langle V_{C,i_{B,l}}c_{i_C}, V_{C,i_{B,l+1}}c_{i'_C}\rangle.\end{aligned} \tag{E51}$$

Since $\langle b_{i_{B,l}}, b_{i_{B,l+1}}\rangle \neq 0$ and the sets $\{c_{i_C}\}_{i_C\in\mathcal{I}_{C,i_{B,l}}}$ and $\{c_{i'_C}\}_{i'_C\in\mathcal{I}_{C,i_{B,l+1}}}$ span the space $\mathcal{H}_C$, we find that $\gamma(i_{B,l})\gamma(i_{B,l+1})V^\dagger_{C,i_{B,l}}V_{C,i_{B,l+1}}$ is identity. Then, we find that

$$V_C := V_{C,i_{B,0}} = \gamma(i_{B,l})V_{C,i_{B,l}}. \tag{E52}$$

That is, we have

$$V_C = \gamma(i_B)V_{C,i_B}. \tag{E53}$$

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

$$\begin{aligned}\langle b_{i_B}, b_{i'_B}\rangle\langle c_{i_C}, c_{i'_C}\rangle &= \langle b_{i_B} \otimes c_{i_C}, b_{i'_B} \otimes c_{i'_C}\rangle \\ &= \beta(i_B, i_C)\beta(i'_B, i'_C)\langle b'_{i_B} \otimes c'_{i_C}, b'_{i'_B} \otimes c'_{i'_C}\rangle \\ &= \langle b'_{i_B}, b'_{i'_B}\rangle\beta(i_B, i_C)\beta(i'_B, i'_C)\langle c'_{i_C}, c'_{i'_C}\rangle \\ &= \langle b'_{i_B}, b'_{i'_B}\rangle\gamma(i_B)\gamma(i'_B)\langle V_C c_{i_C}, V_C c_{i'_C}\rangle \\ &= \gamma(i_B)\gamma(i'_B)\langle b'_{i_B}, b'_{i'_B}\rangle\langle c_{i_C}, c_{i'_C}\rangle.\end{aligned} \tag{E54}$$

Since $\langle c_{i_C}, c_{i'_C}\rangle \neq 0$, we have

$$\langle b_{i_B}, b_{i'_B}\rangle = \gamma(i_B)\gamma(i'_B)\langle b'_{i_B}, b'_{i'_B}\rangle. \tag{E55}$$

Also, we define the isometry V_B from $\mathcal{H}_B$ to $\mathcal{H}'_B$ such that

$$V_B b_{i_B} = \gamma(i_B)b'_{i_B} \quad \text{for } i_B \in \mathcal{I}_B. \tag{E56}$$

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

$$V_{BC}b_{i_B} \otimes c_{i_C} = b'_{i_B} \otimes c'_{i_C} = (V_B \otimes V_C)b_{i_B} \otimes c_{i_C}. \tag{E57}$$

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

$$V_{BC} = V_B \otimes V_C. \tag{E58}$$

Combining Eqs. (E46) and (E58), we have

$$V = V_A \otimes V_B \otimes V_C. \tag{E59}$$

This completes the proof. ■

b. General case

We consider the general case. We define $|v'_i\rangle := \eta_i^{-1}\Pi^A_{i_A} \otimes \Pi^B_{i_B} \otimes \Pi^C_{i_C}|\psi'\rangle$. Let $\bar{\mathcal{I}}_A, \bar{\mathcal{I}}_B, \bar{\mathcal{I}}_C$ be the sets of indices of the spaces $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C$.

To show Theorem 5, we focus on conditions (A8) and (A9) for the optimal maximizer given in Eq. (E22) as a generalization of (A3) and (A4) as well as condition (C1), which were introduced in the main text.

Proof of Theorem 5. Similar to the proof of Theorem 3 , we define orthogonal projections $\bar{\Pi}^X_{j_X}$ on $\mathcal{H}_X$ such that the projection $\Pi^X := \sum_{j_X} \bar{\Pi}^X_{j_A}$ satisfies $\Pi^X\psi' = \psi'$ for $X = A, B, C$. Then, we define the projection $\bar{\Pi}_{(j_A,j_B,j_C)} := \bar{\Pi}^A_{j_A}\bar{\Pi}^B_{j_B}\bar{\Pi}^C_{j_C}$. In the same way as in the proof of Theorem 3, we define $\alpha_{(j_A,j_B,j_C)}$, β_{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

$$|\text{junk}\rangle := \sum_{j_A, j_B, j_C} \beta^{-1}_{j_A, j_B, j_C} \alpha^{-1}_{(j_A, j_B, j_C)} |j_A, j_B, j_C\rangle. \tag{E60}$$

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

$$V_X := \sum_{j_X} V_{X, j_X} \langle j_X | \tag{E61}$$

for $X = A, B, C$. The isometries V_A, V_B, and V_C satisfy conditions (39) and (40). ■

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