



Scalable noncontextuality inequalities and certification of multiqubit quantum systemsRafael Santos , Chellasamy Jebarathinam , and Remigiusz Augusiak *Center for Theoretical Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland*

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We propose a family of noncontextuality inequalities and show that they can be used for certification of multiqubit quantum systems. Our scheme, unlike those based on nonlocality, does not require spatial separation between the subsystems, yet it makes use of certain compatibility relations between measurements. Moreover, it is scalable in the sense that the number of expectation values that are to be measured to observe contextuality scales polynomially with the number of qubits that are being certified. In a particular case we also show our scheme to be robust to errors and experimental imperfections. Our results seem promising as far as certification of physical setups is concerned in scenarios where spatial separation between the subsystems cannot be guaranteed.

DOI: [10.1103/PhysRevA.106.012431](https://doi.org/10.1103/PhysRevA.106.012431)**I. INTRODUCTION**

Multiqubit entangled states constitute a key resource for various quantum information tasks such as quantum computation [1,2] and error correction [3,4], quantum communication [5,6], quantum simulations [7,8], and cryptographic protocols [9,10]. To realize genuine quantum technologies employing such tasks, the back-end user should be guaranteed that the quantum devices work as specified by the provider. The standard state verification schemes based on quantum tomography [11,12], however, suffer from two problems: they are unfeasible for larger systems and require using trusted and well-characterized measuring devices.

Observing nonclassical correlations through the violation of a Bell-type inequality [13] can be used to detect entanglement in a device-independent way; i.e., it implies the presence of entanglement without the need to have a trust in the measurement devices. This property of the violation of Bell inequalities makes them a useful resource for implementing quantum information protocols such as quantum key distribution in a device-independent way [14]. Remarkably, maximal quantum violation of certain Bell inequalities can be used to demonstrate a phenomenon called “self-testing of quantum states and measurements” [15,16], which can be used to provide device-independent characterization of quantum devices. Recently, such a form of certification based on the phenomenon of nonlocality has been explored extensively. For instance, several self-testing statements for multiqubit graph states were recently derived in Refs. [17–19]. However, genuine demonstration of the violation of Bell inequalities requires a spatial separation between the subsystems.

Sequential quantum measurements on a single system can be used to observe quantum contextuality [20] and temporal quantum correlations [21–23] through the violation of suitable inequalities. Apart from the foundational relevance of these two notions of nonclassicality, on one side, they have been explored as a resource for quantum information applications such as measurement-based quantum computation [24–27]. On the other side, they have also been used for certification of relevant quantum properties such as the

dimension of the underlying quantum system [28,29]. More importantly, contextuality and temporal correlations have also been exploited for certification of quantum states and/or measurements [30–34].

Motivated by the above results, in this work we introduce a family of noncontextuality inequalities that are maximally violated by many-qubit quantum systems and certain pairs of anticommuting observables. In constructing our inequalities we exploit the multiqubit stabilizer formalism known for its use in quantum error correction [35–37]. These inequalities are scalable in the sense that the number of expectation values they are built from scales polynomially with the number of observables, $2n$, that are measured; yet their maximal violation can be achieved by quantum systems of dimension at least 2^n . From this point of view they can be seen as dimension witnesses. In the particular case $n = 3$ our family reproduces an inequality that in the nonlocality context is known as the Mermin-Ardehali-Belinskii-Klyshko (MABK) inequality [38–40] (see also Refs. [41–43] for other approaches to reveal Bell nonlocality or quantum contextuality based on stabilizer formalism). Yet for $n > 3$ these families are distinct. We then show that our inequalities can be used for certification of multiqubit quantum systems in the sense of Ref. [32]. In fact, we generalize the results of that work to any number of qubits.

Our work is organized as follows. In Sec. II we outline the contextuality scenario and provide the definitions of graph states and self-testing. In Sec. III we present the simplest inequality designed to certify the three-qubit graph state corresponding to the complete graph together with three pairs of anticommuting observables. In Sec. IV we present a scalable family of inequalities designed to certify multiqubit quantum systems. In Sec. V we investigate whether our certification schemes are robust.

II. PRELIMINARIES

We begin by illustrating our scenario and introducing the relevant notations and definitions.

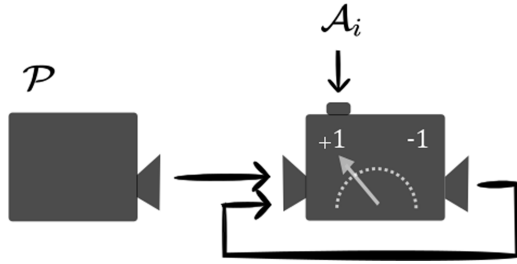


FIG. 1. Measurement setup. A contextuality experiment comprises of a preparation device \mathcal{P} that prepares some quantum state ρ which is later measured sequentially by the nondemolishing measurement device with settings \mathcal{A}_i ; each of these measurements yields the ± 1 outcome. Figure from Ref. [33].

A. Contextuality scenario

A standard contextuality scenario is defined by a triple of sets: a set of measurements, a set of outcomes of the measurements, and a set of contexts, which are the subsets of compatible measurements. The notion of compatibility in a contextuality scenario means that the measurements that belong to the same context can be performed jointly or in a sequence in such a way that the observed statistics are independent of the order in which these measurements were performed. In the latter case, however, the measurements are nondemolishing, meaning that they do not physically destroy the system.

Each run of the experimental observation comprises of preparation of a physical system followed by a sequence of nondemolishing measurements in a device as depicted in Fig. 1. The measurement device has no memory and returns only the actual postmeasurement state. The measurement device has different settings, each of which yields two outcomes which we label by ± 1 . The contexts will be defined in the specific scenarios studied. Let us stress here that in the quantum case the above scenario comprises the most general situation in which the physical system is described by a mixed state and the measurements need not be projective.

After repeating this experiment many times, one estimates the joint probabilities of obtaining the outcomes of measurements that are performed on the preparation and, consequently, their correlation functions, which are average values over the outcomes of the measurements. For instance, if the measurements A_1 , A_2 , and A_3 , which belong to the same context, are performed in sequence or jointly, we can estimate the 2^3 joint probabilities $p(a_1, a_2, a_3 | A_1, A_2, A_3)$ as well as the correlation function

$$\langle A_1 A_2 A_3 \rangle = \sum_{a_i = \pm 1} a_1 a_2 a_3 p(a_1, a_2, a_3 | A_1, A_2, A_3). \quad (1)$$

This notation can be naturally extended to any sets of compatible measurements.

To reveal contextuality in the experiment one typically uses noncontextuality inequalities as violation of such inequalities by the joint probabilities implies that any noncontextual hidden variable model cannot reproduce them [20]. Typically such inequalities are defined in terms of linear expressions composed of correlation functions. For instance, in a scenario where the measurements are performed in triples, we can

consider the following form of inequality:

$$\mathcal{I} := \sum_{i,j,k} c_{i,j,k} \langle A_i A_j A_k \rangle \leq \eta_C \leq \eta_Q, \quad (2)$$

where $c_{i,j,k}$ are real coefficients to be chosen, and η_C and η_Q are the classical and quantum bounds.

If there is a noncontextual hidden variable model that describes the joint probabilities, then the inequality with the classical bound η_C is satisfied. Here, the meaning of classically is mathematically defined as the existence of a noncontextual hidden variable model, for which the expectation values in Eq. (2) factorize and each individual expectation value is deterministic, i.e., $\langle A_i A_j A_k \rangle = a_i a_j a_k$, with $a_i \in \{+1, -1\}$. Consequently, the classical bound η_C of Eq. (2) can be derived as the maximum value that can be attained by any such model,

$$\eta_C = \max_{a_i = \pm 1} \left(\sum_{i,j,k} c_{i,j,k} a_i a_j a_k \right). \quad (3)$$

On the other hand, the quantum bound of the inequality is defined as the optimal value of the linear expression obtained over all the possible quantum states and measurements in any Hilbert space. Since we do not specify the dimension of the underlying Hilbert space, without any loss of generality, we can assume that the measurements are projective and the state is pure (see, e.g., Ref. [32], where an extension of the Neumark dilation theorem is proven). In other words, any correlations obtained within the above experiment can always be reproduced with a pure state and projective measurements satisfying the same compatibility relations.

For instance, in the case of the inequality given in Eq. (2) the quantum bound is evaluated to be

$$\eta_Q = \sup_{A_i; \rho} \left[\sum_{i,j,k} c_{i,j,k} \text{tr}(\rho A_i A_j A_k) \right], \quad (4)$$

where the observables A_i are Hermitian operators acting on a Hilbert space \mathcal{H} and satisfying $A_i^2 = \mathbb{1}$ for any i and $\rho = |\psi\rangle\langle\psi|$ is some pure state that describes the preparation.

Our aim here is to introduce certain noncontextuality inequalities that are scalable in the sense that the number of expectation values they consist of grows polynomially with n and, at the same time, their maximal violation can be achieved only by quantum systems of dimension 2^n . We also explore whether these inequalities can be used for certification of quantum states and measurements.

B. Graph states

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a mathematical object defined by a set of vertices \mathcal{V} and a set of edges \mathcal{E} that connect some pairs of vertices. By $\mathcal{N}(i)$ we denote the neighborhood of the vertex i , that is, a set of those vertices that are connected to i by an edge. Also, we call a graph connected if any two vertices are connected by a path composed of edges.

Interestingly, one can exploit the notion of a graph to define classes of pure entangled multipartite states. While in principle there are many ways of doing that, here we follow the definition based on the stabilizer formalism [44] (see also

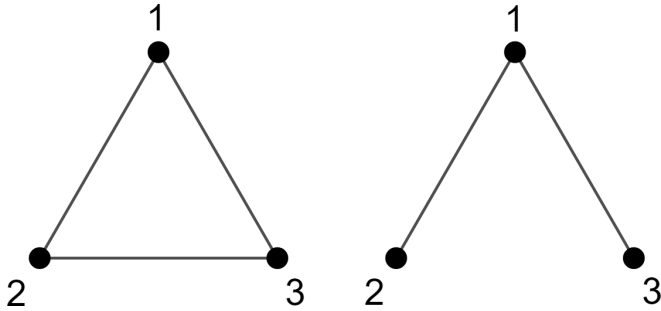


FIG. 2. Two nonisomorphic graphs with three vertices.

Ref. [45] for a review on graph states). It allows one to associate an N -qubit entangled state to any connected N -vertex graph \mathcal{G} .

In order to present the construction consider the Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5)$$

Now, to each vertex $i \in \mathcal{V}$ one associates an N -qubit operator G_i defined as

$$G_i = X_i \otimes \bigotimes_{j \in \mathcal{N}(i)} Z_j, \quad (6)$$

where the single X acts on site i , whereas the Z operators act on all sites that belong to the neighborhood $\mathcal{N}(i)$ of i . Having introduced the G_i operators we define the graph state.

Definition 1. We define the graph state $|G\rangle$ associated to the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ as the unique state stabilized by the corresponding operators G_i (6), that is,

$$G_i |G\rangle = |G\rangle, \quad \forall i = 1, \dots, N. \quad (7)$$

In other words, $|G\rangle$ is the unique common eigenstate of all G_i corresponding to eigenvalue $+1$.

The operators G_i are usually called the stabilizing operators. Notice also that they mutually commute and the Abelian group generated by them is called a stabilizer.

Two simple examples of connected graphs with three vertices are depicted in Fig. 2. The graph on the left is a complete graph, i.e., one in which any vertex is connected to any other vertex by an edge. The unique three-qubit state associated to this graph is stabilized by the following three stabilizing operators,

$$G_1 = X \otimes Z \otimes Z, \quad (8)$$

$$G_2 = Z \otimes X \otimes Z, \quad (9)$$

$$G_3 = Z \otimes Z \otimes X, \quad (10)$$

and can be stated as

$$|G'\rangle = \frac{1}{\sqrt{8}}(|000\rangle + |100\rangle + |010\rangle - |110\rangle + |001\rangle - |101\rangle - |011\rangle - |111\rangle). \quad (11)$$

The graph on the right-hand side in Fig. 2 is nonisomorphic to the complete graph. The unique three-qubit state associated with this graph is stabilized by

$$G_1 = X \otimes Z \otimes Z, \quad (12)$$

$$G_2 = Z \otimes X \otimes \mathbb{1}, \quad (13)$$

$$G_3 = Z \otimes \mathbb{1} \otimes X, \quad (14)$$

and is given by

$$|G''\rangle = \frac{1}{\sqrt{8}}(|000\rangle + |100\rangle + |010\rangle - |110\rangle + |001\rangle + |101\rangle - |011\rangle + |111\rangle). \quad (15)$$

Let us notice that although both these exemplary states $|G'\rangle$ and $|G''\rangle$ correspond to nonisomorphic graphs, they are actually equivalent to the same three-qubit Greenberger-Horne-Zeilinger (GHZ) state,

$$|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle - |111\rangle), \quad (16)$$

by suitable local unitary transformations.

In the context of multipartite qubit states such a vertex is associated to a qubit and edges represent entanglement between qubits. However, in our scheme that we propose for certification of such a multiqubit state, we do not assume that there exists a local Hilbert space corresponding to each vertex.

Let us finally notice that the construction of the graph state corresponding to the three-vertex complete graph can be generalized to any number of qubits. The corresponding stabilizing operators are given by

$$G_i = Z_1 \cdots Z_{i-1} X_i Z_{i+1} \cdots Z_n, \quad (17)$$

with $i = 1, \dots, n$. They stabilize an n -qubit graph state that is local-unitary equivalent to the GHZ state $(1/\sqrt{2})(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$.

C. Self-testing

Self-testing, originally defined in Ref. [15] in the context of nonlocality, aims to certify an unknown quantum state and a set of measurements based on statistics obtained in an experiment, up to certain unitary equivalence and the existence of auxiliary degrees of freedom. Self-testing based on violation of Bell inequalities is by definition a device-independent task as it does not depend on any assumption on the state and measurements. In a Bell test, the assumption of commutativity between the measurements arises due to the fact that spatially separated subsystems cannot communicate instantaneously with each other.

Self-testing statements based on violation of noncontextuality inequalities require, on the other hand, the assumption of compatibility of measurements. First, contextuality-based self-testing was defined in Ref. [31] in a similar way to how self-testing is defined within the Bell scenario. Here we provide a slightly different definition that takes inspiration from Ref. [32] (see also Ref. [33]) and fits better the inequalities introduced here.

To this aim, let us consider again the experiment described in Sec. II A, but now we assume that both the state (in general mixed) and measurements (in general nonprojective) are unknown; still, the measurements obey certain compatibility relations. Since we do not specify the dimension of the underlying Hilbert space, without loss of generality, we can assume that the measurements are projective and the state is pure (see, e.g., Ref. [32]). In other words, any correlations giving rise to the violation of the noncontextuality inequality can always be reproduced with a pure state $\rho = |\psi\rangle\langle\psi|$ and observables A_i obeying $A_i^2 = \mathbb{1}$, all acting on some Hilbert space of unknown dimension \mathcal{H} . These observables obey the same compatibility relations.

At the same time we consider a reference experiment with a known pure state $|\tilde{\psi}\rangle \in \mathbb{C}^d$ for some d and known observables \tilde{A}_i acting on \mathbb{C}^d that obey the same compatibility relations.

Definition 2. Suppose an unknown state $|\psi\rangle \in \mathcal{H}$ and a set of measurements A_i violate a given noncontextuality inequality maximally; then this maximal quantum violation self-tests the state $|\tilde{\psi}\rangle \in \mathbb{C}^d$ and the set of measurements \tilde{A}_i if there exists a projection $P : \mathcal{H} \rightarrow \mathbb{C}^d$ and a unitary U acting on \mathbb{C}^d such that

$$U^\dagger(PA_iP^\dagger)U = \tilde{A}_i, \quad (18)$$

$$U(P|\psi\rangle) = |\tilde{\psi}\rangle. \quad (19)$$

Speaking alternatively, the above definition says that based on the observed nonclassicality one is able to identify a subspace $V = \mathbb{C}^d$ in \mathcal{H} on which all the observables act invariantly. Equivalently, A_i can be decomposed as $A_i = \hat{A}_i \oplus A'_i$, where \hat{A}_i act on V , whereas A'_i act on the orthocomplement of V in \mathcal{H} ; in particular, $A'_i|\psi\rangle = 0$. Moreover, there is a unitary $U^\dagger \hat{A}_i U = \tilde{A}_i$.

III. THE SIMPLEST INEQUALITY AND SELF-TESTING OF THREE-QUBIT GRAPH STATE

A. Simplest inequality

Here, we consider a noncontextuality inequality that allows for self-testing the complete graph state of three qubits and simultaneously a set of six dichotomic observables denoted by A_i and B_j ($i, j \in \{1, 2, 3\}$) such that $\{A_i, B_i\} = 0$ ($i = 1, 2, 3$). The measurement outcomes are labeled by ± 1 , which means that the measurement operators have eigenvalues ± 1 and thus they satisfy $A_i^2 = B_i^2 = \mathbb{1}$.

The compatibility hypergraph of the scenario is depicted in Fig. 3. A compatibility hypergraph is one in which the vertices are associated with the measurements of the scenario and the hyperedges represent the contexts which are subsets of compatible measurements. The noncontextuality inequality we consider is given by

$$\begin{aligned} \mathcal{I}_3 &:= \langle A_1 B_2 B_3 \rangle + \langle B_1 A_2 B_3 \rangle + \langle B_1 B_2 A_3 \rangle - \langle A_1 A_2 A_3 \rangle \\ &\leq \eta_C = 2 < \eta_Q = 4. \end{aligned} \quad (20)$$

The above inequality is equivalent to a noncontextuality inequality employed in Ref. [46] to demonstrate quantum contextuality of a single eight-dimensional quantum system. In the context of the Bell scenario it is the well-known MABK

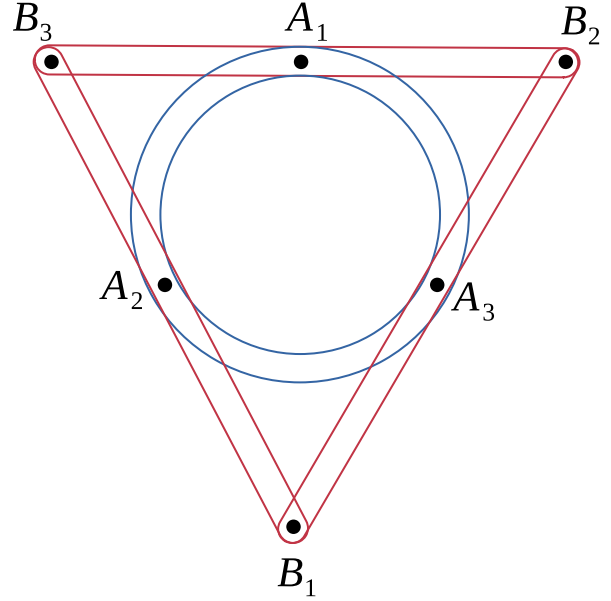


FIG. 3. Hypergraph [47] of compatibility of the Kochen-Specker contextuality scenario associated to inequality (20). In this hypergraph, the vertices represent the observables of the scenario and the hyperedges represent the contexts. The red hyperedges are associated to the correlators which enter inequality (20) with $+1$ and the blue to correlators corresponding to the negative sign. Here the colors are conveniently chosen in order to elucidate symmetric properties of the inequality.

inequality [38–40] for which a non-locality-based self-testing statement was derived in Ref. [17].

Following the argument in the previous section, the classical bound of the above expression can be obtained by assigning the values ± 1 to each variable A_i and B_j which implies $\eta_C = 2$. At the same time, the algebraic maximum of \mathcal{I}_3 is four since the correlators can take a value between -1 and $+1$, and, importantly, it equals the maximal quantum value of \mathcal{I}_3 , that is, $\eta_Q = 4$. Indeed, it can be checked that the following set of measurements,

$$\begin{aligned} A_1 &= X \otimes \mathbb{1} \otimes \mathbb{1}, & B_1 &= Z \otimes \mathbb{1} \otimes \mathbb{1}, \\ A_2 &= \mathbb{1} \otimes X \otimes \mathbb{1}, & B_2 &= \mathbb{1} \otimes Z \otimes \mathbb{1}, \\ A_3 &= \mathbb{1} \otimes \mathbb{1} \otimes X, & B_3 &= \mathbb{1} \otimes \mathbb{1} \otimes Z, \end{aligned} \quad (21)$$

together with the complete graph state $|G'\rangle$ given by Eq. (11) give rise to the algebraic maximum. This follows from the fact that for this choice of observables, the first three terms of the inequality correspond to the stabilizing operators G_i given in Eq. (8), whereas the last one corresponds to their product $G_1 G_2 G_3 = -X_1 X_2 X_3$.

Let us notice that almost all pairs of these observables commute except for those with the same subscripts which anticommute, that is,

$$[A_i, A_j] = [A_i, B_j] = [B_i, B_j] = 0 \quad (i \neq j) \quad (22)$$

and

$$\{A_i, B_i\} = 0 \quad (i = 1, 2, 3). \quad (23)$$

For further convenience let us also comment on the symmetries of inequality (20). A simple way to visualize these symmetries is by using the compatibility hypergraph of the scenario that is represented in Fig. 3. For instance, note that under the relabeling of the measurements $A_i \leftrightarrow A_j$ together with $B_i \leftrightarrow B_j$, i.e., a permutation of subscripts $i \leftrightarrow j$, the inequality remains the same. We can also observe that a cyclic permutation of measurements $A_1 \rightarrow A_2 \rightarrow A_3 \rightarrow A_1$ together with $B_3 \rightarrow B_1 \rightarrow B_2 \rightarrow B_3$ does not change the structure of the hypergraph and therefore the inequality remains the same. Other symmetries can be found just by looking at the hypergraph since it captures the intrinsic structure of the associated inequality. The above symmetries as well as the structure of the \mathcal{I}_3 expression will be vital for our considerations, in particular, for generalizing this inequality into a family of inequalities maximally violated by n -qubit GHZ states and n pairs of anticommuting observables.

B. Self-testing

We now prove that the maximal quantum violation of inequality (20) can be used for certification of the GHZ state (11) along with the observables (21). To this aim, consider a quantum realization given by a pure state $|\psi\rangle \in \mathcal{H}$ and a set of quantum observables A_i, B_j with $i, j = 1, 2, 3$ acting on \mathcal{H} , where \mathcal{H} is some unknown Hilbert space. We additionally assume that these observables obey the compatibility relations presented in Fig. 3, which translate into the commutation relations in Eq. (22).

Assume then the correlations obtained by measuring A_i and B_j on the state $|\psi\rangle$ attain the quantum bound of inequality (20). This directly implies that the first three terms in \mathcal{I}_3 take value 1, whereas the last term equals -1 , which via the Cauchy-Schwarz inequality translate to the following equations:

$$A_1 B_2 B_3 |\psi\rangle = |\psi\rangle \quad \text{and permutations,} \quad (24)$$

$$B_1 A_2 B_3 |\psi\rangle = |\psi\rangle \quad \text{and permutations,} \quad (25)$$

$$B_1 B_2 A_3 |\psi\rangle = |\psi\rangle \quad \text{and permutations,} \quad (26)$$

$$A_1 A_2 A_3 |\psi\rangle = -|\psi\rangle \quad \text{and permutations,} \quad (27)$$

where ‘‘permutations’’ refers to the fact that the above relations also hold if we permute the observables, which is a consequence of the commutation relations (22). One directly deduces from these identities that

$$\begin{aligned} A_1 B_1 |\psi\rangle &= A_1 A_2 B_3 |\psi\rangle = -B_3 A_3 |\psi\rangle \\ &= A_1 A_3 B_2 |\psi\rangle = A_3 B_3 |\psi\rangle, \end{aligned} \quad (28)$$

where in the first line we used $B_1 |\psi\rangle = A_2 B_3 |\psi\rangle$ from Eq. (25) and then the fact that B_3 commutes with A_1 and A_2 along with the relation $A_1 A_2 |\psi\rangle = -A_3 |\psi\rangle$ that stems from Eq. (27). On the other hand, in the second line, we used $B_1 |\psi\rangle = A_3 B_2 |\psi\rangle$ from Eq. (26) and $A_1 B_2 |\psi\rangle = A_3 |\psi\rangle$ from Eq. (27).

Let us now employ the symmetries of the inequality. Indeed, as already mentioned, it is invariant under simultaneous permutations $A_i \leftrightarrow A_j$ and $B_i \leftrightarrow B_j$ for any $i \neq j$, and therefore one can straightforwardly infer from Eq. (28) that the

following chain of equalities holds true:

$$\begin{aligned} A_1 B_1 |\psi\rangle &= A_2 B_2 |\psi\rangle = A_3 B_3 |\psi\rangle \\ &= -B_1 A_1 |\psi\rangle = -B_2 A_2 |\psi\rangle = -B_3 A_3 |\psi\rangle. \end{aligned} \quad (29)$$

From the above equations it follows that the operators A_i and B_i with $i = 1, 2, 3$ anticommute when acting on the state $|\psi\rangle$, i.e.,

$$\{A_i, B_i\} |\psi\rangle = \{A_2, B_2\} |\psi\rangle = \{A_3, B_3\} |\psi\rangle = 0. \quad (30)$$

Inspired by the approach of Ref. [32], we now define a subspace

$$\begin{aligned} V := \text{span}\{&|\psi\rangle, A_1 |\psi\rangle, A_2 |\psi\rangle, A_3 |\psi\rangle, \\ &B_1 |\psi\rangle, B_2 |\psi\rangle, B_3 |\psi\rangle, A_1 B_1 |\psi\rangle\}, \end{aligned} \quad (31)$$

and prove the following fact for it.

Lemma 1. V is an invariant subspace of all the observables A_i and B_j for $i, j \in \{1, 2, 3\}$.

Proof. One can verify with the aid of Eqs. (24)–(27) that the action of the operator A_1 on the eight vectors spanning V is a permutation of these vectors up to the factor -1 . In exactly the same way, one shows that $B_1 V \subseteq V$. Therefore, we conclude that the subspace V is invariant under the action of the observables A_1 and B_1 . By the symmetry of inequality (20) it then follows that the subspace V is invariant under the action of all observables A_i and B_j for $i, j \in \{1, 2, 3\}$. ■

It should be noticed that due to Eq. (29), the subspace V stays the same if one replaces the last vector $A_1 B_1 |\psi\rangle$ in Eq. (31) by $A_2 B_2 |\psi\rangle$ or $A_3 B_3 |\psi\rangle$.

Due to Lemma 1, it suffices for our purpose to identify the form of the state $|\psi\rangle$ and the operators A_i and B_j restricted to the subspace V . In fact, the whole Hilbert space splits as $\mathcal{H} = V \oplus V^\perp$, where V^\perp is an orthocomplement of V in \mathcal{H} . Then, the fact that V is an invariant subspace of all the observables A_i and B_j means that they have the following block structure:

$$A_i = \hat{A}_i \oplus A'_i, \quad B_j = \hat{B}_j \oplus B'_j, \quad (32)$$

where $\hat{A}_i = P A_i P$ and analogously $\hat{B}_i = P B_i P$ with $P : \mathcal{H} \rightarrow V$ being a projection onto V . Since A'_i and B'_j act trivially on V , that is, $A'_i V = B'_j V = 0$, which means that the observed correlations giving rise to the maximal violation of inequality (20) come solely from the subspace V , in what follows we can restrict our attention to the operators \hat{A}_i and \hat{B}_j .

First, from the fact that A_i and B_j are observables obeying $A_i^2 = B_j^2 = \mathbb{1}$, it directly follows that \hat{A}_i, \hat{B}_j are observables too and satisfy

$$\hat{A}_i^2 = \hat{B}_j^2 = \mathbb{1}_V \quad (i, j = 1, 2, 3), \quad (33)$$

where $\mathbb{1}_V$ is the identity acting on V . Second, Eq. (32) implies that the hatted observables must obey the same commutation relations as A_i and B_j , that is,

$$[\hat{A}_i, \hat{A}_j] = [\hat{A}_i, \hat{B}_j] = [\hat{B}_i, \hat{B}_j] = 0 \quad (i \neq j). \quad (34)$$

Third, it turns out that relations (30) force \hat{A}_i and \hat{B}_i to anticommute on the subspace V .

Lemma 2. Suppose the maximal quantum violation of inequality (20) is observed. Then, $\{\hat{A}_i, \hat{B}_i\} = 0$ for all $i \in \{1, 2, 3\}$.

Proof. Let us focus on the first pair \hat{A}_1 and \hat{B}_1 . By checking the action of $\{A_1, B_1\}$ on all the eight vectors that span the subspace V we can conclude that $\{\hat{A}_1, \hat{B}_1\} = 0$. Indeed, Eq. (30) implies that $\{A_1, B_1\}$ vanishes when acting on $|\psi\rangle$. Then, for $A_1|\psi\rangle$ one has

$$\{A_1, B_1\}A_1|\psi\rangle = (A_1B_1A_1 + B_1)|\psi\rangle = 0, \quad (35)$$

where the second equality follows again from Eq. (30). For $A_2|\psi\rangle$ and $A_3|\psi\rangle$ we can use the fact that A_1 and B_1 commute with A_2 and A_3 , which gives

$$\{A_1, B_1\}A_i|\psi\rangle = A_i\{A_1, B_1\}|\psi\rangle = 0 \quad (i = 2, 3). \quad (36)$$

In exactly the same way one deals with the vectors $B_i|\psi\rangle$. Finally, for the last vector in Eq. (31), $A_1B_1|\psi\rangle$, one has

$$\{A_1, B_1\}A_1B_1|\psi\rangle = (A_1B_1A_1B_1 + \mathbb{1})|\psi\rangle = 0, \quad (37)$$

where to get the last equality we use Eq. (30). Owing to the block form of A_1 and B_1 in Eq. (32), all this implies that $\{\hat{A}_1, \hat{B}_1\} = 0$.

One more time, by the symmetries of the inequality, we can draw the same conclusions for the remaining pairs of the observables A_i and B_i . As a result $\{\hat{A}_i, \hat{B}_i\} = 0$ for $i = 1, 2, 3$, which completes the proof. ■

With Lemma 2 at hand, we can now employ the standard approach that has already been used in many non-locality-based self-testing schemes [17,18,48,49]. Precisely, using this approach we can first infer that the dimension d of the subspace V is even. To see this, note that from the above anticommutation relation between \hat{A}_i and \hat{B}_i we have

$$\hat{A}_i = -\hat{B}_i\hat{A}_i\hat{B}_i \quad \text{or} \quad \hat{B}_i = -\hat{A}_i\hat{B}_i\hat{A}_i, \quad (38)$$

which after taking trace on both sides simplifies to $\text{tr}(\hat{A}_i) = \text{tr}(\hat{B}_i) = 0$. It then follows that both the eigenvalues ± 1 of each observable \hat{A}_i or \hat{B}_i have equal multiplicities. This clearly implies that the dimension $d = \dim V$ is an even number, $d = 2k$ for some $k \in \mathbb{N}$, and thus $V = \mathbb{C}^2 \otimes \mathbb{C}^k$. On the other hand, since $\dim V \leq 8$, one concludes that $k = 2, 3, 4$.

The fact that \hat{A}_1 and \hat{B}_1 are traceless means also that the operators \hat{A}_1 and \hat{B}_1 are equivalent to $X \otimes \mathbb{1}_k$ and $Z \otimes \mathbb{1}_k$ for some $k = 2, 3, 4$ up to some unitary operation (see for instance Appendix B in Ref. [48] for the proof of this statement). This observation is one of the key ideas behind the proof of the following lemma.

Lemma 3. Suppose the maximal quantum violation of inequality (20) is observed. Then, there exists a basis in V such that

$$\begin{aligned} \hat{A}_1 &= X \otimes \mathbb{1} \otimes \mathbb{1}, & \hat{B}_1 &= Z \otimes \mathbb{1} \otimes \mathbb{1}, \\ \hat{A}_2 &= \mathbb{1} \otimes X \otimes \mathbb{1}, & \hat{B}_2 &= \mathbb{1} \otimes Z \otimes \mathbb{1}, \\ \hat{A}_3 &= \mathbb{1} \otimes \mathbb{1} \otimes X, & \hat{B}_3 &= \mathbb{1} \otimes \mathbb{1} \otimes Z. \end{aligned} \quad (39)$$

Proof. First, from Lemma 2 we have $\{\hat{A}_1, \hat{B}_1\} = 0$ which implies that there exists a unitary U_1 acting on V such that

$$U_1^\dagger \hat{A}_1 U_1 = X \otimes \mathbb{1}_k, \quad (40)$$

$$U_1^\dagger \hat{B}_1 U_1 = Z \otimes \mathbb{1}_k, \quad (41)$$

where, as already mentioned, the dimension d of the subspace V is given by $d = 2k$ for some $k = 2, 3, 4$. Using then the

above form of \hat{A}_1 and \hat{B}_1 and the commutation relations (22) we can write the other operators as follows:

$$U_1^\dagger \hat{A}_2 U_1 = \mathbb{1}_2 \otimes M, \quad (42)$$

$$U_1^\dagger \hat{B}_2 U_1 = \mathbb{1}_2 \otimes N, \quad (43)$$

$$U_1^\dagger \hat{A}_3 U_1 = \mathbb{1}_2 \otimes O, \quad (44)$$

$$U_1^\dagger \hat{B}_3 U_1 = \mathbb{1}_2 \otimes P, \quad (45)$$

where M, N, O , and P are Hermitian involutions acting on the subspace of dimension k . To show explicitly how the above equations are obtained let us focus on \hat{A}_2 ; the proof for the other observables is basically the same. Since \hat{A}_2 acts on $\mathbb{C}^2 \otimes \mathbb{C}^k$, it can be decomposed in the Pauli basis as

$$U_1^\dagger \hat{A}_2 U_1 = \mathbb{1}_2 \otimes M_1 + X \otimes M_2 + Y \otimes M_3 + Z \otimes M_4, \quad (46)$$

where Y is the third Pauli matrix and M_i are some Hermitian matrices acting on \mathbb{C}^k . Now, it follows from the fact that \hat{A}_2 commutes with \hat{A}_1 , that $M_3 = M_4 = 0$. Then, from $[\hat{A}_2, \hat{B}_1]$ one obtains that $M_2 = 0$, and, by putting $M_1 = M$, we arrive at Eq. (42).

Second, from Lemma 2, we have $\{\hat{A}_2, \hat{B}_2\} = 0$ which is equivalent to $\{M, N\} = 0$. Since both M and N are involutions, one concludes, as before, that $k = 2k'$ for $k' = 1, 2$, or, equivalently, that $\mathbb{C}^k = \mathbb{C}^2 \otimes \mathbb{C}^{k'}$. Moreover, there exists another unitary transformation $U_2 : \mathbb{C}^k \rightarrow \mathbb{C}^k$ such that

$$U_2^\dagger M U_2 = X \otimes \mathbb{1}_{k'}, \quad (47)$$

$$U_2^\dagger N U_2 = Z \otimes \mathbb{1}_{k'}. \quad (48)$$

Finally, to learn the form of O and P we can again employ the commutation relations (22). They imply in particular that $[M, O] = [N, O] = [M, P] = [N, P] = 0$, and consequently,

$$O = \mathbb{1}_2 \otimes O', \quad P = \mathbb{1}_2 \otimes P', \quad (49)$$

where O' and P' are some operators acting on $\mathbb{C}^{k'}$ such that $[O']^2 = [P']^2 = \mathbb{1}_{k'}$. Additionally, due to the fact that $\{\hat{A}_3, \hat{B}_3\} = 0$, they must anticommute, $\{O', P'\} = 0$. This means that $k' = 2$ and that there exists a unitary operation U_3 acting on this qubit Hilbert space such that

$$U_3^\dagger O' U_3 = X, \quad U_3^\dagger P' U_3 = Z. \quad (50)$$

Taking all this into account, one finds that $V \cong \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ and that there exists a single unitary operation $U = U_1(\mathbb{1}_2 \otimes U_2)(\mathbb{1}_2 \otimes \mathbb{1}_2 \otimes U_3)$ on V which brings all the observables \hat{A}_i and \hat{B}_i to the form in Eqs. (39). ■

We have thus arrived at one of our main results of this paper.

Theorem 1. If a quantum state $|\psi\rangle$ and a set of measurements A_i and B_j with $i, j \in \{1, 2, 3\}$ maximally violate inequality (20), then there exist a projection $P : \mathcal{H} \rightarrow V$ with $V = (\mathbb{C}^2)^{\otimes 3}$ and a unitary U acting on V such that

$$U^\dagger (P A_i P^\dagger) U = X_i, \quad (51)$$

$$U^\dagger (P B_i P^\dagger) U = Z_i, \quad (52)$$

where X_i and Z_i are X and Z Pauli matrices acting on qubit i , and

$$U(P|\psi\rangle) = |G\rangle \quad (53)$$

with $|G\rangle$ being the three-qubit complete graph state defined in Eq. (11).

Proof. A quantum state $|\psi\rangle$ that belongs to a Hilbert space \mathcal{H} and a set of observables A_i, B_j acting on \mathcal{H} attain the maximal quantum violation of inequality (20) if and only if they satisfy the set of Eqs. (24)–(27). The algebraic relations induced by this set of equations let us prove Lemmas 1–3 which imply that there exists a projection $P : \mathcal{H} \rightarrow V \cong \mathbb{C}^8$ and a unitary $U = U_1(\mathbb{1}_2 \otimes U_2)(\mathbb{1}_2 \otimes \mathbb{1}_2 \otimes U_3)$ acting on $V \cong \mathbb{C}^8$ for which Eqs. (51) hold true.

From the above characterization of the observables we can infer the form of the state $|\psi\rangle$. Indeed, after plugging Eqs. (78) into the conditions (24) one realizes that the latter are simply the stabilizing conditions of the graph state associated to the complete graph of three vertices given in Eq. (11) and thus $U|\psi\rangle = |G'\rangle$. This completes the proof. ■

A few comments are in order. The first is that the tensor product structure here is just a suitable mathematical tool we used to represent our results. We know that in composite quantum systems the Hilbert space of the whole system is a tensor product of the Hilbert spaces of the separate subsystems; however, it has to be clear that in Theorem 1 we do not assume the whole system to be composite.

The second comment is that the certification statement made in Theorem 1 involves a global unitary operation which means that any state from V can in fact be chosen as the reference state, even a fully product one. Thus, Theorem 1 cannot be understood as a certification of only the state, but rather as a certification of a state and a set of measurements at the same time. Or, more precisely, it is a certification of how measurements act on the state or what the relation between a state and measurements is; this relation is basis independent.

One way to get rid of the above ambiguity is to assume that the quantum system at hand is composed of spatially separated subsystems on which the verifier can perform local measurements. Such an assumption allows them to use Bell nonlocality to deduce the form of the state. For instance for the GHZ state of three qubits a self-testing statement based on the violation of inequality (20) was derived in Ref. [17].

To illustrate the difference between contextuality and nonlocality-based certification let us consider another set of quantum observables on \mathbb{C}^8 defined as

$$\begin{aligned} A_1 &= X \otimes \mathbb{1} \otimes \mathbb{1}, & A_2 &= \mathbb{1} \otimes X \otimes Z, & A_3 &= \mathbb{1} \otimes Z \otimes X, \\ B_1 &= Z \otimes \mathbb{1} \otimes \mathbb{1}, & B_2 &= \mathbb{1} \otimes Z \otimes \mathbb{1}, & B_3 &= \mathbb{1} \otimes \mathbb{1} \otimes Z. \end{aligned} \tag{54}$$

Clearly, these observables, similarly to those in Eq. (21), satisfy the commutation and anticommutation relations in

Eqs. (22) and (30). Moreover, they give rise to the maximal violation of inequality (20) together with the graph state $|G''\rangle$ corresponding to the linear graph in Fig. 2. However, while both the graph states $|G'\rangle$ and $|G''\rangle$ are equivalent under local unitary operations and thus cannot be distinguished within both approaches to self-testing, the sets of observables in Eqs. (21) and (54) are certainly not; they are equivalent under global unitary operations. Thus, the maximal violation of the Bell inequality (20) would allow one to distinguish between these two sets, while standard quantum contextuality does not allow to do that.

IV. A SCALABLE INEQUALITY AND SELF-TESTING OF MULTIQUBIT GRAPH STATES

In this section we design a family of noncontextuality inequalities which is scalable and aimed to certify multiqubit quantum systems. These inequalities are scalable since the numbers of measurements and correlators increase polynomially with the number of vertices of the respective graph state. The inequality we propose in Eq. (57) generalizes the inequality given in Eq. (20) and has this inequality in the heart of the construction since the structure of the simplest inequality appears as the building blocks of the general construction. We prove that the inequalities are useful for certification purposes.

A. Scalable noncontextuality inequalities

First, let us consider a set of $2n$ observables denoted by A_1, \dots, A_n and B_1, \dots, B_n . They are assumed to mutually commute except for pairs A_i, B_i with $i \in \{1, \dots, n\}$, that is,

$$[A_i, A_j] = [B_i, B_j] = [A_i, B_j] = 0 \quad (i \neq j). \tag{55}$$

We now describe our construction of the noncontextuality inequalities. We first consider a sum of n expectation values of the form $C_i = \langle B_1 \cdots B_{i-1} A_i B_{i+1} \cdots B_n \rangle$ for $i = 1, \dots, n$ which involve $n - 1$ different B_j observables and a single observable A_i . Then, for any choice of three out of n such different correlators C_i, C_j and C_k ($i \neq j \neq k$) we consider another correlator that we subtract from the sum. It is given by

$$\langle B_1 \cdots A_i \cdots A_j \cdots A_k \cdots B_n \rangle \tag{56}$$

and consists of three observables A_i, A_j , and A_k and $n - 3$ observables B_m with $m \neq i, j, k$. In this way we obtain $n + \binom{n}{3}$ expectation values from which we construct our noncontextuality inequality,

$$\begin{aligned} \mathcal{I}_n &= \alpha_n (\langle A_1 B_2 B_3 B_4 \cdots B_n \rangle + \langle B_1 A_2 B_3 B_4 \cdots B_n \rangle + \langle B_1 B_2 A_3 B_4 \cdots B_n \rangle + \cdots + \langle B_1 B_2 B_3 B_4 \cdots A_n \rangle) \\ &\quad - \langle A_1 A_2 A_3 B_4 \cdots B_n \rangle - \langle A_1 A_2 B_3 A_4 \cdots B_n \rangle - \cdots - \langle B_1 \cdots B_{n-3} A_{n-2} A_{n-1} A_n \rangle \leq \eta_C^{(n)} < \eta_Q^{(n)} = \alpha_n n + \binom{n}{3}, \end{aligned} \tag{57}$$

where the constant $\alpha_n = \binom{n-1}{2}$ has been added for further convenience.

It is not difficult to see that for the case $n = 3$ the above inequality reproduces the one in Eq. (20). While, as already

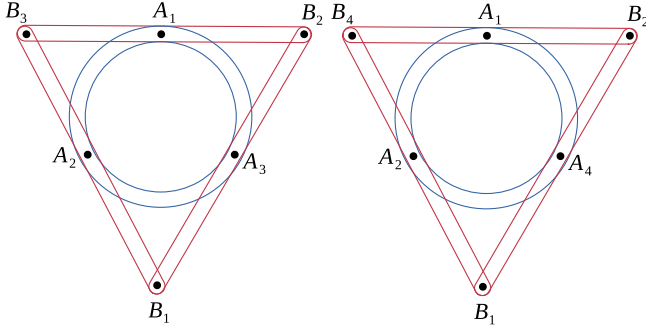


FIG. 4. Hypergraphs of compatibility of subsets of observables related with two choices of subsets of correlators in Eq. (58). On the left we have the hypergraph associated with the subscripts 1, 2, and 3, and on the right side with the subscripts 1, 2, and 4. These two hypergraphs also represent the compatibility structures of the observables corresponding to the simpler inequality (20) and another such simpler inequality with the observables A_i and B_j , with $i, j = 1, 2, 4$, respectively. These two compatibility structures serve as the building blocks to construct inequality (58).

mentioned, for $n = 3$ it is equivalent to the MABK inequality [38–40] if the commutation relations between the observables are satisfied due to the spatial separation between the subsystems, for $n > 3$ this is not the case. The number of terms in the MABK Bell-type inequalities grows exponentially with n , whereas in our noncontextuality inequalities this number scales only polynomially with n . In Refs. [18,42,50] other Bell-type inequalities were designed for the graph states which again scale exponentially or linearly; thus, they differ from our inequalities. Our inequalities (57) are designed such that they are suitable for the purpose of certification. It is also important to notice that our inequality is constructed in such a way that for every three different correlators that enter \mathcal{I}_n with + and the associated “negative” one, the noncommon observables appearing in all these four correlators adopt the compatibility structure from the simplest inequality for $n = 3$. To illustrate this with an example let us consider the inequality for $n = 4$:

$$\begin{aligned} \mathcal{I}_4 &= 3(\langle A_1 B_2 B_3 B_4 \rangle + \langle B_1 A_2 B_3 B_4 \rangle + \langle B_1 B_2 A_3 B_4 \rangle \\ &\quad + \langle B_1 B_2 B_3 A_4 \rangle) - \langle B_1 A_2 A_3 A_4 \rangle - \langle A_1 B_2 A_3 A_4 \rangle \\ &\quad - \langle A_1 A_2 B_3 A_4 \rangle - \langle A_1 A_2 A_3 B_4 \rangle \\ &\leq \eta_C^{(4)} < \eta_Q^{(4)} = 16. \end{aligned} \quad (58)$$

Figure 4 presents the compatibility structures of the common observables for two choices of such four-element subsets of expectation values in \mathcal{I}_4 . The first subset consists of the first three terms with a + sign and the last one with a – sign, all containing observables A_1, A_2 , and A_3 , whereas the second set is composed of the first, the second, and the fourth “+” terms in \mathcal{I}_4 and the third “negative one,” all of them containing A_1, A_2 , and A_4 .

Inequality (57) is nontrivial for any n , i.e., $\eta_C^{(n)} < \eta_Q^{(n)}$. To prove this statement, let us first notice that its quantum bound is $\eta_Q^{(n)} = n\alpha_n + \binom{n}{3}$ and can be attained by the following observables,

$$A_i = X_i, \quad B_j = Z_j, \quad (59)$$

and the unique graph state $|G_n\rangle$ associated to the complete graph of n qubits and stabilized by the operators in Eq. (17). In fact, plugging Eqs. (59) into the expression for \mathcal{I}_n one realizes that all correlators with + correspond to the stabilizing operators G_i , whereas those entering \mathcal{I}_n with a minus sign correspond to products of triples of different G_i 's.

Let us then estimate the maximal classical value $\eta_C^{(n)}$, and, for pedagogical purposes, we first consider the case $n = 4$ for which the expression \mathcal{I}_4 can be stated as

$$\begin{aligned} \mathcal{I}_4 &= (\langle A_1 B_2 B_3 B_4 \rangle + \langle B_1 A_2 B_3 B_4 \rangle + \langle B_1 B_2 A_3 B_4 \rangle \\ &\quad - \langle A_1 A_2 A_3 B_4 \rangle) + (\langle A_1 B_2 B_3 B_4 \rangle + \langle B_1 A_2 B_3 B_4 \rangle \\ &\quad + \langle B_1 B_2 B_3 A_4 \rangle - \langle A_1 A_2 B_3 A_4 \rangle) + (\langle A_1 B_2 B_3 B_4 \rangle \\ &\quad + \langle B_1 B_2 A_3 B_4 \rangle + \langle B_1 B_2 B_3 A_4 \rangle - \langle A_1 B_2 A_3 A_4 \rangle) \\ &\quad + ((\langle B_1 A_2 B_3 B_4 \rangle + \langle B_1 B_2 A_3 B_4 \rangle + \langle B_1 B_2 B_3 A_4 \rangle \\ &\quad - \langle B_1 A_2 A_3 A_4 \rangle), \end{aligned} \quad (60)$$

where each line in the right-hand side of the above equation corresponds to a lifting of \mathcal{I}_3 to $n = 4$. Due to the fact that in each line we have basically the inequality for $n = 3$, it is not difficult to see that for noncontextual models, $|\mathcal{I}_4| \leq 4 \times 2 = 8$, which is clearly smaller than the maximal quantum value $\eta_Q^{(4)} = 16$. To prove that the same holds true for any n , it suffices to notice that, analogously to \mathcal{I}_4 , \mathcal{I}_n can be rewritten as a sum of $\binom{n}{3}$ terms that are liftings of \mathcal{I}_3 , and thus $\eta_C^{(n)} \leq 2\binom{n}{3}$. At the same time, $\eta_Q^{(n)} = n\binom{n-1}{2} + \binom{n}{3}$ and thus $\eta_Q^{(n)} > \eta_C^{(n)}$ for any $n \geq 3$.

B. Certification based on the noncontextuality inequality

Let us now show how the above inequality can be used for certification of the complete graph state and n pairs of anti-commuting observables. To this aim, we assume that a state $|\psi\rangle \in \mathcal{H}$ together with a set of $2n$ dichotomic observables A_i and B_i acting on \mathcal{H} maximally violate Eq. (57). Then, as in the case $n = 3$, this implies the following set of $n + \binom{n}{3}$ equations:

$$B_1 \cdots B_{i-1} A_i B_{i+1} |\psi\rangle = |\psi\rangle \quad (61)$$

with $i = 1, \dots, n$, and

$$B_1 \cdots A_i \cdots A_j \cdots A_k \cdots B_n |\psi\rangle = -|\psi\rangle \quad (62)$$

for any choice of $i, j, k = 1, \dots, n$ such that $i \neq j \neq k$.

As a consequence of these equations, we have

$$A_1 B_1 |\psi\rangle = A_1 A_2 B_3 B_4 \cdots B_n |\psi\rangle = A_2 B_2 |\psi\rangle, \quad (63)$$

where the first and the second equality stem from Eq. (61) for $i = 2$ and Eq. (61) for $i = 1$, respectively. Then, by applying Eq. (62) for $i = 1, j = 2$, and $k = 3$, one obtains

$$A_1 B_1 |\psi\rangle = -B_3 A_3 |\psi\rangle. \quad (64)$$

On the other hand, using Eq. (61) with $i = 3$ we can write

$$A_1 B_1 |\psi\rangle = A_1 A_3 B_2 B_4 \cdots B_n |\psi\rangle = A_3 B_3 |\psi\rangle, \quad (65)$$

where the second equation is a consequence of Eq. (61) for $i = 1$. Simultaneously, an application of Eq. (62) for $i = 1, j = 2$, and $k = 3$ to the second terms in the above gives

$$A_1 B_1 |\psi\rangle = -B_2 A_2 |\psi\rangle. \quad (66)$$

Note that our inequality is designed in a such way that it is symmetric under any permutation of subscripts; i.e., it is invariant under the transformations $A_i \leftrightarrow A_j$ together with $B_i \leftrightarrow B_j$. This when applied to Eqs. (63)–(66) results in the following relations:

$$A_i B_i |\psi\rangle = A_j B_j |\psi\rangle = -B_i A_i |\psi\rangle \quad (67)$$

for $i, j \in \{1, 2, \dots, n\}$. In particular, A_i and B_i anticommute:

$$\{A_i, B_i\} |\psi\rangle = 0 \quad (i = 1, \dots, n). \quad (68)$$

Having established the key relations between the state and the observables, let us now, analogously to the case $n = 3$, identify a subspace of the Hilbert space \mathcal{H} which is invariant under the action of all observables A_i and B_i . The subspace is given by

$$V_n = \text{span}\{|\psi\rangle, B_{i_1} |\psi\rangle, B_{i_1} B_{i_2} |\psi\rangle, \dots, B_{i_1} B_{i_2} \dots B_{i_k} |\psi\rangle, \dots, B_{i_1} B_{i_2} \dots B_{i_{n-1}} |\psi\rangle, B_1 \dots B_n |\psi\rangle\}, \quad (69)$$

where $i_j = 1, \dots, n$ for any j and $i_1 < i_2 < \dots < i_k < \dots < i_{n-1}$.

For instance, in the simplest cases of $n = 3$ and $n = 4$, the above construction gives

$$V_3 = \text{span}\{|\psi\rangle, B_i |\psi\rangle, B_i B_j |\psi\rangle, B_1 B_2 B_3 |\psi\rangle\} \quad (70)$$

and

$$V_4 = \text{span}\{|\psi\rangle, B_i |\psi\rangle, B_i B_j |\psi\rangle, B_i B_j B_k |\psi\rangle, B_1 B_2 B_3 B_4 |\psi\rangle\} \quad (71)$$

with $i, j, k = 1, \dots, n$ and $i < j < k$. In particular, V_3 is exactly the same as the one defined in Eq. (31); due to Eq. (61), $B_i B_j |\psi\rangle = A_k |\psi\rangle$ with $i \neq j \neq k$ and $B_1 B_2 B_3 |\psi\rangle = A_1 B_1 |\psi\rangle$.

Let us then notice that the number of vectors spanning V_n is 2^n . This is because each subset of vectors of the form $A_{i_1} \dots A_{i_k} |\psi\rangle$ for $i_1 < \dots < i_k$ contains $\binom{n}{k}$ elements, and we have $n + 1$ such subsets indexed by $k = 0, \dots, n$. Thus the total number of vectors can be counted as

$$\sum_{k=0}^n \binom{n}{k} = (1 + 1)^n = 2^n, \quad (72)$$

meaning that $\dim V_n \leq 2^n$. In fact, as we show later $\dim V_n$ is exactly 2^n .

Our aim now is to identify the form of the operators A_i and B_j projected onto the subspace V_n . The idea of the proof of self-testing is similar to those we used in the case $n = 3$.

Lemma 4. The subspace V_n of \mathcal{H}_n is invariant under the action of the operators A_i and B_j for $i, j = \{1, 2, \dots, n\}$.

Proof. It can be checked that the action of any operator A_i or B_j over all the set of 2^n elements that generate the subspace V_n is, up to the factor -1 , a permutation over this set. Indeed, the action of B_m on vectors of the form $B_{i_1} \dots B_{i_k} |\psi\rangle$ with $i_1 < \dots < i_k$ for $k = 1, \dots, n$ returns vectors of a similar form with $k \rightarrow k - 1$ if m equals one of the subscripts i_1, \dots, i_k , or with $k \rightarrow k + 1$ otherwise. In both cases the resulting vectors are already in V_n .

Let us then consider the A_i observables. Due to Eq. (61) and taking into account the commutation (55) or anticommutation (68) their action on the vectors spanning V_n can always be represented as an action of a product of $n - 1$ different B_i observables. Thus, when applied to $B_{i_1} \dots B_{i_k} |\psi\rangle$

with $i_1 < \dots < i_k$ for $k = 1, \dots, n$ they will again produce vectors involving products of B_i operators that are already in V_n . This completes the proof. ■

This is a key step of our considerations because, taking into account the fact that A_i and B_i are quantum observables, Lemma 4 implies that they can be represented as a direct sum of two blocks,

$$A_i = \hat{A}_i \oplus A'_i, \quad B_j = \hat{B}_j \oplus B'_j, \quad (73)$$

where \hat{A}_i and \hat{B}_i are projections of A_i and B_i onto V_n , that is, $\hat{A}_i = P_n A_i P_n$ and $\hat{B}_i = P_n B_i P_n$ with $P_n : \mathcal{H}_n \rightarrow V_n$ denoting the projector onto V_n . On the other hand, A'_i and B'_j are defined on the orthocomplement of V_n in the Hilbert space \mathcal{H}_n that we denote V_n^\perp ; clearly, $\mathcal{H}_n = V_n \oplus V_n^\perp$.

Importantly, A'_i and B'_i act trivially on the subspace V_n , in particular $A'_i |\psi\rangle = B'_i |\psi\rangle = 0$, and consequently it is enough for our purposes to characterize \hat{A}_i and \hat{B}_j . Our first step to achieve this goal is to prove the following lemma.

Lemma 5. $\{\hat{A}_i, \hat{B}_i\} = 0$ for all $i \in \{1, \dots, n\}$.

Proof. In order to prove this statement we will show that $\{A_i, B_i\} V_n = 0$; that is, all these anticommutators act trivially on any vector from V_n . To this aim, let us investigate how $\{A_i, B_i\}$ acts on the vectors spanning V_n . We first see that $\{A_i, B_i\} |\psi\rangle = 0$ as a direct consequence of Eq. (67). Let us then consider vectors $B_j |\psi\rangle$. If $i \neq j$, we can directly use the commutation relations (55) to write

$$\{A_i, B_i\} B_j |\psi\rangle = B_j \{A_i, B_i\} |\psi\rangle = 0. \quad (74)$$

On the other hand, if $i = j$, one has

$$\{A_i, B_i\} B_i |\psi\rangle = (A_i + B_i A_i B_i) |\psi\rangle = 0, \quad (75)$$

where the last equality is again a consequence of the facts that $A_i B_i |\psi\rangle = -B_i A_i |\psi\rangle$ and that $B_i^2 = \mathbb{1}$.

It is not difficult to realize that the above reasoning extends to any vector spanning the subspace V_n . Indeed, let us consider vectors of the form $B_{i_1} \dots B_{i_k} |\psi\rangle$ with $i_1 < \dots < i_k$ for $k = 1, \dots, n$ and assume first that all i_1, \dots, i_k differ from i . Then, due to the commutation relations, one directly has

$$\{A_i, B_i\} B_{i_1} \dots B_{i_k} |\psi\rangle = B_{i_1} \dots B_{i_k} \{A_i, B_i\} |\psi\rangle = 0. \quad (76)$$

On the other hand, if one of the subscripts, say, i_1 , equals i , then

$$\begin{aligned} \{A_i, B_i\} B_{i_1} \dots B_{i_k} |\psi\rangle &= B_{i_2} \dots B_{i_k} \{A_i, B_i\} B_1 |\psi\rangle \\ &= B_{i_2} \dots B_{i_k} (A_i + B_i A_i B_i) |\psi\rangle \\ &= 0, \end{aligned} \quad (77)$$

where the last equality follows from the fact that A_i and B_i anticommute when acting on $|\psi\rangle$ and from $B_i^2 = \mathbb{1}$.

Taking into account that each $\{A_i, B_i\}$ is a Hermitian operator and that it acts trivially on the whole subspace V_n , one directly concludes that $\{\hat{A}_i, \hat{B}_i\} = 0$. ■

Our next lemma is a straightforward generalization of Lemma 3.

Lemma 6. Suppose the maximal quantum violation of our inequality (57) is observed. Then, there exists a basis of V_n for which

$$\hat{A}_i = X_i, \quad \hat{B}_j = Z_j. \quad (78)$$

Proof. We will proceed recursively starting from the pair \hat{A}_1 and \hat{B}_1 . It follows from Lemma 5 that $\{\hat{A}_1, \hat{B}_1\} = 0$ which means that the dimension $d = \dim V_n$ is an even number, i.e., $d = 2k$ for some $k = 1, \dots, 2^{n-1}$ (recall that $d \leq 2^n$), and that there exists a unitary U_1 acting on V_n such that

$$U_1^\dagger \hat{A}_1 U_1 = X \otimes \mathbb{1}_k, \quad (79)$$

$$U_1^\dagger \hat{B}_1 U_1 = Z \otimes \mathbb{1}_k, \quad (80)$$

where $\mathbb{1}_k$ is an identity acting on \mathbb{C}^k .

Next, to determine the remaining observables \hat{A}_i and \hat{B}_i we exploit the fact that they all must commute with both \hat{A}_1 and \hat{B}_1 . With this aim, we use the fact that $V_n = \mathbb{C}^2 \otimes \mathbb{C}^k$ to decompose \hat{A}_i and \hat{B}_i ($i = 2, \dots, n$) in terms of the Pauli basis as

$$U_1^\dagger \hat{R}_i U_1 = \mathbb{1} \otimes M_0^R + X \otimes M_1^R + Y \otimes M_2^R + Z \otimes M_3^R, \quad (81)$$

where $R = A, B$, and M_i^R are some Hermitian matrices acting on \mathbb{C}^k . Now, $[\hat{R}_i, \hat{A}_1] = 0$ implies that $M_2^R = M_3^R = 0$, whereas from $[\hat{R}_i, \hat{B}_1] = 0$ one concludes that $M_1^R = 0$. As a result, all \hat{A}_i and \hat{B}_i with $i = 2, \dots, n$ admit the following representation,

$$U_1^\dagger \hat{A}_i U_1 = \mathbb{1}_2 \otimes M_i, \quad U_1^\dagger \hat{B}_i U_1 = \mathbb{1}_2 \otimes N_i, \quad (82)$$

where M_i and N_i act on \mathbb{C}^k ; in fact, they are Hermitian and obey $M_A^2 = M_B^2 = \mathbb{1}_k$, and thus are quantum observables. Moreover, it follows from Lemma 5 that $\{M_i, N_i\} = 0$ for all $i = 2, \dots, n$.

We have thus a set of $2(n-1)$ quantum observables M_i and N_i that satisfy the same commutation and anticommutation relations as \hat{A}_i and \hat{B}_i , and therefore we can use the above reasoning again to conclude that the dimension k is even, that is, $k = 2k'$ for some $k' = 1, \dots, 2^{n-4}$, and that there is a unitary operation $U_2 : \mathbb{C}^k \rightarrow \mathbb{C}^{k'}$ such that

$$U_2^\dagger M_2 U_2 = X \otimes \mathbb{1}_{k'}, \quad U_2^\dagger N_2 U_2 = Z \otimes \mathbb{1}_{k'}, \quad (83)$$

where $\mathbb{1}_{k'}$ is an identity acting on $\mathbb{C}^{k'}$. We then use the fact that the other operators M_i and N_i with $i = 3, \dots, n$ commute with both M_2 and N_2 to see that they are of the form $M_i = \mathbb{1}_2 \otimes P_i$ and $N_i = \mathbb{1}_2 \otimes Q_i$, where P_i and Q_i are quantum observables acting on $\mathbb{C}^{k'}$.

It is now clear that the above procedure can be applied iteratively many times until all the observables are proven to be of the form (78), of course, up to certain unitary operation. In fact, one finds that $V_n = (\mathbb{C}^2)^{\otimes n}$; that is, it is an n -qubit Hilbert space. Moreover, there is a unitary operation U composed of all the intermediate unitary operations U_i such that

$$U^\dagger \hat{A}_i U = X_i, \quad U^\dagger \hat{B}_i U = Z_i, \quad (84)$$

for any $i = 1, \dots, n$. \blacksquare

One of the main messages that one takes from this lemma is that the dimension of V_n is exactly 2^n ; in other words, V_n is isomorphic to an n -qubit Hilbert space. In this sense our inequalities can be seen as dimension witnesses: the dimension of the Hilbert space supporting a state and observables giving rise to the maximal violation of our inequalities must be at least 2^n . Moreover, the above lemma implies that a set of n pairs of anticommuting quantum observables with outcomes ± 1 that satisfy the commutation relations (55) can always

be represented, up to a single unitary operation, as a tensor product of single-qubit operators (78). We have thus arrived at our main result.

Theorem 2. If a quantum state $|\psi\rangle$ and a set of dichotomic observables A_i and B_j with $i, j = \{1, 2, \dots, n\}$ give rise to maximal violation of inequality (57), then there exist a projection $P_n : \mathcal{H}_n \rightarrow \mathbb{C}^{2^n}$ and a unitary U acting on \mathbb{C}^{2^n} such that

$$U^\dagger (P A_i P^\dagger) U = \hat{A}_i, \quad (85)$$

$$U^\dagger (P B_j P^\dagger) U = \hat{B}_j, \quad (86)$$

$$U(P|\psi\rangle) = |G_n\rangle, \quad (87)$$

where \hat{A}_i and \hat{B}_j are defined in Eq. (78) and $|G_n\rangle$ is the complete graph state of n qubits.

Proof. The state $|\psi\rangle \in \mathcal{H}_n$ and observables A_i and B_j acting on the Hilbert space \mathcal{H}_n attain the maximal quantum violation of inequality (57) if, and only if, they satisfy the set of $n + \binom{n}{3}$ equations (61) and (62). The algebra induced by this set of equations allows us to prove Lemmas 4, 5, and 6; in particular, it follows that there exists a projection $P_n : \mathcal{H} \rightarrow V_n \cong \mathbb{C}^{2^n}$ and a unitary U acting on V_n such that

$$U^\dagger (P A_i P^\dagger) U = X_i, \quad (88)$$

$$U^\dagger (P B_j P^\dagger) U = Z_j. \quad (89)$$

In this way, the products of observables that appear in the first n correlators in inequality (57) give stabilizing operators of the graph state associated to the complete graph with n vertices, whereas the correlators with negative sign correspond to products of three different stabilizing operators for which the graph state $|G_n\rangle$ is an eigenvector with associated eigenvalue -1 . Thus the complete graph state will be the unique state that attains the maximal quantum violation; then

$$U(P|\psi\rangle) = |G_n\rangle. \quad (90)$$

This completes the proof. \blacksquare

V. ROBUSTNESS

Here we obtain fidelity bounds on the state and measurements leading to the given nonmaximal violation of inequality (57) to demonstrate that our scheme is robust to errors and experimental imperfections. For simplicity, let us focus on the case of $n = 3$. Let us say that the maximal quantum violation of inequality (20) is observed with an ϵ error, i.e., a non-maximal violation of $4 - \epsilon$ is observed. Then, the correlators satisfy the following bounds:

$$\begin{aligned} \langle \psi | A_1 B_2 B_3 | \psi \rangle &\geq 1 - \epsilon, \\ \langle \psi | B_1 A_2 B_3 | \psi \rangle &\geq 1 - \epsilon, \\ \langle \psi | B_1 B_2 A_3 | \psi \rangle &\geq 1 - \epsilon, \\ -\langle \psi | A_1 A_2 A_3 | \psi \rangle &\geq 1 - \epsilon, \end{aligned} \quad (91)$$

for some $\epsilon > 0$. We demonstrate that for a small enough value of ϵ , the quantum realization is close enough to the optimal quantum realization which leads to the maximal quantum violation of the inequality. This is the purpose of robustness analysis that will be presented here; i.e., we show that in the

limit $\epsilon \rightarrow 0$ the quantum realization is close to the optimal one.

In the presence of errors, it is not straightforward to guarantee the existence of an invariant subspace under the action of the operators A_i and B_j , as we have in the self-testing of the optimal quantum realization. However, the robustness of the protocol can be demonstrated, in a similar way to that of Ref. [32], by proving the existence of an eight-dimensional ideal subspace \hat{V} together with a state $|\hat{\psi}\rangle \in \hat{V}$ and observables \hat{A}_i and \hat{B}_i acting on it such that their fidelities with the actual state and measurements approach one in the limit of $\epsilon \rightarrow 0$. We define the state fidelity as $F(|\hat{\psi}\rangle, |\psi\rangle) := |\langle \hat{\psi} | \psi \rangle|^2$, and the operator fidelity as $F(\hat{X}_i, X_i) := (1/8)\text{Tr}(\hat{X}_i X_i)$ (with $X_i = A_i$), where the $1/8$ factor is used to normalize the fidelity since $\text{Tr}(\hat{X}_i X_i) \leq 8$, and similarly defined between \hat{B}_j and B_j . Formally, we have the following theorem.

Theorem 3. Suppose a quantum state $|\psi\rangle$ and a set of measurements A_i, B_j with $i, j = \{1, 2, 3\}$ in a Hilbert space \mathcal{H} satisfy the ideal expectations corresponding to the maximal quantum violation of inequality (20) to within error ϵ . Then there exists a projection $P : \mathcal{H} \rightarrow \hat{V}$, where $\dim(\hat{V}) = 8$, a state $|\hat{\psi}\rangle \in \hat{V}$ and \hat{A}_i, \hat{B}_j which are Hermitian involutions acting on \hat{V} for all i and j such that

$$\begin{aligned} \langle \hat{\psi} | \hat{A}_1 \hat{B}_2 \hat{B}_3 | \hat{\psi} \rangle &= 1, \\ \langle \hat{\psi} | \hat{B}_1 \hat{A}_2 \hat{B}_3 | \hat{\psi} \rangle &= 1, \\ \langle \hat{\psi} | \hat{B}_1 \hat{B}_2 \hat{A}_3 | \hat{\psi} \rangle &= 1, \end{aligned}$$

and there exists some unitary U acting on \hat{V} such that

$$\begin{aligned} F(U|\hat{\psi}\rangle, |\psi\rangle) &\geq 1 - \epsilon_0, \\ F(U\hat{A}_i U^\dagger, A_i) &\geq 1 - \epsilon_1 \quad \forall i, \\ F(U\hat{B}_j U^\dagger, B_j) &\geq 1 - \epsilon_2 \quad \forall i, \end{aligned}$$

where $\epsilon_0 = 25\epsilon$, $\epsilon_1 = 0$, and $\epsilon_2 = 4\epsilon$.

The proof of the above theorem is given in Appendix A. This theorem implies that there exists a subspace in which, up to a small enough error, the quantum realization leading to the nonmaximal quantum violation is close to the optimal quantum realization up to a unitary. For instance, an error of 0.1% in each expectation value implies that the state fidelity is not less than 97.5% and the operator fidelities of B_j are not less than 99.6%. Following the proof of Theorem 3, one can also obtain the fidelity bounds for any n demonstrating the robustness of the scheme similarly as presented in Theorem 4.

In order to obtain a tight self-testing bound that is applicable to a more noisy practical scenario in which the given nonmaximal violation is not almost perfect, one may employ the numerical method to bound the state fidelity as a function of violation of the noncontextual inequality based on semidefinite programming relaxations of quantum contextual sets introduced in Ref. [51] or the analytical method based on operator inequalities introduced in Ref. [17].

VI. CONCLUSIONS

Quantum contextuality provides a notion of nonclassicality for single systems. Motivated by extending the task of self-testing based on Bell inequalities to scenarios where en-

tanglement is not necessary or spatial separation between the subsystems is not required, self-testing of quantum devices based on quantum contextuality has recently been explored. In this work we have followed this research direction and have introduced a family of inequalities revealing quantum contextuality and have shown that they can be used for certification of multiqubit quantum systems. An interesting feature of our scheme is that it is scalable: the amount of information about the observed nonclassical correlations needed to certify the underlying quantum system grows only polynomially with the number of qubits that are certified.

Such contextuality-based certification schemes rely, however, on compatibility relations between the involved measurements and are thus generally difficult to implement in practice. A natural follow-up of this work would be therefore to design a scheme for certification built on our inequalities that does not rely on the compatibility relations, but rather allows one to deduce them from the observed nonclassicality. Such schemes for single quantum systems have recently been proposed in Refs. [33,34] within the sequential measurements or temporal correlations scenario. It would be thus interesting to see whether our results can be mapped to this scenario. Another possible direction for further research is to explore whether one can improve the scalability of our scheme with the number of the certified qubits. From a general perspective it is a highly nontrivial question to ask what is the minimal information about the observed nonclassical correlations that enables making nontrivial statements about the underlying quantum system.

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APPENDIX A: PROOF OF THEOREM 3

Here we present the derivation of robustness of the scheme given in Theorem 3. This will be similar to the proof of robustness of the certification scheme given in Ref. [32].

For providing robust self-testing statements in the Bell tests where dichotomic measurements are implemented [17], Jordan decomposition for the state and measurements has been employed to simplify the derivation. In Ref. [32], Jordan decomposition has also been extended to the contextuality scenario to provide robust certification of the two-qubit system. In Appendix B, we extend this Jordan decomposition to our scenario to provide the robust certification. According to this decomposition, we can decompose the Hilbert space \mathcal{H} in which the state and measurements leading to the violation of our inequality act as

$$\mathcal{H} = \bigoplus_l \mathcal{H}_l, \quad (\text{A1})$$

where each \mathcal{H}_l has dimension at most eight and is invariant under the action of A_i and B_j .

With respect to decomposition (A1), the state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_l \sqrt{p_l} |\psi_l\rangle, \quad (\text{A2})$$

where $|\psi_l\rangle \in \mathcal{H}_l$ and $\sum_l p_l = 1$. We express each $|\psi_l\rangle$ in the computational basis $\{|abc\rangle_l : a, b, c \in \{0, 1\}\}$ as

$$|\psi_l\rangle = \sum_{a,b,c=0,1} c_{abc}^{(l)} |abc\rangle_l, \quad (\text{A3})$$

where $c_{abc}^{(l)}$ satisfies $\sum_{a,b,c} |c_{abc}^{(l)}|^2 = 1$.

We define the subspace $\hat{V} \subseteq \mathcal{H}$ as the linear span of $\{|\hat{a}\hat{b}\hat{c}\rangle := \sum_l \sqrt{p_l} |abc\rangle_l\}$. We define the ideal state in this subspace as

$$|\hat{\psi}\rangle := \frac{1}{\sqrt{2}} (|\hat{0}\hat{0}\hat{0}\rangle - |\hat{1}\hat{1}\hat{1}\rangle), \quad (\text{A4})$$

which can be reexpressed as

$$|\hat{\psi}\rangle = \sum_l \sqrt{p_l} |\hat{\psi}_l\rangle, \quad (\text{A5})$$

where

$$|\hat{\psi}_l\rangle := \frac{1}{\sqrt{2}} (|000\rangle_l - |111\rangle_l). \quad (\text{A6})$$

Note that for the ideal observables defined as

$$\begin{aligned} \hat{A}_1 &:= \bigoplus_l (\hat{A}_l \otimes \mathbb{1}_l \otimes \mathbb{1}_l), & \hat{B}_1 &:= \bigoplus_l (\hat{B}_l \otimes \mathbb{1}_l \otimes \mathbb{1}_l), \\ \hat{A}_2 &:= \bigoplus_l (\mathbb{1}_l \otimes \hat{A}_l \otimes \mathbb{1}_l), & \hat{B}_2 &:= \bigoplus_l (\mathbb{1}_l \otimes \hat{B}_l \otimes \mathbb{1}_l), \\ \hat{A}_3 &:= \bigoplus_l (\mathbb{1}_l \otimes \mathbb{1}_l \otimes \hat{A}_l), & \hat{B}_3 &:= \bigoplus_l (\mathbb{1}_l \otimes \mathbb{1}_l \otimes \hat{B}_l), \end{aligned}$$

where

$$\hat{A}_i = X_i, \quad \hat{B}_j = Y_j, \quad (\text{A7})$$

where X_i and Y_j are the Pauli operators acting on the i th qubit, the ideal state defined in Eq. (A4) violates the noncontextuality inequality (20) maximally. Note that the ideal state projected onto \mathcal{H}_l , i.e., $|\hat{\psi}_l\rangle$, has the form of the GHZ state (16). We have chosen the above particular form of the ideal state for our convenience.

We now express the nonideal observables with respect to the Jordan decomposition. Due to the fact that we have three pairs of dichotomic observables that do not commute on the quantum state, which is a consequence of Lemma 7, the dimension of each of the subspaces \mathcal{H}_l in Eq. (A1) can be taken to be eight. From Corollary 1, it follows that

$$\begin{aligned} A_1 &= \bigoplus_l (A_l \otimes \mathbb{1}_l \otimes \mathbb{1}_l), & B_1 &= \bigoplus_l (B_l \otimes \mathbb{1}_l \otimes \mathbb{1}_l), \\ A_2 &= \bigoplus_l (\mathbb{1}_l \otimes A_l \otimes \mathbb{1}_l), & B_2 &= \bigoplus_l (\mathbb{1}_l \otimes B_l \otimes \mathbb{1}_l), \\ A_3 &= \bigoplus_l (\mathbb{1}_l \otimes \mathbb{1}_l \otimes A_l), & B_3 &= \bigoplus_l (\mathbb{1}_l \otimes \mathbb{1}_l \otimes B_l), \end{aligned}$$

where by using ‘‘local’’ unitary operations we can always choose A_i and B_i acting on \mathcal{H}_l to be other following forms:

$$\begin{aligned} A_1 &= X_1, & B_1 &= \cos \theta_1 Y_1 + \sin \theta_1 X_1, \\ A_2 &= X_2, & B_2 &= \cos \phi_1 Y_2 + \sin \phi_1 X_2, \\ A_3 &= X_3, & B_3 &= \cos \nu_1 Y_3 + \sin \nu_1 X_3, \end{aligned} \quad (\text{A8})$$

with $\theta_l, \phi_l, \nu_l \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.

We now proceed to calculate the state fidelity given by $|\langle \hat{\psi} | \psi \rangle|^2$, where $|\hat{\psi}\rangle$ is the ideal state given by Eq. (A4). Using the fact that the global phase on each subspace can be chosen freely, we can always set $\langle \hat{\psi}_l | \psi_l \rangle \geq 0$, and therefore,

$$\langle \hat{\psi} | \psi \rangle = \sum_l p_l \langle \hat{\psi}_l | \psi_l \rangle \geq \sum_l p_l |\langle \hat{\psi}_l | \psi_l \rangle|^2. \quad (\text{A9})$$

Now, using the expressions of $|\psi_l\rangle$ and $|\hat{\psi}_l\rangle$ given by Eqs. (A3) and (A6), respectively, $\sum_l p_l |\langle \hat{\psi}_l | \psi_l \rangle|^2$ can be written as

$$\sum_l p_l |\langle \hat{\psi}_l | \psi_l \rangle|^2 = \sum_l p_l \frac{1}{2} |c_{000}^{(l)} - c_{111}^{(l)}|^2.$$

The expression in the right-hand side of the above equation can be written as

$$\frac{1}{2} |c_{000}^{(l)} - c_{111}^{(l)}|^2 = |c_{000}^{(l)}|^2 + |c_{111}^{(l)}|^2 - \frac{1}{2} |c_{000}^{(l)} + c_{111}^{(l)}|^2.$$

Using $\sum_{abc} |c_{abc}^{(l)}|^2 = 1$ in the first term in the right-hand side of the above equation, we arrive at

$$\begin{aligned} \sum_l p_l |\langle \hat{\psi}_l | \psi_l \rangle|^2 &= 1 - \sum_l p_l \sum_{abc \neq 000, 111} |c_{abc}^{(l)}|^2 \\ &\quad - \sum_l p_l \frac{1}{2} |c_{000}^{(l)} + c_{111}^{(l)}|^2. \end{aligned} \quad (\text{A10})$$

We will use the following lemma to obtain a lower bound on the right-hand side of the above equation.

Lemma 7. Suppose that inequalities (91) are satisfied for some $\epsilon > 0$. Then, $\|\{A_i, B_i\}|\psi\rangle\| \leq 4\sqrt{2\epsilon}$ for all i .

Proof. We show that $\|\{A_1, B_1\}|\psi\rangle\| \leq 4\sqrt{2\epsilon}$. From Eqs. (91) and assuming that $0 \leq \epsilon \leq 1$, we have that

$$\begin{aligned} \|A_1|\psi\rangle + A_2A_3|\psi\rangle\| &= \sqrt{2(1 + \langle \psi | A_1A_2A_3 | \psi \rangle)} \\ &\leq \sqrt{2[1 - (1 - \epsilon)]} \\ &= \sqrt{2\epsilon}, \end{aligned} \quad (\text{A11})$$

and, similarly, we have

$$\|B_2|\psi\rangle - B_1A_3|\psi\rangle\| \leq \sqrt{2\epsilon}, \quad (\text{A12})$$

$$\|B_1|\psi\rangle - A_2B_3|\psi\rangle\| \leq \sqrt{2\epsilon}, \quad (\text{A13})$$

$$\|B_2|\psi\rangle - A_1B_3|\psi\rangle\| \leq \sqrt{2\epsilon}. \quad (\text{A14})$$

Using then the triangle inequality for the vector norm and the fact that it is unitarily invariant, we have

$$\begin{aligned} \|(A_1B_1 + B_1A_1)|\psi\rangle\| &\leq \|(B_1A_1 + B_1A_2A_3)|\psi\rangle\| \\ &\quad + \|(-B_1A_2A_3 + A_2B_2)|\psi\rangle\| \\ &\quad + \|(-A_2B_2 + A_1A_2B_3)|\psi\rangle\| \\ &\quad + \|(-A_1A_2B_3 + A_1B_1)|\psi\rangle\| \\ &\leq 4\sqrt{2\epsilon}. \end{aligned} \quad (\text{A15})$$

Due to the symmetry of the inequality, the same will hold for any other i , which completes the proof. \blacksquare

First, let us bound $\sum_l p_l |c_{000}^{(l)} + c_{111}^{(l)}|^2$ in Eq. (A10). From Eqs. (A11) and (A12), respectively, we obtain

$$\begin{aligned} & \sum_l p_l (|c_{000}^{(l)} + c_{111}^{(l)}|^2 + |c_{001}^{(l)} + c_{110}^{(l)}|^2 \\ & \quad + |c_{010}^{(l)} + c_{101}^{(l)}|^2 + |c_{011}^{(l)} + c_{100}^{(l)}|^2) \leq \epsilon, \\ & \sum_l p_l (|e^{-i\phi_l} c_{000}^{(l)} - e^{i\theta_l} c_{111}^{(l)}|^2 + |e^{i\phi_l} c_{010}^{(l)} + e^{i\theta_l} c_{101}^{(l)}|^2 \\ & \quad + |e^{-i\phi_l} c_{001}^{(l)} - e^{i\theta_l} c_{110}^{(l)}|^2 + |e^{i\phi_l} c_{011}^{(l)} + e^{i\theta_l} c_{100}^{(l)}|^2) \leq \epsilon. \end{aligned}$$

From the first of these equations, it follows that

$$\sum_l p_l |c_{000}^{(l)} + c_{111}^{(l)}|^2 \leq \epsilon. \quad (\text{A16})$$

It also follows that

$$\sum_l p_l |c_{001}^{(l)} + c_{110}^{(l)}|^2 \leq \epsilon, \quad (\text{A17})$$

$$\sum_l p_l |e^{-i\phi_l} c_{001}^{(l)} - e^{i\theta_l} c_{110}^{(l)}|^2 \leq \epsilon. \quad (\text{A18})$$

Next, we proceed to bound $\sum_l p_l \sum_{abc \neq 000, 111} |c_{abc}^{(l)}|^2$ in Eq. (A10). We have

$$\begin{aligned} & |c_{110}^{(l)}|^2 |e^{i\theta_l} + e^{-i\phi_l}|^2 \\ & = |(e^{i\theta_l} c_{110}^{(l)} - e^{-i\phi_l} c_{001}^{(l)}) + e^{-i\phi_l} (c_{001}^{(l)} + c_{110}^{(l)})|^2. \end{aligned}$$

Using the fact that $|x + y|^2 \leq 2(|x|^2 + |y|^2)$ for any $x, y \in \mathbb{C}$ in the above equation, we arrive at

$$\begin{aligned} & |c_{110}^{(l)}|^2 |e^{i\theta_l} + e^{-i\phi_l}|^2 \\ & \leq 2(|e^{i\theta_l} c_{110}^{(l)} - e^{-i\phi_l} c_{001}^{(l)}|^2 + |c_{001}^{(l)} + c_{110}^{(l)}|^2). \end{aligned}$$

From Eqs. (A17) and (A18),

$$\begin{aligned} & \sum_l p_l |c_{110}^{(l)}|^2 |e^{i\theta_l} + e^{-i\phi_l}|^2 \\ & = \sum_l p_l |c_{110}^{(l)}|^2 (2 + 2 \cos(\theta_l + \phi_l)) \leq 4\epsilon. \quad (\text{A19}) \end{aligned}$$

Similarly,

$$\begin{aligned} & |c_{001}^{(l)}|^2 |e^{i\theta_l} + e^{-i\phi_l}|^2 \\ & = |(-e^{i\theta_l} c_{110}^{(l)} + e^{-i\phi_l} c_{001}^{(l)}) + e^{i\theta_l} (c_{001}^{(l)} + c_{110}^{(l)})|^2 \\ & \leq 2(|-e^{i\theta_l} c_{110}^{(l)} + e^{-i\phi_l} c_{001}^{(l)}|^2 + |c_{001}^{(l)} + c_{110}^{(l)}|^2), \end{aligned}$$

from which it follows that

$$\begin{aligned} & \sum_l p_l |c_{001}^{(l)}|^2 |e^{i\theta_l} + e^{-i\phi_l}|^2 \\ & = \sum_l p_l |c_{001}^{(l)}|^2 (2 + 2 \cos(\theta_l + \phi_l)) \leq 4\epsilon. \quad (\text{A20}) \end{aligned}$$

Adding Eqs. (A19) and (A20),

$$\sum_l p_l (|c_{001}^{(l)}|^2 + |c_{110}^{(l)}|^2) (1 + \cos(\theta_l + \phi_l)) \leq 4\epsilon. \quad (\text{A21})$$

We now need the following lemma, which is similar to Lemma 7.

Lemma 8. Suppose the ideal expectations are satisfied to within error ϵ . Then $\|A_1 B_2 |\psi\rangle + B_1 A_2 |\psi\rangle\| \leq 2\sqrt{2\epsilon}$.

Proof.

$$\begin{aligned} & \|A_1 B_2 |\psi\rangle + B_1 A_2 |\psi\rangle\| \leq \|(A_1 B_2 - A_1 B_1 A_3) |\psi\rangle\| \\ & \quad + \|(A_1 B_1 A_3 + B_1 A_2) |\psi\rangle\| \leq 2\sqrt{2\epsilon}, \end{aligned}$$

where the last inequality follows from Eqs. (A11) and (A12). ■

From the result of the lemma, we obtain

$$\begin{aligned} & \sum_l p_l (|c_{001}^{(l)}|^2 + |c_{110}^{(l)}|^2) |e^{i\theta_l} + e^{i\phi_l}|^2 \\ & \quad + (|c_{011}^{(l)}|^2 + |c_{100}^{(l)}|^2) |e^{i\theta_l} - e^{-i\phi_l}|^2 \\ & \quad + \sum_l p_l (|c_{000}^{(l)}|^2 + |c_{111}^{(l)}|^2) |e^{-i\theta_l} + e^{-i\phi_l}|^2 \\ & \quad + (|c_{010}^{(l)}|^2 + |c_{101}^{(l)}|^2) |e^{-i\theta_l} - e^{i\phi_l}|^2 \leq 8\epsilon, \end{aligned}$$

and therefore,

$$\sum_l p_l (|c_{001}^{(l)}|^2 + |c_{110}^{(l)}|^2) |e^{i\theta_l} + e^{i\phi_l}|^2 \leq 8\epsilon,$$

or

$$\sum_l p_l (|c_{001}^{(l)}|^2 + |c_{110}^{(l)}|^2) (1 + \cos(\theta_l - \phi_l)) \leq 4\epsilon. \quad (\text{A22})$$

Adding Eqs. (A21) and (A22),

$$\begin{aligned} & \frac{8}{2}\epsilon \geq \sum_l p_l (|c_{001}^{(l)}|^2 + |c_{110}^{(l)}|^2) (1 + \cos \theta_l \cos \phi_l) \\ & \geq \sum_l p_l (|c_{001}^{(l)}|^2 + |c_{110}^{(l)}|^2), \quad (\text{A23}) \end{aligned}$$

where in the last inequality we used $\theta_l, \phi_l \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, and so $\cos \theta_l \geq 0$ and $\cos \phi_l \geq 0$. Similarly, from Eqs. (A13) and (A14), we have found the following bounds on $\sum_l p_l (|c_{010}^{(l)}|^2 + |c_{101}^{(l)}|^2)$ and $\sum_l p_l (|c_{011}^{(l)}|^2 + |c_{100}^{(l)}|^2)$:

$$\frac{8}{2}\epsilon \geq \sum_l p_l (|c_{010}^{(l)}|^2 + |c_{101}^{(l)}|^2), \quad (\text{A24})$$

$$\frac{8}{2}\epsilon \geq \sum_l p_l (|c_{011}^{(l)}|^2 + |c_{100}^{(l)}|^2), \quad (\text{A25})$$

respectively. Summing Eqs. (A23)–(A25), we obtain

$$\sum_l p_l \sum_{abc \neq 000, 111} |c_{abc}^{(l)}|^2 \leq \frac{24}{2}\epsilon. \quad (\text{A26})$$

Substituting Eqs. (A26) and (A16) in Eq. (A10), we obtain the state fidelity as

$$\begin{aligned} & F(|\hat{\psi}\rangle, |\psi\rangle) \geq \left(1 - \frac{25}{2}\epsilon\right)^2 \\ & \geq 1 - 25\epsilon. \quad (\text{A27}) \end{aligned}$$

Next we bound the fidelity of the operators. From Eq. (A8) and the definition of the ideal operators (up to a unitary freedom), it follows that for all i , $\text{tr}(\hat{A}_i A_i) = 8$ which implies that

$F(\hat{A}_i, A_i) = 1$. From Eq. (A8), it also follows that

$$F(\hat{B}_1, B_1) = \sum_l p_l \cos \theta_l. \quad (\text{A28})$$

Let us now obtain a lower bound on $\sum_l p_l \cos \theta_l$. Using both the result of Lemma 7 and Eq. (A8), we obtain

$$\begin{aligned} 4\epsilon &\geq \frac{1}{8} \|\{A_1, B_1\}|\psi\rangle\|^2 \\ &= \sum_l p_l \sin^2 \theta_l. \end{aligned} \quad (\text{A29})$$

Using $\cos^2 \theta_l + \sin^2 \theta_l = 1$ and $\sum_l p_l = 1$, we can write $\sum_l p_l \sin^2 \theta_l$ as

$$\begin{aligned} \sum_l p_l \sin^2 \theta_l &= 1 - \sum_l p_l \cos^2 \theta_l \\ &\geq 1 - \sum_l p_l \cos \theta_l, \end{aligned} \quad (\text{A30})$$

where the inequality follows from $\theta_l \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ and therefore $\cos \theta_l \geq 0$. From the above two equations, it follows that

$$1 - \sum_l p_l \cos \theta_l \leq 4\epsilon. \quad (\text{A31})$$

Using the above equation in Eq. (A28), we obtain

$$F(\hat{B}_1, B_1) \geq 1 - 4\epsilon.$$

This ends the proof of Theorem 3.

Theorem 3 can be straightforwardly extended to any n as follows. Here the state fidelity is defined as earlier and the operator fidelity is defined with the different normalization factor as $F(\hat{X}_i, X_i) := (1/\dim(\hat{V}_n))\text{Tr}(\hat{X}_i X_i)$, where $\dim(\hat{V}_n)$ is the dimension of the invariant subspace.

Theorem 4. If a quantum state $|\psi\rangle$ and a set of measurements A_i, B_j with $i, j = \{1, 2, \dots, n\}$ in a Hilbert space \mathcal{H}_n satisfy the ideal expectations corresponding to the maximal quantum violation of inequality (57) to within error ϵ , then there exists a projection $P: \mathcal{H}_n \rightarrow \hat{V}_n$, where $\dim(\hat{V}_n) = 2^n$, a state $|\hat{\psi}\rangle \in \hat{V}_n$, and \hat{A}_i, \hat{B}_j which are Hermitian involutions acting on \hat{V}_n for all i and j such that

$$\begin{aligned} \langle \hat{\psi} | \hat{A}_1 \hat{B}_2 \hat{B}_3 \hat{B}_4 \cdots \hat{B}_n | \hat{\psi} \rangle &= 1, \\ \langle \hat{\psi} | \hat{B}_1 \hat{A}_2 \hat{B}_3 \hat{B}_4 \cdots \hat{B}_n | \hat{\psi} \rangle &= 1, \\ &\vdots \\ \langle \hat{\psi} | \hat{B}_1 \hat{B}_2 \hat{B}_3 \hat{B}_4 \cdots \hat{A}_n | \hat{\psi} \rangle &= 1, \end{aligned}$$

and there also exists a unitary U acting on \hat{V} such that

$$\begin{aligned} F(U|\hat{\psi}\rangle, |\psi\rangle) &\geq 1 - \epsilon_0, \\ F(U\hat{A}_i U^\dagger, A_i) &\geq 1 - \epsilon_1 \quad \forall i, \\ F(U\hat{B}_i U^\dagger, B_i) &\geq 1 - \epsilon_2 \quad \forall i, \end{aligned}$$

where $\epsilon_0 = [8(2^{n-1} - 1) + 1]\epsilon$, $\epsilon_1 = 0$, and $\epsilon_2 = 2^{5-n}\epsilon$.

Proof. The bounds of this theorem are obtained using the similar steps used in the proof of Theorem 3. With respect to the Jordan decomposition,

$$\mathcal{H}_n = \bigoplus_l \mathcal{H}_l, \quad (\text{A32})$$

where each \mathcal{H}_l has dimension at most 2^n and is invariant under the action of A_i and B_j . As before, the state $|\psi\rangle$ can be decomposed as

$$|\psi\rangle = \sum_l \sqrt{p_l} |\psi_l\rangle, \quad (\text{A33})$$

where $|\psi_l\rangle \in \mathcal{H}_l$ and $\sum_l p_l = 1$. With respect to the computational basis $\{|n_1 n_2 \cdots n_n\rangle_l : n_i \in \{0, 1\}\}$, we express each $|\psi_l\rangle$ as

$$|\psi_l\rangle = \sum_{n_i \in \{0,1\}} c_{n_1 n_2 \cdots n_n}^{(l)} |n_1 n_2 \cdots n_n\rangle_l,$$

where $\sum_{n_1 n_2 \cdots n_n} |c_{n_1 n_2 \cdots n_n}^{(l)}|^2 = 1$.

We define the subspace $\hat{V}_n \subseteq \mathcal{H}_n$ as the linear span of $\{|\tilde{n}_1 \tilde{n}_2 \cdots \tilde{n}_n\rangle := \sum_l \sqrt{p_l} |n_1 n_2 \cdots n_n\rangle_l\}$. We define the ideal state in this subspace as

$$|\hat{\psi}\rangle := \frac{1}{\sqrt{2}} (|\tilde{0}_1 \tilde{0}_2 \cdots \tilde{0}_n\rangle - |\tilde{1}_1 \tilde{1}_2 \cdots \tilde{1}_n\rangle), \quad (\text{A34})$$

which can be reexpressed as

$$|\hat{\psi}\rangle = \sum_l \sqrt{p_l} |\hat{\psi}_l\rangle, \quad (\text{A35})$$

where

$$|\hat{\psi}_l\rangle := \frac{1}{\sqrt{2}} (|0_1 0_2 \cdots 0_n\rangle_l - |1_1 1_2 \cdots 1_n\rangle_l). \quad (\text{A36})$$

Note that for the ideal observables defined as

$$\begin{aligned} \hat{A}_i &:= \bigoplus_l \left(\bigotimes_{i=1}^{k-1} \mathbb{1}_l \otimes \hat{A}_i^l \otimes \bigotimes_{i=k+1}^n \mathbb{1}_l \right), \\ \hat{B}_j &:= \bigoplus_l \left(\bigotimes_{i=1}^{k-1} \mathbb{1}_l \otimes \hat{B}_j^l \otimes \bigotimes_{i=k+1}^n \mathbb{1}_l \right), \end{aligned}$$

where

$$\hat{A}_{ii} = X_i, \quad \hat{B}_{ji} = Y_j,$$

with $i, j = 1, 2, 3$, and, for $i, j = 4, 5, \dots, n$,

$$\hat{A}_{ii} = -Y_i, \quad \hat{B}_{ji} = X_j,$$

the ideal state defined in Eq. (A34) violates the noncontextuality inequality (20) maximally.

From Appendix B, it follows that the nonideal observables can be written as

$$\begin{aligned} A_i &= \bigoplus_l \left(\bigotimes_{i=1}^{k-1} \mathbb{1}_l \otimes A_i^l \otimes \bigotimes_{i=k+1}^n \mathbb{1}_l \right), \\ B_j &= \bigoplus_l \left(\bigotimes_{j=1}^{k-1} \mathbb{1}_l \otimes B_j^l \otimes \bigotimes_{j=k+1}^n \mathbb{1}_l \right), \end{aligned}$$

for all $i, j = 1, 2, \dots, n$. We choose a unitary such that the operators A_i and B_j acting on \mathcal{H}_l can be written as follows:

$$A_i = X_j, \quad B_{ji} = \cos \theta_{ji} Y_j + \sin \theta_{ji} X_j, \quad i, j = 1, 2, 3, \quad (\text{A37})$$

$$B_{ii} = X_k, \quad A_{ji} = \cos \theta_{ji} Y_k + \sin \theta_{ji} X_k, \quad i, j = 4, 5, \dots, n, \quad (\text{A38})$$

with $\theta_{ji} \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ for all j and k .

Using the similar steps used to obtain Eq. (A10), we have

$$\begin{aligned} \langle \hat{\psi} | \psi \rangle &\geq 1 - \sum_l p_l \sum_{n_1 n_2 \dots n_n \neq 0, 0_2 \dots 0_n, 1_1 1_2 \dots 1_n} |c_{n_1 n_2 \dots n_n}^{(l)}|^2 \\ &\quad - \frac{1}{2} \sum_l p_l |c_{0_1 0_2 \dots 0_n}^{(l)} + c_{1_1 1_2 \dots 1_n}^{(l)}|^2. \end{aligned} \quad (\text{A39})$$

Similarly to the case of $n = 3$, a bound on the right-hand side of the above equation can be obtained as follows. The term $\frac{1}{2} \sum_l p_l |c_{0_1 0_2 \dots 0_n}^{(l)} + c_{1_1 1_2 \dots 1_n}^{(l)}|^2$ in Eq. (A39) can be bounded using the inequality given by

$$\|A_1 |\psi\rangle + A_2 A_3 B_4 \dots B_n |\psi\rangle\| \leq \sqrt{2\epsilon}. \quad (\text{A40})$$

From this equation, we obtain

$$\begin{aligned} \sum_l p_l (|c_{0_1 0_2 0_3 \dots 0_n}^{(l)} + c_{1_1 1_2 1_3 \dots 1_n}^{(l)}|^2 \\ + \dots + |c_{0_1 1_2 1_3 \dots 1_n}^{(l)} + c_{1_1 0_2 0_3 \dots 0_n}^{(l)}|^2) \leq \epsilon, \end{aligned} \quad (\text{A41})$$

from which it follows that

$$\sum_l p_l |c_{0_1 0_2 \dots 0_n}^{(l)} + c_{1_1 1_2 \dots 1_n}^{(l)}|^2 \leq \epsilon. \quad (\text{A42})$$

Next, the second term in Eq. (A39) can be bounded using the other inequalities such as

$$\|B_2 |\psi\rangle - B_1 A_3 B_4 \dots B_n |\psi\rangle\| \leq \sqrt{2\epsilon}, \quad (\text{A43})$$

from which we obtain

$$\begin{aligned} \sum_l p_l \left(\sum_{n_4, \dots, n_n} |e^{-i\theta_{2l}} c_{000n_4 \dots n_n}^{(l)} - e^{i\theta_{1l}} c_{111\bar{n}_4 \dots \bar{n}_n}^{(l)}|^2 \right. \\ + \sum_{n_4, \dots, n_n} |e^{i\theta_{2l}} c_{010n_4 \dots n_n}^{(l)} + e^{i\theta_{1l}} c_{101\bar{n}_4 \dots \bar{n}_n}^{(l)}|^2 \\ + \sum_{n_4, \dots, n_n} |e^{-i\theta_{2l}} c_{001n_4 \dots n_n}^{(l)} - e^{i\theta_{1l}} c_{110\bar{n}_4 \dots \bar{n}_n}^{(l)}|^2 \\ \left. + \sum_{n_4, \dots, n_n} |e^{i\theta_{2l}} c_{011n_4 \dots n_n}^{(l)} + e^{i\theta_{1l}} c_{100\bar{n}_4 \dots \bar{n}_n}^{(l)}|^2 \right) \leq \epsilon, \end{aligned}$$

where \bar{n}_i , with $i = 4, 5, \dots, n$, denotes $n_i \oplus 1$. From the above equation, using the steps similar to the ones used to obtain the bound given by Eq. (A23), we obtain a bound on $\sum_l p_l (|c_{0010 \dots 0}^{(l)}|^2 + |c_{1101 \dots 1}^{(l)}|^2)$ as follows:

$$\sum_l p_l (|c_{0010 \dots 0}^{(l)}|^2 + |c_{1101 \dots 1}^{(l)}|^2) \leq \frac{8}{2}\epsilon. \quad (\text{A44})$$

The sum $\sum_{n_1 n_2 \dots n_n \neq 0_0 \dots 0, 1_1 \dots 1} \sum_l p_l |c_{n_1 n_2 \dots n_n}^{(l)}|^2$ can be spilt into the sum of $(2^{n-1} - 1)$ terms which are a sum of the modulus of two coefficients $c_{n_1 n_2 \dots n_n}^{(l)}$ as in the left-hand side of Eq. (A44). These $(2^{n-1} - 1)$ terms have the same bound as given in Eq. (A44). Therefore, we obtain

$$\sum_l p_l \sum_{n_1 n_2 \dots n_n \neq 0_0 \dots 0, 1_1 \dots 1} |c_{n_1 n_2 \dots n_n}^{(l)}|^2 \leq \frac{8(2^{n-1} - 1)}{2}\epsilon. \quad (\text{A45})$$

Using Eqs. (A42) and (A45) in Eq. (A39), we obtain the bound on the fidelity as given in Theorem 4.

Next, we bound the fidelity of the operators. As in the case of $n = 3$, we also have $\|\{A_1, B_1\}|\psi\rangle\| \leq 4\sqrt{2\epsilon}$ which implies that

$$\begin{aligned} 2^{5-n}\epsilon &\geq \frac{1}{2^n} \|\{A_1, B_1\}|\psi\rangle\|^2 \\ &\geq 1 - \sum_l p_l \cos \theta_l, \end{aligned} \quad (\text{A46})$$

leading to the following bound on the fidelity between \hat{B}_1 and B_1 :

$$F(\hat{B}_1, B_1) \geq 1 - 2^{5-n}\epsilon,$$

employing the similar steps as in the case of $n = 3$. This ends the proof of Theorem 4. \blacksquare

APPENDIX B: JORDAN'S LEMMA

In this section we prove a corollary to Jordan's lemma which is a direct generalization of Corollary 7.1 proven in Ref. [32]. For completeness we also state Jordan's lemma (see, e.g., Ref. [32] for a proof).

Lemma 9 (Jordan's lemma). Let A and B be a pair of Hermitian operators acting on a Hilbert space \mathcal{H} such that $A^2 = B^2 = \mathbb{1}$. Then, \mathcal{H} decomposes as a direct sum $\mathcal{H} = \bigoplus_l \mathcal{H}_l$, with $\dim \mathcal{H}_l \in \{1, 2\}$, and A and B act invariantly on each \mathcal{H}_l .

In this way, since the set of eigenvectors of AB span \mathcal{H} , we can decompose the Hilbert space $\mathcal{H} = \bigoplus_l \mathcal{H}_l$ where the dimension of such \mathcal{H}_l is at most 2.

Corollary 1. Let A_i and B_j with $i = 1, 2, 3$ be Hermitian operators acting on a Hilbert space \mathcal{H} that square to identity and satisfy the following commutation relations:

$$[A_i, A_j] = [A_i, B_j] = 0 \quad (i \neq j). \quad (\text{B1})$$

Then, \mathcal{H} can be decomposed as

$$\mathcal{H} = \bigoplus_l (\mathcal{H}_l^1 \otimes \mathcal{H}_l^2 \otimes \mathcal{H}_l^3), \quad (\text{B2})$$

where each local Hilbert space \mathcal{H}_l^i is of dimension at most two. Moreover, $A_1 = \bigoplus_l (A_{1l} \otimes \mathbb{1}_l \otimes \mathbb{1}_l)$, $B_1 = \bigoplus_l (B_{1l} \otimes \mathbb{1}_l \otimes \mathbb{1}_l)$, $A_2 = \bigoplus_l (\mathbb{1}_l \otimes A_{2l} \otimes \mathbb{1}_l)$, $B_2 = \bigoplus_l (\mathbb{1}_l \otimes B_{2l} \otimes \mathbb{1}_l)$, $A_3 = \bigoplus_l (\mathbb{1}_l \otimes \mathbb{1}_l \otimes A_{3l})$, and $B_3 = \bigoplus_l (\mathbb{1}_l \otimes \mathbb{1}_l \otimes B_{3l})$.

Proof. This proof is a direct generalization of that of Corollary 7.1 proven in Ref. [32].

First, let us notice that Eq. (B1) implies that $[A_i B_i, A_j B_j] = 0$ for any $i, j = 1, 2, 3$, which means that all three Hermitian operators $A_i B_i$ can be jointly diagonalized.

Let then $|\alpha, \beta, \gamma\rangle$ be an eigenvector of these operators such that $A_1 B_1 |\alpha, \beta, \gamma\rangle = \alpha |\alpha, \beta, \gamma\rangle$ and $A_2 B_2 |\alpha, \beta, \gamma\rangle = \beta |\alpha, \beta, \gamma\rangle$ and $A_3 B_3 |\alpha, \beta, \gamma\rangle = \gamma |\alpha, \beta, \gamma\rangle$. Define the following vectors: $|\bar{\alpha}, \beta, \gamma\rangle = A_1 |\alpha, \beta, \gamma\rangle$, $|\alpha, \bar{\beta}, \gamma\rangle = A_2 |\alpha, \beta, \gamma\rangle$, $|\alpha, \beta, \bar{\gamma}\rangle = A_3 |\alpha, \beta, \gamma\rangle$, $|\bar{\alpha}, \bar{\beta}, \gamma\rangle = A_1 A_2 |\alpha, \beta, \gamma\rangle$, $|\bar{\alpha}, \beta, \bar{\gamma}\rangle = A_1 A_3 |\alpha, \beta, \gamma\rangle$, $|\alpha, \bar{\beta}, \bar{\gamma}\rangle = A_2 A_3 |\alpha, \beta, \gamma\rangle$, and $|\bar{\alpha}, \bar{\beta}, \bar{\gamma}\rangle = A_1 A_2 A_3 |\alpha, \beta, \gamma\rangle$. Then, the subspace

$$\begin{aligned} \text{span}\{|\alpha, \beta, \gamma\rangle, |\bar{\alpha}, \beta, \gamma\rangle, |\alpha, \bar{\beta}, \gamma\rangle, |\alpha, \beta, \bar{\gamma}\rangle, \\ |\bar{\alpha}, \bar{\beta}, \gamma\rangle, |\bar{\alpha}, \beta, \bar{\gamma}\rangle, |\alpha, \bar{\beta}, \bar{\gamma}\rangle, |\bar{\alpha}, \bar{\beta}, \bar{\gamma}\rangle\} \end{aligned} \quad (\text{B3})$$

is isomorphic to $\text{span}\{|\alpha\rangle, |\bar{\alpha}\rangle\} \otimes \text{span}\{|\beta\rangle, |\bar{\beta}\rangle\} \otimes \text{span}\{|\gamma\rangle, |\bar{\gamma}\rangle\}$. It follows from Lemma 9 that both A_1 and B_1 , both A_2 and B_2 , as well as both A_3 and B_3 act invariantly on the first, second, and third tensor factors, and trivially on the others, respectively. ■

The above corollary can be trivially generalized to any $n \geq 3$: let A_i and B_j ($i, j = 1, \dots, n$) be Hermitian operators acting on \mathcal{H}_n that square to the identity and satisfy

$$[A_i, A_j] = [B_i, B_j] = 0 \quad (i \neq j). \quad (\text{B4})$$

Then, \mathcal{H}_n decomposes as $\mathcal{H}_n = \bigoplus_l (\mathcal{H}_l^1 \otimes \mathcal{H}_l^2 \otimes \dots \otimes \mathcal{H}_l^n)$, with $\dim \mathcal{H}_l^i \leq 2$, and

$$A_j = \bigoplus_l \left(\bigotimes_{i=1}^{j-1} \mathbb{1}_l \otimes A_j^l \otimes \bigotimes_{i=j+1}^n \mathbb{1}_l \right) \quad (\text{B5})$$

and

$$B_j = \bigoplus_l \left(\bigotimes_{i=1}^{j-1} \mathbb{1}_l \otimes B_j^l \otimes \bigotimes_{i=j+1}^n \mathbb{1}_l \right). \quad (\text{B6})$$

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