





Certification of two-qubit quantum systems with temporal inequality

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Self-testing of quantum devices based on observed measurement statistics is a method to certify quantum systems using minimal resources. In Irfan *et al.* [A. A. M. Irfan, K. Mayer, G. Ortiz, and E. Knill, *Phys. Rev. A* **101**, 032106 (2020)] a scheme based on observing measurement statistics that demonstrate Kochen-Specker contextuality has been shown to certify two-qubit entangled states and measurements without the requirement of spatial separation between the subsystems. However, this scheme assumes a set of compatibility conditions on the measurements which are crucial to demonstrating Kochen-Specker contextuality. In this paper, we propose a self-testing protocol to certify the above two-qubit states and measurements without the assumption of the compatibility conditions, and at the same time without requiring the spatial separation between the subsystems. Our protocol is based on the observation of sequential correlations leading to the maximal violation of a temporal inequality derived from noncontextuality inequality. Moreover, our protocol is robust to small experimental errors or noise.

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I. INTRODUCTION

Realizing fault-tolerant quantum computation plays a key role in achieving quantum technologies. A fault-tolerant quantum computer may be achieved by making use of topological qubits in which qubits are encoded as the subspace of a high-dimensional space of a suitable physical system such as Majorana fermions [1,2]. The circuit model of quantum computing can be replaced by Pauli-based computing which makes use of only a minimal number of Pauli measurements [3]. Such Pauli-based computing can be realized by topological qubits [4].

Before performing any quantum information processing task, it is important to certify how close are the relevant quantum devices to the ideal ones. There are the certification methods such as tomography [5–7] and self-testing [8] that have been explored to certify the relevant quantum devices. While certifying quantum devices, it is desirable to use methods that make use of a limited number of resources and minimize the assumptions on the quantum devices. Certification schemes based on tomography can become resource consuming depending on the quantum system to be certified and they require that certain assumptions such as the Hilbert-space dimension of the quantum system have to be trusted. On the other hand, self-testing of quantum devices aims to provide certification using a minimal number of resources and a minimal number of assumptions. Self-testing was originally introduced as a device-independent certification of quantum state and measurements for quantum cryptographic applications [9]. Device-independent certification schemes are based on the observation of nonclassical correlations that imply Bell nonlocality [10,11]. These schemes do not depend on the detailed characterization of the quantum devices; importantly, they do not assume the Hilbert-space dimension of the quantum systems to be certified.

Self-testing based on Bell nonlocality has a restriction that it can be used to certify composite quantum systems that have entanglement and admit spatial separation between the subsystems and local measurements on subsystems. Recently, self-testing based on observation of Kochen-Specker contextuality [12] has been explored to certify quantum systems which do not have entanglement or do admit a spatial separation between the subsystems [13–16]. Such a certification method is relevant in the context of certification quantum devices for quantum computation purposes as computation typically happens in a local fashion. Note, however, that contextuality-based certification methods require the measurements to obey certain compatibility relations in order to observe the nonclassical correlations, whereas it is in general difficult to assess whether such relations are satisfied in an experiment.

Sequential correlation inequalities, on the other hand, such as the Leggett-Garg inequality [17] or temporal inequality [18] can be used to demonstrate nonclassicality based on quantum measurements on single quantum systems without the need of assuming that the measurements are jointly measurable. Motivated by this, such inequalities have also been explored to certify quantum measurements on single quantum systems without the requirement of any compatibility conditions on the quantum measurements [19–22]. However, these certification schemes also make a few minimal assumptions; for instance, in Refs. [19–21] it is assumed that (a) the preparation device always prepares a maximally mixed state and (b) measurements do not have any memory and they return only the postmeasurement state, while in Ref. [22] one can certify only the temporal correlation matrix. Moreover, one can lift the assumption of producing maximally mixed states by the measurement device with (a) ensuring that the input state to the device is always a full rank state and (b) sequential

action of the same measurement will output a certain outcome always [23].

In Ref. [15], a certification scheme has been proposed to certify quantum measurements of a fermionic system for topological quantum computing. These quantum measurements are a subset of two-qubit Pauli measurements that demonstrate Kochen-Specker contextuality. As this scheme is based on observed statistics that imply Kochen-Specker contextuality, it assumes certain compatibility conditions on the quantum measurements. In this paper, we propose a certification scheme based on a temporal inequality to certify the same subset of two-qubit Pauli measurements along with the same quantum state. Our scheme may be applied to certify those two-qubit quantum states and measurements for topological quantum computing without assuming the compatibility relations to hold, unlike the approach of Ref. [15]. However, we assume that the measurements are projective. In this respect, we would like to mention that the previous approaches such as the one in Ref. [21] also make this assumption. In fact, in that work it is assumed that the measurement device produces always a maximally mixed state as well as that the same measurement applied many times in a sequence yields the same outcome. As proven in Ref. [21] (see Appendix there), these assumptions imply that the involved measurements are projective. Yet, in our paper we do not assume the input state to be maximally mixed. Let us finally mention that we also show our self-testing scheme to be robust to small experimental errors or noise.

Before we discuss our methodology and main results, we provide some background information necessary for further considerations.

A. Sequential correlations

We consider a sequential measurements scenario to observe a violation of a temporal inequality. The scenario consists of a preparation device that prepares a single quantum system in an unknown quantum state ρ and a sequence of two and three black-box operations. These operations are dichotomic measurements denoted by A_i , with $i = 1, \dots, 6$. The outcomes of these measurements are denoted by a_i which can take the values ± 1 . We then assume that these measurements are projective, and so A_i are the standard quantum observables such that $A_i^2 = \mathbb{1}$. Notice here that, while we do not restrict the dimension of the underlying Hilbert space, we cannot, however, exploit here the Naimark dilation argument that allows one to represent generalized measurements in terms of projective ones acting on a higher-dimensional Hilbert space. This is because we do not impose any commutation relations for the measurements.

In our sequential scenario, we finally need to assume that the measurements A_i are nondemolishing, i.e., they do not destroy the physical system, and also that each black box has no memory and returns the actual postmeasurement state.

In an experiment that realizes this scenario, the joint probabilities corresponding to the sequences of two measurements and three measurements can be observed. For instance, the joint probabilities of measuring $\{A_1, A_4\}$ in the temporal order $A_1 \rightarrow A_4$ and $\{A_1, A_2, A_3\}$ in the temporal order $A_1 \rightarrow A_2 \rightarrow A_3$ are given by $P(a_1, a_4|A_1, A_4)$ and $P(a_1, a_2, a_3|A_1, A_2, A_3)$,

respectively. In terms of these joint probabilities, the second- and third-order sequential correlations denoted by $\langle A_1 A_4 \rangle_\pi$ and $\langle A_1 A_2 A_3 \rangle_\pi$ are defined as

$$\langle A_1 A_4 \rangle_\pi = \sum_{a_1, a_4} a_1 a_4 P(a_1, a_4|A_1, A_4),$$

$$\langle A_1 A_2 A_3 \rangle_\pi = \sum_{a_1, a_2, a_3} a_1 a_2 a_3 P(a_1, a_2, a_3|A_1, A_2, A_3),$$

respectively.

Quantum-mechanical versions of the sequential correlations, such as $\langle A_1 A_4 \rangle_\pi$ and $\langle A_1 A_2 A_3 \rangle_\pi$, can then be written as

$$\langle A_1 A_4 \rangle_\pi = \frac{1}{2} \text{tr}(\rho \{A_1, A_4\}), \quad (1)$$

$$\langle A_1 A_2 A_3 \rangle_\pi = \frac{1}{4} \text{tr}(\rho \{A_1, \{A_2, A_3\}\}), \quad (2)$$

respectively, where $\rho = |\psi\rangle\langle\psi|$ (see the Appendix in Ref. [24] for the derivation of such formulas) and $\{A, B\} = AB + BA$ is the standard anticommutator. The other sequential correlations can also be similarly expressed in terms of the anticommutator.

B. Noncontextuality inequality

Using these sequential correlations one can demonstrate both contextual and temporal correlations. We will now first describe how to demonstrate contextual correlation here. Suppose the sets of measurements $\{A_1, A_4\}$, $\{A_2, A_5\}$, $\{A_3, A_6\}$, $\{A_1, A_2, A_3\}$, and $\{A_4, A_5, A_6\}$ that are measured sequentially are treated as contexts, i.e., the measurements in these sets commute with each other:

$$\begin{aligned} [A_1, A_4] &= [A_2, A_5] = [A_3, A_6] = [A_1, A_2] = [A_1, A_3] \\ &= [A_2, A_3] = [A_4, A_5] = [A_4, A_6] = [A_5, A_6] = 0, \end{aligned} \quad (3)$$

where $[A, B] = AB - BA$. Then, the quantum-mechanical versions of the sequential correlations simplify as $\langle A_1 A_4 \rangle_\pi = \langle A_1 A_4 \rangle$ and $\langle A_1 A_2 A_3 \rangle_\pi = \langle A_1 A_2 A_3 \rangle$, such that these sets of measurements can be used to demonstrate Kochen-Specker contextuality. For instance, the sequential measurements of these contexts with the two-qubit observables

$$\begin{aligned} A_1 &= X \otimes \mathbb{1}, & A_4 &= \mathbb{1} \otimes X, \\ A_2 &= \mathbb{1} \otimes Z, & A_5 &= Z \otimes \mathbb{1}, \\ A_3 &= X \otimes Z, & A_6 &= Z \otimes X \end{aligned} \quad (4)$$

on the two-qubit maximally entangled state,

$$|\phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}, \quad (5)$$

imply Kochen-Specker contextuality through a logical contradiction by providing noncontextual value assignments to each observable in the context. The above contexts form a subset of the contexts pertaining to the famous Peres-Mermin square demonstrating Kochen-Specker contextuality for any two-qubit state [25,26]. Moreover, one can consider a non-contextuality inequality as used in Ref. [27] in terms of the expectation values corresponding to joint measurements of the observables in the above contexts as follows:

$$\begin{aligned} \mathcal{I}_{NC} &= \langle A_1 A_2 A_3 \rangle + \langle A_4 A_5 A_6 \rangle \\ &+ \langle A_1 A_4 \rangle + \langle A_2 A_5 \rangle - \langle A_3 A_6 \rangle \leq \eta_C, \end{aligned} \quad (6)$$

where $\eta_C = 3$ is the classical bound of the inequality. The quantum bound $\eta_Q = 5$ of the above inequality can be obtained from the state given by Eq. (5) for the measurements given by Eq. (4). In Ref. [15], the measurement statistics pertaining to the maximal violation of the inequality (6) have been shown to provide robust certification of two-qubit Pauli measurements in a setup such as Majorana fermions.

Now, the stage is set to discuss our setup and main results regarding certification of the two-qubit state and measurements using a temporal inequality. In the next section (Sec. II), we discuss the procedure to obtain the temporal inequality from the noncontextuality inequality considered earlier within the sequential correlations scenario. We also discuss how such inequality can be used to certify the two-qubit systems with permissible small experimental errors and noises. We conclude in Sec. III.

II. ROBUST CERTIFICATION OF THE TWO-QUBIT SYSTEMS USING TEMPORAL INEQUALITY

A. Temporal inequality

Our goal is to propose a temporal extension of the inequality (6) to certify the two-qubit maximally entangled state (5) and measurements (4) without assuming the compatibility relations (3). To this aim, we consider the following temporal inequality:

$$\begin{aligned} \mathcal{I}_T := & \frac{1}{2}(\langle A_1 A_2 A_3 \rangle_\pi + \langle A_2 A_1 A_3 \rangle_\pi + \langle A_4 A_5 A_6 \rangle_\pi \\ & + \langle A_5 A_4 A_6 \rangle_\pi) + \langle A_1 A_4 \rangle_\pi + \langle A_2 A_5 \rangle_\pi - \langle A_3 A_6 \rangle_\pi \leq \eta_C, \end{aligned} \quad (7)$$

where no compatibility relations for the measurements are assumed. It has been argued in Ref. [18] that the existence of a single joint probability distribution for all the outcomes of the measurements is the common underpinning assumption for the Bell-type, Kochen-Specker noncontextuality, and temporal inequalities. Therefore, in order to derive the maximal classical value of the inequality η_C one optimizes the expression \mathcal{I}_T over all deterministic strategies in which all measurements have definite values independently of the measurement sequence. In other words, all expectation values in \mathcal{I}_T split into products of expectation values of individual observables, and each such expectation value takes the values ± 1 . Hence, for the inequality (7) we have

$$\begin{aligned} \eta_C = & \max_{a_i \in \{\pm 1\}} \left[\frac{1}{2}(a_1 a_2 a_3 + a_2 a_1 a_3 + a_4 a_5 a_6 + a_5 a_4 a_6) \right. \\ & \left. + a_1 a_4 + a_2 a_5 - a_3 a_6 \right], \\ = & \max_{a_i \in \{\pm 1\}} [a_1 a_2 a_3 + a_4 a_5 a_6 + a_1 a_4 + a_2 a_5 - a_3 a_6] \end{aligned}$$

which gives $\eta_C = 3$.

Then, in order to determine the maximal quantum value η_Q of \mathcal{I}_T let us observe that it directly follows from the definitions (1) that the sequential expectation values are bounded as

$$-1 \leq \langle A_i A_j \rangle_\pi \leq 1, \quad -1 \leq \langle A_i A_j A_k \rangle_\pi \leq 1$$

for any i, j , and k . As a consequence $\eta_Q = 5$. What is more, this value is achieved by the same quantum state and measurements that lead to the maximal quantum violation of the noncontextuality inequality (6). In the next section, we

demonstrate that the quantum bound of the inequality (7) can be used to certify this quantum realization without the assumption of the compatibility relations as used in the case of the inequality (6).

B. Robust self-testing of two-qubit systems

Consider an experimental situation that realizes the sequential scenario, in which we assume that both the state and measurements and their compatibility relations are unknown. Together, we consider a reference experiment with a known pure state $|\hat{\psi}\rangle \in \mathbb{C}^d$ for $d = 4$ and known observables \hat{A}_i acting on \mathbb{C}^4 that obey the compatibility relations given by Eq. (3). We assume that our reference experiment leads to the maximal violation of the temporal inequality given by Eq. (7). With these two experiments at hand, for our purpose, we adopt the definition of self-testing used in Ref. [15] (see also Ref. [20]) as given below.

Definition 1. Given that the state $|\psi\rangle \in \mathcal{H}$ and a set of measurements A_i with $i \in [1, 6]$ maximally violate the given temporal inequality (7), then the self-testing of the state $|\hat{\psi}\rangle \in \mathbb{C}^4$ and the set of observables \hat{A}_i acting on \mathbb{C}^4 is defined by the existence of a projection $P : \mathcal{H} \rightarrow \mathbb{C}^4$ and a unitary U acting on \mathbb{C}^4 such that

$$U^\dagger (P A_i P^\dagger) U = \hat{A}_i, \quad (8)$$

$$U(P|\psi\rangle) = |\hat{\psi}\rangle. \quad (9)$$

In other words, the above definition implies that based on the observed maximal violation of the inequality, one is able to identify a subspace $V = \mathbb{C}^4$ in \mathcal{H} on which all the observables act invariantly. Equivalently, A_i s 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 $U^\dagger \hat{A}_i U = \hat{A}_i$.

C. Symmetries of the inequality

Before we proceed with the self-testing proof, let us observe the following symmetries of the inequality (7):

$$(1) \quad A_1 \leftrightarrow A_2 \quad \text{and} \quad A_4 \leftrightarrow A_5, \quad (10)$$

$$(2) \quad A_1 \leftrightarrow A_3 \quad \text{and} \quad A_4 \leftrightarrow -A_6, \quad (11)$$

$$(3) \quad A_2 \leftrightarrow -A_3 \quad \text{and} \quad A_5 \leftrightarrow A_6, \quad (12)$$

$$(4) \quad A_1 \leftrightarrow A_4 \quad \text{and} \quad A_2 \leftrightarrow A_5 \quad \text{and} \quad A_3 \leftrightarrow A_6. \quad (13)$$

It can be checked that in any of these four cases, the inequality (7) remains invariant. In the following, we will employ these symmetries to prove our self-testing statement.

Now, assume that our first experiment achieves the quantum bound of the inequality (7). This directly implies that all except the last correlation functions of the inequality take value 1, whereas the last term equals -1 , which via the Cauchy-Schwartz inequality translate to the following equations:

$$A_1 A_2 A_3 |\psi\rangle = |\psi\rangle \quad \text{and permutations}, \quad (14)$$

$$A_4 A_5 A_6 |\psi\rangle = |\psi\rangle \quad \text{and permutations}, \quad (15)$$

$$A_1 A_4 |\psi\rangle = |\psi\rangle \quad \text{and permutations}, \quad (16)$$

$$A_2 A_5 |\psi\rangle = |\psi\rangle \quad \text{and permutations,} \quad (17)$$

$$A_3 A_6 |\psi\rangle = -|\psi\rangle \quad \text{and permutations,} \quad (18)$$

where *permutations* refers to the fact that the above relations also hold if we permute the observables. Using these identities, we now proceed to show the following anticommutation relations:

$$\begin{aligned} \{A_1, A_5\}|\psi\rangle &= \{A_1, A_6\}|\psi\rangle = \{A_2, A_4\}|\psi\rangle \\ &= \{A_2, A_6\}|\psi\rangle = \{A_3, A_4\}|\psi\rangle \\ &= \{A_3, A_5\}|\psi\rangle = 0. \end{aligned} \quad (19)$$

One directly deduces from the identities given by Eqs. (14)–(18) that

$$\begin{aligned} A_1 A_5 |\psi\rangle &= A_1 A_2 |\psi\rangle = A_3 |\psi\rangle = -A_6 |\psi\rangle \\ &= -A_5 A_4 |\psi\rangle = -A_5 A_1 |\psi\rangle, \end{aligned} \quad (20)$$

where in the first line we used $A_5 |\psi\rangle = A_2 |\psi\rangle$ from Eq. (17) and $A_1 A_2 |\psi\rangle = A_3 |\psi\rangle$ that stems from Eq. (14). On the other hand, in the second line, we used $A_3 |\psi\rangle = -A_6 |\psi\rangle$ from Eq. (18), $A_6 |\psi\rangle = A_5 A_4 |\psi\rangle$ from Eq. (15), and $A_4 |\psi\rangle = A_1 |\psi\rangle$ from Eq. (16).

In the following, we employ the symmetries in Eqs. (10)–(13) to obtain other similar relations. Employing the first, second, and third symmetries (10)–(12) of the inequality in the argument given by Eq. (20), we can get

$$A_2 A_4 |\psi\rangle = -A_4 A_2 |\psi\rangle, \quad (21)$$

$$A_3 A_5 |\psi\rangle = -A_5 A_3 |\psi\rangle, \quad (22)$$

$$A_1 A_6 |\psi\rangle = -A_6 A_1 |\psi\rangle, \quad (23)$$

respectively. Now, employing the second and first symmetries of the inequality in Eqs. (21) and (22), respectively, we get the remaining anticommutation relations:

$$A_2 A_6 |\psi\rangle = -A_6 A_2 |\psi\rangle, \quad (24)$$

$$A_3 A_4 |\psi\rangle = -A_4 A_3 |\psi\rangle. \quad (25)$$

Now, as in Ref. [15] we define the subspace

$$V := \text{span}\{|\psi\rangle, A_1 |\psi\rangle, A_5 |\psi\rangle, A_1 A_5 |\psi\rangle\}, \quad (26)$$

and prove the following fact for it.

Lemma 1. V is an invariant subspace under the action of all the observables A_i for $i \in [1, 6]$.

Proof. First, under the action of A_1 , V is trivially invariant. Next, using the fact that $A_5^2 = \mathbb{1}$ and $\{A_1, A_5\}|\psi\rangle = 0$, it follows that $A_5 V$ belongs to V up to the phase factor -1 . Having established that V is invariant under the action of A_1 and A_5 , from the first symmetry (10) of the inequality, it follows that A_2 and A_4 also leave the subspace V invariant.

Next, we proceed to see the action of A_3 on all the elements of V . Using the relations given by Eqs. (14) and (17), it follows that $A_3 |\psi\rangle = A_1 A_5 |\psi\rangle$, $A_3 A_1 |\psi\rangle = A_5 |\psi\rangle$, $A_3 A_5 |\psi\rangle = A_1 |\psi\rangle$, and $A_3 A_1 A_5 |\psi\rangle = |\psi\rangle$. Therefore, we have arrived at $A_3 V \subseteq V$. Using the fourth symmetry in (13) of the inequality in these arguments used to establish invariance of V under the action of A_3 , it then follows that $A_6 V \subseteq V$. ■

Due to Lemma 1, it suffices for our purpose to identify the form of the state $|\psi\rangle$ and the operators A_i 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 means that they have the following block structure:

$$A_i = \hat{A}_i \oplus A'_i, \quad (27)$$

where $\hat{A}_i = P A_i P$ with $P : \mathcal{H} \rightarrow V$ being a projection onto V . Since A'_i act trivially on V , that is, $A'_i V = 0$, which means that the observed correlations giving rise to the maximal violation of the inequality (7) come solely from the subspace V , in what follows we can restrict our attention to the operators \hat{A}_i .

Lemma 2. Suppose the maximal quantum violation of the inequality (7) is observed. Then, $[\hat{A}_1, \hat{A}_2] = [\hat{A}_1, \hat{A}_3] = [\hat{A}_2, \hat{A}_3] = [\hat{A}_4, \hat{A}_5] = [\hat{A}_4, \hat{A}_6] = [\hat{A}_5, \hat{A}_6] = [\hat{A}_1, \hat{A}_4] = [\hat{A}_2, \hat{A}_5] = [\hat{A}_3, \hat{A}_6] = 0$.

Proof. It is enough to show explicitly that $[\hat{A}_1, \hat{A}_2] = [\hat{A}_1, \hat{A}_4] = 0$. Then, by using symmetries of the inequality (7), the other commutators can be argued to vanish.

To show that $[\hat{A}_1, \hat{A}_2] = 0$, we prove that the action of the commutator $[A_1, A_2]$ on the invariant subspace vanishes. First, from the relations given by Eq. (14), we have $A_1 A_2 |\psi\rangle = A_2 A_1 |\psi\rangle = A_3 |\psi\rangle$ which implies that $[A_1, A_2]|\psi\rangle = 0$. Second, it also follows from the relations given by Eq. (14) that $A_1 A_2 A_1 |\psi\rangle = A_2 A_1 A_1 |\psi\rangle = A_2 |\psi\rangle$ which implies that $[A_1, A_2] A_1 |\psi\rangle = 0$. Third, using the relation given by Eq. (17), we have $A_1 A_2 A_5 |\psi\rangle = A_1 |\psi\rangle$. On the other hand, using the relations given by Eqs. (17) and (14), we have $A_2 A_1 A_5 |\psi\rangle = A_2 A_1 A_2 |\psi\rangle = A_1 |\psi\rangle$. Therefore, $[A_1, A_2] A_5 |\psi\rangle = 0$. Finally, let us check whether $[A_1, A_2] A_1 A_5 |\psi\rangle$ also vanishes. In the third case above, we have shown that $A_2 A_1 A_5 |\psi\rangle = A_1 |\psi\rangle$. Using this relation, it follows that $A_1 A_2 A_1 A_5 |\psi\rangle = |\psi\rangle$. On the other hand, using the relations given by Eqs. (17) and (14), we have $A_2 A_1 A_1 A_5 |\psi\rangle = |\psi\rangle$. Therefore, we have arrived at $[A_1, A_2] A_1 A_5 |\psi\rangle = 0$.

Using the symmetries (11) and (12) of the inequality in the above arguments, we also have $[A_2, A_3]V = 0$ and $[A_1, A_3]V = 0$, respectively. The fact that the action of the commutators $[A_1, A_2]$, $[A_2, A_3]$, and $[A_1, A_3]$ vanishes on V implies that the action of the commutators $[A_4, A_5]$, $[A_5, A_6]$, and $[A_4, A_6]$ on V vanishes as well. This follows from the fourth symmetry (13) of the inequality.

Next, we proceed to demonstrate that the action of the commutator $[A_1, A_4]$ on the invariant subspace vanishes. First, using Eq. (16), we have $A_1 A_4 |\psi\rangle = A_4 A_1 |\psi\rangle = |\psi\rangle$ which implies that $[A_1, A_4]|\psi\rangle = 0$. Second, using the same relation, we have $A_1 A_4 A_1 |\psi\rangle = A_4 |\psi\rangle$; on the other hand, $A_4 A_1 A_1 |\psi\rangle = A_4 |\psi\rangle$. From this, it follows that $[A_1, A_4] A_1 |\psi\rangle = 0$. Third,

$$A_1 A_4 A_5 |\psi\rangle = A_1 A_6 |\psi\rangle = -A_1 A_3 |\psi\rangle = -A_2 |\psi\rangle,$$

where we have used relations given by Eqs. (15), (18), and (14), respectively. On the other hand, we also have

$$\begin{aligned} A_4 A_1 A_5 &= A_4 A_1 A_2 |\psi\rangle = A_4 A_3 |\psi\rangle = -A_4 A_6 |\psi\rangle \\ &= -A_4 A_4 A_5 |\psi\rangle = -A_2 |\psi\rangle \end{aligned}$$

where in the first line we have used relations given by Eqs. (17), (14), and (18), respectively, and then we have employed the relations given by Eqs. (15) and (17), respectively. Combining the above two equations implies that $[A_1, A_4]A_5|\psi\rangle = 0$. Finally,

$$\begin{aligned} A_1A_4A_1A_5|\psi\rangle &= A_1A_4A_1A_2|\psi\rangle = A_1A_4A_3|\psi\rangle \\ &= -A_1A_4A_6|\psi\rangle = -A_1A_5|\psi\rangle \\ &= -A_1A_2|\psi\rangle = -A_3|\psi\rangle \end{aligned}$$

where in the first line we have used the relations given by Eqs. (17) and (14), respectively, and then we have employed the relations given by Eqs. (18), (15), (17), and (14), respectively. On the other hand, we also have

$$A_4A_1A_1A_5|\psi\rangle = A_6|\psi\rangle = -A_3|\psi\rangle,$$

where we have employed the relations given by Eqs. (15) and (18), respectively. Combining these two equations, we get that $[A_1, A_4]A_1A_5|\psi\rangle = 0$.

Using the symmetries of the inequality in (10) and (11) in the above arguments used to demonstrate that the action of the commutator $[A_1, A_4]$ vanishes on V , we will get $[A_2, A_5]V = 0$ and $[A_3, A_6]V = 0$, respectively. ■

Lemma 3. Suppose the maximal quantum violation of the inequality (7) is observed. Then,

$$\begin{aligned} \{\hat{A}_1, \hat{A}_5\} &= \{\hat{A}_1, \hat{A}_6\} \\ &= \{\hat{A}_2, \hat{A}_4\} = \{\hat{A}_2, \hat{A}_6\} \\ &= \{\hat{A}_3, \hat{A}_4\} = \{\hat{A}_3, \hat{A}_5\} = 0. \end{aligned} \quad (28)$$

Proof. It is enough to show explicitly that $\{\hat{A}_1, \hat{A}_5\} = 0$, by demonstrating that the anticommutator $\{A_1, A_5\}$ vanishes on the invariant subspace. First, in Eq. (20), it has been shown that $\{A_1, A_5\}|\psi\rangle = 0$. Second, using the fact that $A_1A_5|\psi\rangle = -A_5A_1|\psi\rangle$, we have $A_1A_5A_1|\psi\rangle = -A_5|\psi\rangle$; on the other hand, $A_5A_1A_1|\psi\rangle = A_5|\psi\rangle$, which implies $\{A_1, A_5\}A_1|\psi\rangle = 0$. Third, using the fact that $A_1A_5|\psi\rangle = -A_5A_1|\psi\rangle$, we have $A_1A_5A_5|\psi\rangle = A_1|\psi\rangle$; on the other hand, $A_5A_1A_5|\psi\rangle = -A_1|\psi\rangle$. Therefore, we get $\{A_1, A_5\}A_5|\psi\rangle = 0$. Finally, using the anticommutation relation $\{A_1, A_5\}|\psi\rangle = 0$, we obtain $A_1A_5A_1A_5|\psi\rangle = -|\psi\rangle$ and $A_1A_5A_5A_1|\psi\rangle = |\psi\rangle$. Therefore, we have $\{A_1, A_5\}A_1A_5|\psi\rangle = 0$.

Using symmetries of the inequality (7) in Eqs. (10)–(13) as used to demonstrate Eq. (19), it then follows that the other anticommutators in Lemma 3 can similarly be shown to vanish. ■

Having proven Lemma 3, we can infer that the dimension d of the subspace V is an even number by using the techniques as adopted in Refs. [16,28–31]. Thus, we can write the dimension $d = 2k$ for some $k \in \mathbb{N}$, and thus $V = \mathbb{C}^2 \otimes \mathbb{C}^k$. Moreover, since $\dim V \leq 4$, one concludes that $k = 1, 2$.

Lemma 4. Suppose the maximal quantum violation of the inequality (7) is observed. Then, there exists a unitary $U = U_1(\mathbb{1}_2 \otimes U_2)$ acting on V such that

$$\begin{aligned} U\hat{A}_1U^\dagger &= X \otimes \mathbb{1}, & U\hat{A}_2U^\dagger &= \mathbb{1} \otimes Z, \\ U\hat{A}_3U^\dagger &= \pm X \otimes Z, & U\hat{A}_4U^\dagger &= \mathbb{1} \otimes X, \\ U\hat{A}_5U^\dagger &= Z \otimes \mathbb{1}, & U\hat{A}_6U^\dagger &= \pm Z \otimes X. \end{aligned} \quad (29)$$

Proof. First, from Lemma 3, we have $\{\hat{A}_1, \hat{A}_5\} = 0$ which implies that there exists a unitary U_1 acting on V such that

$$U_1^\dagger \hat{A}_1 U_1 = X \otimes \mathbb{1}_k, \quad (30)$$

$$U_1^\dagger \hat{A}_5 U_1 = Z \otimes \mathbb{1}_k, \quad (31)$$

where, as already mentioned, the dimension d of the subspace V is given by $d = 2k$ for some $k = 1, 2$. Using then the above form of \hat{A}_1 and \hat{A}_5 and the relations in Lemmas 2 and 3 we can write the remaining operators as follows:

$$U_1^\dagger \hat{A}_2 U_1 = \mathbb{1}_2 \otimes M, \quad (32)$$

$$U_1^\dagger \hat{A}_3 U_1 = X \otimes N, \quad (33)$$

$$U_1^\dagger \hat{A}_4 U_1 = \mathbb{1}_2 \otimes O, \quad (34)$$

$$U_1^\dagger \hat{A}_6 U_1 = Z \otimes P, \quad (35)$$

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 observable 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

$$U_1^\dagger \hat{A}_2 U_1 = \mathbb{1}_2 \otimes M_1 + X \otimes M_2 + Y \otimes M_3 + Z \otimes M_4, \quad (36)$$

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 $[\hat{A}_2, \hat{A}_5] = 0$, one obtains that $M_2 = 0$, and, by putting $M_1 = M$, we arrive at Eq. (32).

Second, from Lemma 3, we also have $\{\hat{A}_2, \hat{A}_4\} = 0$ which is equivalent to $\{M, O\} = 0$. Since both M and O are involutions, one concludes that $k = 2$, or, equivalently, that $\mathbb{C}^k = \mathbb{C}^2$. In what follows, using $\{M, O\} = 0$, we can fix $M = Z$ and $O = X$. Now, from Lemmas 2 and 3, using $[\hat{A}_2, \hat{A}_3] = 0$ and $\{\hat{A}_3, \hat{A}_4\} = 0$, we find that $[N, Z] = 0$ as well as $\{N, X\} = 0$. This is possible if $N = \pm Z$. Similarly, using $\{\hat{A}_2, \hat{A}_6\} = 0$ and $[\hat{A}_4, \hat{A}_6] = 0$, we find that $O = \pm X$. Therefore, there exists another unitary transformation $U_2 : \mathbb{C}^k \rightarrow \mathbb{C}^k$ such that

$$U_2^\dagger M U_2 = Z, \quad U_2^\dagger N U_2 = \pm Z,$$

$$U_2^\dagger O U_2 = X, \quad U_2^\dagger P U_2 = \pm X.$$

Then, we find the relations in Eq. (29). ■

We have thus arrived at the main result of this paper.

Theorem 1. If a quantum state $|\psi\rangle$ and a set of measurements A_i with $i \in [1, 6]$ maximally violate the inequality (7), then there exists a projection $P : \mathcal{H} \rightarrow V$ with $V = \mathbb{C}^2 \otimes \mathbb{C}^2$

and a unitary U acting on V such that

$$\begin{aligned} U^\dagger (P\hat{A}_1P^\dagger)U &= X \otimes \mathbb{1}_2, & U^\dagger (P\hat{A}_4P^\dagger)U &= \mathbb{1}_2 \otimes X, \\ U^\dagger (P\hat{A}_2P^\dagger)U &= \mathbb{1}_2 \otimes Z, & U^\dagger (P\hat{A}_5P^\dagger)U &= Z \otimes \mathbb{1}_2, \\ U^\dagger (P\hat{A}_3P^\dagger)U &= X \otimes Z, & U^\dagger (P\hat{A}_6P^\dagger)U &= Z \otimes X, \end{aligned} \quad (37)$$

$$U(P|\psi\rangle) = |\phi^+\rangle, \quad (38)$$

where $|\phi^+\rangle$ is the two-qubit maximally entangled state Eq. (5).

Proof. A quantum state $|\psi\rangle$ that belongs to a Hilbert space \mathcal{H} and a set of observables A_i acting on \mathcal{H} attain the maximal quantum violation of the inequality (7) if and only if they satisfy the set of Eqs. (14)–(18). The algebraic relations induced by this set of equations let us prove Lemmas 1–4 which imply that there exists a projection $P : \mathcal{H} \rightarrow V \cong \mathbb{C}^4$ and a unitary $U = U_1(\mathbb{1}_2 \otimes U_2)$ acting on $V \cong \mathbb{C}^4$ for which Eqs. (29) hold true. Now, using stabilizer condition Eq. (14), we find that the sign in front of $U^\dagger \hat{A}_3 U$ can only be $+1$. Similarly, using Eq. (15), we can fix the sign of $U^\dagger \hat{A}_6 U$ to be $+1$.

From the above characterization of the observables, we can infer the form of the state $|\psi\rangle$. Indeed, after plugging $A_i = \hat{A}_i \oplus A_i$ with \hat{A}_i as given by Eq. (37), into the conditions (16) and (17) one realizes that the latter is simply the stabilizing conditions of the two-qubit maximally entangled state and thus $U(P|\psi\rangle) = |\phi^+\rangle$. This completes the proof. ■

Given this self-testing statement, we will now show in the following theorem that the above self-testing protocol is robust to very small errors (ϵ) which might come from noise or experimental imperfections. A rigorous proof of the following fact has been furnished in the Appendix.

Theorem 2. Suppose a quantum state $|\psi\rangle$ and a set of measurements A_i with $i \in [1, 6]$ in \mathcal{H} provide a nonmaximal violation $5 - \epsilon$ of the inequality (7). Then, there exists a projection $P : \mathcal{H} \rightarrow V$ (with $V = \mathbb{C}^2 \otimes \mathbb{C}^2$) and a unitary U acting on V such that the measurements \hat{A}_i and the state $|\hat{\psi}\rangle$ acting on V satisfy the following relations:

$$\begin{aligned} \|U^\dagger \hat{A}_i^{\text{noisy}} U - \hat{A}_i^{\text{opt}}\| &\leq m_1 \sqrt{\epsilon} + m_2 \epsilon^{1/4}, \\ |\langle \hat{\psi} | \phi^+ \rangle|^2 &\geq 1 - (s_1 \epsilon + s_2 \epsilon^{3/4} + s_3 \sqrt{\epsilon}), \end{aligned} \quad (39)$$

where $m_1, m_2, s_1, s_2,$ and s_3 are positive constants and \hat{A}_i^{opt} are the optimal measurements obtained in Eq. (37).

III. CONCLUSIONS AND OUTLOOK

In order to demonstrate Kochen-Specker contextuality via noncontextuality inequalities, we need to assume certain compatibility relations between the measurements by defining ‘‘contexts.’’ On the other hand, with temporal inequalities, we do not need to assume any compatibility conditions on the quantum measurements. In Ref. [15], a self-testing protocol based on observing measurement statistics that imply Kochen-Specker contextuality was proposed. This protocol certifies a two-qubit maximally entangled state and a subset of two-qubit Pauli measurements for realizing a topological quantum computer. In this paper, we proposed a self-testing protocol based on a temporal inequality that certifies this two-qubit entangled state and measurements. Thus, our scheme provides an alternative certification to the approach based on

Kochen-Specker contextuality as it does not assume those compatibility conditions.

As a future direction, it would be interesting to find a self-testing scheme using temporal inequalities which will work for general measurements. In our paper, we need to assume that measurements are projective if we drop the compatibility assumption. Note that Ref. [21] assumes that the measurement device produces a maximally mixed state as well as that the same measurement performed many times produces a particular outcome with certainty always in order to drop compatibility assumptions. Alternatively, it was suggested that one can assume a full rank input state to the measurement device instead of a maximally mixed state in order to remove the compatibility assumptions [23]. Therefore, we are lacking a universal self-testing scheme where such assumptions will be lifted. Also, it would be useful to find temporal inequalities with which we can reproduce self-testing statements for other existing noncontextuality inequalities. In another work, we extend our protocol to certify n -qubit quantum states and measurements with $n \geq 3$ [32].

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APPENDIX: ROBUSTNESS ANALYSIS

In this section we show that our certification scheme is robust to the experimental errors and imperfections, i.e., we can certify the state and measurements within a threshold fidelity close to the ideal state and measurements, even when the inequality (7) is violated nonmaximally. Let us assume that a maximal violation of the inequality (7) is obtained with an ϵ error, i.e., a nonmaximal violation of $5 - \epsilon$ is observed. We will now demonstrate that for $\epsilon \rightarrow 0$, the quantum realization is very close to the optimal quantum realization that gives the maximal bound. For a nonmaximal violation of $5 - \epsilon$ it is implied that the sequential correlations satisfy the following bounds:

$$\begin{aligned} \langle A_1 A_2 A_3 \rangle_\pi &\geq 1 - 2\epsilon, & \langle A_2 A_1 A_3 \rangle_\pi &\geq 1 - 2\epsilon, \\ \langle A_4 A_5 A_6 \rangle_\pi &\geq 1 - 2\epsilon, & \langle A_5 A_4 A_6 \rangle_\pi &\geq 1 - 2\epsilon, \\ \langle A_1 A_4 \rangle_\pi &\geq 1 - \epsilon, & \langle A_2 A_5 \rangle_\pi &\geq 1 - \epsilon, \\ -\langle A_3 A_6 \rangle_\pi &\geq 1 - \epsilon, \end{aligned} \quad (A1)$$

for some $\epsilon > 0$. From these error-prone correlations we will do all the steps that went into the self-testing in the error-free scenario, i.e., we will deduce the commutation relations, anticommutation relations, invariant subspace, and states and measurements within a small error bound. The sequential

correlations in (A1) further bound the quantum expectation values in the following way:

$$\langle (A_1 A_2 A_3 + A_3 A_2 A_1) \rangle \geq 2(1 - 4\epsilon) \quad \forall \text{ permutations,} \quad (\text{A2})$$

$$\langle (A_4 A_5 A_6 + A_6 A_5 A_4) \rangle \geq 2(1 - 4\epsilon) \quad \forall \text{ permutations.} \quad (\text{A3})$$

It can be seen that these relations are an approximate version of the optimal relations in (14)–(18). Equipped with these relations we now present the following lemma that will be useful for further proofs.

Lemma 5. Suppose the relations in (A1)–(A3) are satisfied for some $\epsilon > 0$. Then the following bounds hold true:

$$\|(A_1 - A_2 A_3) |\psi\rangle\| \leq 4\sqrt{\epsilon} \quad \forall \text{ permutations,} \quad (\text{A4})$$

$$\|(A_4 - A_5 A_6) |\psi\rangle\| \leq 4\sqrt{\epsilon} \quad \forall \text{ permutations,} \quad (\text{A5})$$

$$\|(A_1 - A_4) |\psi\rangle\| \leq 2\sqrt{\epsilon}, \quad (\text{A6})$$

$$\|(A_2 - A_5) |\psi\rangle\| \leq 2\sqrt{\epsilon}, \quad (\text{A7})$$

$$\|(A_3 + A_6) |\psi\rangle\| \leq 2\sqrt{\epsilon}. \quad (\text{A8})$$

Proof. We note the following:

$$\|(A_1 - A_2 A_3) |\psi\rangle\| = \sqrt{2 - \langle (A_1 A_2 A_3 + A_3 A_2 A_1) \rangle} \leq 4\sqrt{\epsilon},$$

where we simplify the norm by using the fact that A_i are unitary measurements and then we substitute (A2) to get the inequality. In the noise-free scenario, this reduces to $A_1 |\psi\rangle = A_2 A_3 |\psi\rangle$. In a similar way, we can obtain other relations. ■

Using these relations one can obtain the following error bounds on the anticommutators in Eq. (19):

$$\|\{A_i, A_j\} |\psi\rangle\| \leq 14\sqrt{\epsilon}. \quad (\text{A9})$$

The error bound can be obtained by following the proof of Eq. (19) and replacing each step of “equality” in the proof with a triangle inequality and then using the bounds in (A4)–(A8). For instance, in the anticommutation proof of $\{A_1, A_5\} |\psi\rangle = 0$ in Eq. (20), we do the following:

$$\begin{aligned} & \|(A_1 A_5 + A_5 A_1) |\psi\rangle\| \\ & \leq \|(A_1 A_5 - A_1 A_2) |\psi\rangle\| + \|(A_1 A_2 - A_3) |\psi\rangle\| \\ & \quad + \|(A_3 + A_6) |\psi\rangle\| + \|(-A_6 + A_5 A_4) |\psi\rangle\| \\ & \quad + \|(-A_5 A_4 + A_5 A_1) |\psi\rangle\| \leq 14\sqrt{\epsilon}, \end{aligned} \quad (\text{A10})$$

where we have used a chain of triangle inequalities for the vector norm, the error bounds from (A4)–(A8), and the fact that the vector norm is unitarily invariant. In the same way, we can get error bounds on the other anticommutators from Eq. (19).

Action of A_i on subspace V

Next, we will show that the invariant subspace $V := \text{span}\{|\psi\rangle, A_1 |\psi\rangle, A_5 |\psi\rangle, A_1 A_5 |\psi\rangle\}$ considered in (26) is now approximately invariant under the action of operators A_i for $i \in \{1, \dots, 6\}$. We find that the operator A_1 keeps the space V invariant. For A_5 , the nontrivial transformations are

(1) $A_5 A_1 |\psi\rangle \approx -A_1 A_5 |\psi\rangle + 14\sqrt{\epsilon} |\xi\rangle$ and (2) $A_5 A_1 A_5 |\psi\rangle \approx -A_1 |\psi\rangle + 14\sqrt{\epsilon} |\xi\rangle$ from Eq. (A10). Therefore, A_5 keeps the vectors from V approximately invariant. Note that vector $|\xi\rangle$ is arbitrary, moreover, we can assume without loss of generality that $|\xi\rangle$ lives in a subspace orthogonal to V .

Similarly, one can show that other operators keep the subspace invariant approximately. For example, the operator A_2 acting on V changes its vectors to $A_2 |\psi\rangle \approx A_5 |\psi\rangle + 2\sqrt{\epsilon} |\xi\rangle$ and $A_2 A_5 |\psi\rangle \approx A_2^2 |\psi\rangle + 2\sqrt{\epsilon} A_2 |\xi\rangle$ using Eq. (A7). Now, the vector $A_2 A_1 |\psi\rangle \approx A_1 A_2 |\psi\rangle + 8\sqrt{\epsilon} |\xi\rangle$ due to the relation that $\|A_1 A_2 - A_2 A_1\| \leq \|A_1 A_2 - A_3\| + \|A_3 - A_2 A_1\| \leq 8\sqrt{\epsilon}$ [using (A4)]. Then, it implies using Eq. (A7) that $A_2 A_1 |\psi\rangle \approx A_1 A_5 |\psi\rangle + 2\sqrt{\epsilon}(1 + 4A_1) |\xi\rangle$. The last vector $A_2 A_1 A_5 |\psi\rangle \approx A_2 A_1 A_2 |\psi\rangle + 2\sqrt{\epsilon} A_2 A_1 |\xi\rangle$ first, then $A_2 A_1 A_2 |\psi\rangle \approx A_2^2 A_1 |\psi\rangle + 8\sqrt{\epsilon} A_2 |\xi\rangle$. Therefore, A_2 keeps V invariant approximately. We tabulate all such transformation in Table I.

From Table I, we see that indeed action of A_i keeps V invariant approximately. However, notice that the vectors inside V are not necessarily orthogonal. Therefore, it is not guaranteed that A_i acting on an arbitrary state from V will keep it approximately within V . To proceed, we need to show the following:

$$\max_{|\psi\rangle_1, |\psi\rangle_2 \in V} \|A_i |\psi\rangle_1 - |\psi\rangle_2\| \leq f(\epsilon), \quad (\text{A11})$$

where $f(\epsilon)$ is some well-behaved function of ϵ . This will ensure that the action of A_i on V will be approximately invariant. For this purpose, we state and prove the following lemma. Importantly, we can remove maximization using the Gram-Schmidt orthogonalization procedure.

Lemma 6. Under the action of operators A_i for $i \in \{1, \dots, 6\}$, the subspace $V := \text{span}\{|\psi\rangle, A_1 |\psi\rangle, A_5 |\psi\rangle, A_1 A_5 |\psi\rangle\}$ changes as follows:

$$\forall |\psi\rangle_1 \in V, \quad \exists |\psi\rangle_k \in V, \quad \text{s.t.}$$

$$\|A_i |\psi\rangle_1 - |\psi\rangle_k\| \leq 2C_i \sqrt{\epsilon}, \quad (\text{A12})$$

where C_i with $i \in [1, 6]$ are real, finite, and positive constants and $k \in [1, 5]$.

Proof. Let us denote the vectors that span the subspace V as $|e_1\rangle = |\psi\rangle$, $|e_2\rangle = A_1 |\psi\rangle$, $|e_3\rangle = A_5 |\psi\rangle$, and $|e_4\rangle = A_1 A_5 |\psi\rangle$ and define the Gram matrix (Γ) with the elements $\Gamma_{mn} = \langle e_m | e_n \rangle$. Then, by applying the Gram-Schmidt (GS) orthogonalization procedure one finds an orthogonal basis that spans the subspace V . We denote this basis as $\{|\phi_m\rangle | m = 1, \dots, 4\}$, where $|\phi_m\rangle$ are expressed in terms of the initial vectors $|e_m\rangle$ as [33]

$$|\phi_m\rangle = \sum_n [\Gamma^{-1/2}]_{nm} |e_n\rangle. \quad (\text{A13})$$

Now, we notice that the Gram matrix Γ is invariant when we have following transformation.

- (1) $|e_1\rangle \rightarrow X_2 |e_1\rangle = A_1 |\psi\rangle$, $|e_2\rangle \rightarrow X_2 |e_2\rangle = |\psi\rangle$, $|e_3\rangle \rightarrow X_2 |e_3\rangle = A_1 A_5 |\psi\rangle$, and $|e_4\rangle \rightarrow X_2 |e_4\rangle = A_5 |\psi\rangle$.
- (2) $|e_1\rangle \rightarrow X_3 |e_1\rangle = A_5 |\psi\rangle$, $|e_2\rangle \rightarrow X_3 |e_2\rangle = A_1 A_5 |\psi\rangle$, $|e_3\rangle \rightarrow X_3 |e_3\rangle = |\psi\rangle$, and $|e_4\rangle \rightarrow X_3 |e_4\rangle = A_1 |\psi\rangle$.
- (3) $|e_1\rangle \rightarrow X_4 |e_1\rangle = A_1 A_5 |\psi\rangle$, $|e_2\rangle \rightarrow X_4 |e_2\rangle = A_5 |\psi\rangle$, $|e_3\rangle \rightarrow X_4 |e_3\rangle = A_1 |\psi\rangle$, and $|e_4\rangle \rightarrow X_4 |e_4\rangle = |\psi\rangle$.

Here the symbolic operators, X_2 , X_3 , and X_4 , mimic the action of A_1 , A_5 , and $A_1 A_5$ respectively. Therefore, we have

TABLE I. $A_i V \rightarrow V + f(\epsilon)$. The table describes how the vectors spanning V transform under the action of A_i in the nonideal scenario. Here, we denote $\chi = 2 + A_1$, $\Theta_1 = 1 + 4A_1$, $\Theta_2 = A_2(1 + \Theta_4)$, $\Theta_3 = 2 + A_4\Theta_4$, $\Theta_4 = 1 + \chi$, and $\Theta_5 = 3 + \chi$.

V	$ \psi\rangle$	$A_1 \psi\rangle$	$A_5 \psi\rangle$	$A_1A_5 \psi\rangle$
A_1V	$A_1 \psi\rangle$	$ \psi\rangle$	$A_1A_5 \psi\rangle$	$A_5 \psi\rangle$
A_2V	$A_5 \psi\rangle + 2\sqrt{\epsilon} \xi\rangle$	$A_1A_5 \psi\rangle + 2\sqrt{\epsilon}\Theta_1 \xi\rangle$	$ \psi\rangle + 2\sqrt{\epsilon}A_2 \xi\rangle$	$A_1 \psi\rangle + 2\sqrt{\epsilon}\Theta_2 \xi\rangle$
A_3V	$A_1A_5 \psi\rangle + 2\sqrt{\epsilon}\chi \xi\rangle$	$A_5 \psi\rangle + 6\sqrt{\epsilon} \xi\rangle$	$A_1 \psi\rangle + 2\sqrt{\epsilon}(2 + A_3) \xi\rangle$	$ \psi\rangle + 2\sqrt{\epsilon}A_3\chi \xi\rangle$
A_4V	$A_1 \psi\rangle + 2\sqrt{\epsilon} \xi\rangle$	$ \psi\rangle + 2\sqrt{\epsilon}A_4 \xi\rangle$	$-A_1A_5 \psi\rangle + 2\sqrt{\epsilon}\Theta_5 \xi\rangle$	$-A_5 \psi\rangle + 2\sqrt{\epsilon}\Theta_3 \xi\rangle$
A_5V	$A_5 \psi\rangle$	$-A_1A_5 \psi\rangle + 14\sqrt{\epsilon} \xi\rangle$	$ \psi\rangle$	$-A_1 \psi\rangle + 14\sqrt{\epsilon} \xi\rangle$
A_6V	$-A_1A_5 \psi\rangle + 2\sqrt{\epsilon}\Theta_4 \xi\rangle$	$A_5 \psi\rangle + 2\sqrt{\epsilon}(2 + A_6) \xi\rangle$	$A_1 \psi\rangle + 6\sqrt{\epsilon} \xi\rangle$	$- \psi\rangle + 2\sqrt{\epsilon}A_6\Theta_4 \xi\rangle$

another three GS bases (with the same Gram matrix Γ) which also span V . It is evident from Table I that we only need these four bases, $\{X_k|e_n\rangle\} \in V$ for our analysis below. Now, any vector $|\psi\rangle_k \in V$, $\forall k \in [1, 4]$ can be expressed in terms of these orthogonal bases as

$$|\psi\rangle_k = \sum_m \alpha_m X_k |\phi_m\rangle = \sum_m \alpha_m \sum_n [\Gamma^{-1/2}]_{nm} X_k |e_n\rangle, \quad (\text{A14})$$

where $X_1 = \mathbb{1}$ and α_m are complex coefficients satisfying $\sum_i |\alpha_m|^2 = 1$. Notice here that the action of X_k on the set of vectors $|e_n\rangle \in V$ in Eq. (A14) is listed above.

Equipped with the above relations, we are now ready to prove the lemma. First we prove that $A_1|\psi\rangle_1 = |\psi\rangle_2$ below:

$$\begin{aligned} A_1|\psi\rangle_1 &= A_1 \left(\sum_m \alpha_m \sum_n [\Gamma^{-1/2}]_{nm} |e_n\rangle \right) \\ &= \sum_m \alpha_m \sum_n [\Gamma^{-1/2}]_{nm} X_2 |e_n\rangle = |\psi\rangle_2, \end{aligned}$$

where we use Eq. (A14). Now, consider the action of A_2 on V , and then using Table I

$$\begin{aligned} A_2|\psi\rangle_1 &= \sum_m \alpha_m \sum_n [\Gamma^{-1/2}]_{nm} A_2 |e_n\rangle \\ &\approx \sum_m \alpha_m \sum_n [\Gamma^{-1/2}]_{nm} \{X_3 |e_n\rangle + 2\sqrt{\epsilon}f_n(A_2)|\xi\rangle\} \\ &= |\psi\rangle_3 + 2\sqrt{\epsilon} \sum_m \alpha_m \sum_n [\Gamma^{-1/2}]_{nm} f_n(A_2)|\xi\rangle, \end{aligned}$$

where $f_1(A_2) = 1$, $f_2(A_2) = 1 + 4A_1$, $f_3(A_2) = A_2$, and $f_4(A_2) = A_2(4 + A_1)$ using Table I and we use Eq. (A14) in the second line. Note that in the above equation, we find that the Gram matrix remains invariant also under the action of $\{A_i | i \in [2, 6]\}$ as $\langle e_n | \xi \rangle = 0$. By rearranging the terms, we find the below relation:

$$\begin{aligned} \|A_2|\psi\rangle_1 - |\psi\rangle_3\| &\leq 2\sqrt{\epsilon} \sum_m \left\| \sum_n [\Gamma^{-1/2}]_{nm} f_n(A_2)|\xi\rangle \right\| \\ &\leq 2\sqrt{\epsilon}C_2, \end{aligned}$$

where we used $|\alpha_m| \leq 1$ and identified the real and positive constant C_2 as

$$C_2 = \sum_m \left\| \sum_n [\Gamma^{-1/2}]_{nm} f_n(A_2)|\xi\rangle \right\|.$$

Notice that it is straightforward to find the expression of C_2 by opening the summation over n . In this way a lot of terms will be simplified by noticing that $A_i^2 = \mathbb{1}$.

Similarly, we can prove that all the operators A_i will keep V approximately invariant. In the end, we get the following relations for the rest of the operators for their actions on V :

$$\begin{aligned} \forall |\psi\rangle_1 \in V \quad \exists |\psi\rangle_4 \in V, \text{ s.t. } \|A_3|\psi\rangle_1 - |\psi\rangle_4\| &\leq 2\sqrt{\epsilon}C_3, \\ \forall |\psi\rangle_1 \in V \quad \exists |\psi\rangle_2 \in V, \text{ s.t. } \|A_4|\psi\rangle_1 - |\psi\rangle_2\| &\leq 2\sqrt{\epsilon}C_4, \\ \forall |\psi\rangle_1 \in V \quad \exists |\psi\rangle_3 \in V, \text{ s.t. } \|A_5|\psi\rangle_1 - |\psi\rangle_3\| &\leq 2\sqrt{\epsilon}C_5, \\ \forall |\psi\rangle_1 \in V \quad \exists |\psi\rangle_4 \in V, \text{ s.t. } \|A_6|\psi\rangle_1 - |\psi\rangle_4\| &\leq 2\sqrt{\epsilon}C_6, \end{aligned} \quad (\text{A15})$$

where C_i with $i \in \{3, \dots, 6\}$ are real, finite, and positive constants. Moreover, the constants C_i can in general be estimated by the following relation:

$$C_i = \sum_m \left\| \sum_n [\Gamma^{-1/2}]_{nm} f_n(A_i)|\xi\rangle \right\|, \quad (\text{A16})$$

where the expressions of $f_n(A_i)$ can be found from Table I. Hence, we prove the lemma. \blacksquare

Due to Lemma 6, the operators A_i are approximately restricted to the subspace V , i.e., we can write them as $A_i = \begin{pmatrix} \hat{A}_i & B_i^* \\ \hat{A}_i' & A_i' \end{pmatrix}$, where similar to the error-free scenario $\hat{A}_i = PA_iP$ with $P: \mathcal{H} \rightarrow V$ projects onto V , A_i' acts trivially on V , and the correlation terms between V and V^\perp represented with B are of the order of $2C_i\sqrt{\epsilon}$. Since the action of A_i' on V is trivial and B on V is of the order of $2C_i\sqrt{\epsilon}$, we can conclude that the contribution to the nonmaximal violation comes mostly from the operators \hat{A}_i . For the remaining proof, we can limit ourselves to \hat{A}_i only. Furthermore, due to (A15) all the eigenvalues a_i of operators A_i , respectively, are bounded as follows:

$$|a_1| = 1, \quad 1 - 2C_i\sqrt{\epsilon} \leq |a_i| \leq 1. \quad (\text{A17})$$

Note that since A_1 keeps V invariant, we have the unitary condition $\hat{A}_1^2 = \mathbb{1}$, whereas all the remaining hatted operators are not unitary anymore. For robust self-testing, we also need to show that the commutators and anticommutators from Lemmas 2 and 3 hold within a small error bound proportional to ϵ . We derive these bounds in the next two lemmas. The derivations of the error bounds on the commutators and anticommutators are obtained by following the proofs in the error-free scenario and replacing the ‘‘equalities’’ with the relevant triangle inequalities.

Lemma 7. Suppose a nonmaximal quantum violation $5 - \epsilon$ of the inequality (7) is observed. Then the following error bounds on the commutation relations can be obtained:

$$\begin{aligned} \|\{\hat{A}_1, \hat{A}_2\}\|, \|\{\hat{A}_1, \hat{A}_3\}\|, \|\{\hat{A}_2, \hat{A}_3\}\| &\leq 4(C_2 + C_3)\sqrt{\epsilon}, \\ \|\{\hat{A}_4, \hat{A}_5\}\|, \|\{\hat{A}_4, \hat{A}_6\}\|, \|\{\hat{A}_5, \hat{A}_6\}\| &\leq 4(C_4 + C_5 + C_6)\sqrt{\epsilon}, \\ \|\{\hat{A}_1, \hat{A}_4\}\| &\leq 4C_4\sqrt{\epsilon}, \quad \|\{\hat{A}_2, \hat{A}_5\}\| \leq 4(C_2 + C_5)\sqrt{\epsilon}, \quad \|\{\hat{A}_3, \hat{A}_6\}\| \leq 4(C_3 + C_6)\sqrt{\epsilon}. \end{aligned}$$

Proof. We will show the proof for error bound on $[\hat{A}_1, \hat{A}_2]$, and the remaining bounds are obtained in a similar way. To get a bound on $\|\{\hat{A}_1, \hat{A}_2\}\|$, we will prove that $\|[A_1, A_2]\|$ is bounded by $4(C_2 + C_3)\sqrt{\epsilon}$ in arbitrary vectors from subspace V . Considering the vector $|\psi\rangle_1 \in V$, we have

$$\|[A_1, A_2]|\psi\rangle_1\| \leq \|(A_1A_2 - A_3)|\psi\rangle_1\| + \|(A_3 - A_2A_1)|\psi\rangle_1\|,$$

where we use the triangle inequality. Now, considering the term $\sum_i \|(A_1A_2 - A_3)|\psi\rangle_1\|$ and evaluating it,

$$\|(A_1A_2 - A_3)|\psi\rangle_1\| \leq \|A_1A_2|\psi\rangle_1 - |\psi\rangle_4\| + \|\psi\rangle_4 - A_3|\psi\rangle_1\|,$$

where $|\psi\rangle_4 \in V$. According to Lemma 6, $\|\psi\rangle_4 - A_3|\psi\rangle_1\| \leq 2\sqrt{\epsilon}C_3$. We need to evaluate the first term above. Further notice that

$$\|A_1A_2|\psi\rangle_1 - |\psi\rangle_4\| \leq \|A_1A_2|\psi\rangle_1 - A_1|\psi\rangle_3\| + \|A_1|\psi\rangle_3 - |\psi\rangle_4\|,$$

where $|\psi\rangle_3 \in V$. Using Lemma 6, we conclude that $\|A_1A_2|\psi\rangle_1 - A_1|\psi\rangle_3\| \leq 2\sqrt{\epsilon}C_2$. Note that the relation $A_1|\psi\rangle_3 = |\psi\rangle_4$ holds trivially. Therefore, we reach to the following expression after collecting all such contributions:

$$\|[A_1, A_2]|\psi\rangle_1\| \leq 4\sqrt{\epsilon}(C_2 + C_3).$$

Similarly, we show this for all the commutators. This proves our claim. ■

Next, we find the error bound for the anticommutation relations in the following lemma.

Lemma 8. Suppose a nonmaximal quantum violation $5 - \epsilon$ of the inequality (7) is observed. Then the following error bounds on the anticommutation relations can be obtained:

$$\|\{\hat{A}_1, \hat{A}_5\}\|, \|\{\hat{A}_2, \hat{A}_4\}\|, \|\{\hat{A}_3, \hat{A}_4\}\|, \|\{\hat{A}_3, \hat{A}_5\}\|, \|\{\hat{A}_1, \hat{A}_6\}\|, \|\{\hat{A}_2, \hat{A}_6\}\| \leq 4C_\gamma\sqrt{\epsilon},$$

where $C_\gamma = \sum_{i=2}^6 C_i$ is also a finite constant.

Proof. We consider $\|\{\hat{A}_3, \hat{A}_4\}\|$, and prove the upper bound for it by showing that $\|\{A_3, A_4\}\| \leq 4C_\gamma\sqrt{\epsilon}$ for every element of V . Similar to the proof of Lemma 7, consider any arbitrary $|\psi\rangle_1 \in V$, then

$$\begin{aligned} \|\{A_3, A_4\}|\psi\rangle_1\| &\leq \|(A_3A_4 - A_3A_1)|\psi\rangle_1\| + \|(A_3A_1 - A_2)|\psi\rangle_1\| + \|(A_2 - A_5)|\psi\rangle_1\| \\ &\quad + \|(A_5 - A_4A_6)|\psi\rangle_1\| + \|(A_4A_6 + A_4A_3)|\psi\rangle_1\|, \end{aligned}$$

where we use the triangle inequality. Then from Lemma 6, the first three terms in the right-hand side are easy to compute and, directly, $\|(A_3A_4 - A_3A_1)|\psi\rangle_1\| \leq 2\sqrt{\epsilon}C_4$, $\|(A_3A_1 - A_2)|\psi\rangle_1\| \leq 2\sqrt{\epsilon}(C_2 + C_3)$ and $\|(A_2 - A_5)|\psi\rangle_1\| \leq 2\sqrt{\epsilon}(C_2 + C_5)$. The fourth one can be estimated as $\|(A_5 - A_4A_6)|\psi\rangle_1\| \leq 2\sqrt{\epsilon}(C_4 + C_5 + C_6)$ and the last one can be expressed as $\|(A_4A_6 + A_4A_3)|\psi\rangle_1\| \leq 2\sqrt{\epsilon}(C_6 + C_3)$. Collecting all these contributions, we find that

$$\|\{A_3, A_4\}|\psi\rangle_1\| \leq 4C_\gamma\sqrt{\epsilon},$$

where $C_\gamma = \sum_{i=2}^6 C_i$. In the same way, we can show the other anticommutator bounds by Lemma 6. ■

Having proved Lemma 8, we can show that for a basis $\{|\phi_i\rangle\}$, we have $\text{Tr}(\hat{A}_5\hat{A}_1\hat{A}_5 + \hat{A}_1) = \sum_i \langle\phi_i|\hat{A}_5\hat{A}_1\hat{A}_5 + \hat{A}_1|\phi_i\rangle \leq \sum_i \|\langle\phi_i|\{\hat{A}_1, \hat{A}_5\}|\phi_i\rangle\| \leq 4C_\gamma\sqrt{\epsilon}$, where the first inequality is obtained using the triangle inequality and the next one by using the bound on $\|\{\hat{A}_1, \hat{A}_5\}|\psi\rangle_1\|$. Therefore, we can deduce that $\text{Tr}(\hat{A}_1) \leq 4C_\gamma\sqrt{\epsilon}$ which is possible only when $\text{Tr}(\hat{A}_1) = 0$. A similar situation holds for all other operators \hat{A}_i . As in the noise-free case, we can write the dimension $d = 2k$ for $k \in \mathbb{N}$, and thus $V = \mathbb{C}^2 \otimes \mathbb{C}^k$. Also since, $\dim V \leq 4$, we can only have $k = 1, 2$. Now we are ready to certify the measurements in the following lemma.

Lemma 9. Suppose a nonmaximal quantum violation $5 - \epsilon$ of the inequality (7) is observed. Then, there exists a basis in V such that

$$\begin{aligned} \hat{A}_1 &= X \otimes \mathbb{1}, & \|\hat{A}_2 - \mathbb{1} \otimes Z\| &\leq 2c_2\sqrt{\epsilon} + 8C\epsilon^{1/4}, \\ \|\hat{A}_3 - X \otimes Z\| &\leq 2c_3\sqrt{\epsilon} + 16C\epsilon^{1/4}, & \|\hat{A}_4 - \mathbb{1} \otimes X\| &\leq 2c_4\sqrt{\epsilon} + 16C\epsilon^{1/4}, \\ \|\hat{A}_5 - Z \otimes \mathbb{1}\| &\leq 6C_\gamma\sqrt{\epsilon} + 2C\epsilon^{\frac{1}{4}}, & \|\hat{A}_6 - Z \otimes X\| &\leq 2c_6\sqrt{\epsilon} + 16C\epsilon^{1/4}, \end{aligned} \tag{A18}$$

where $c_2 = C_2 + 2\bar{C}_2$, $c_3 = C_3 + 2\bar{C}_3 + 2\bar{C}_4 + 2C_\gamma - 2C_2$, $c_4 = C_2 + 2\bar{C}_2 + 2\bar{C}_4 + C_\gamma$, and $c_6 = C_\gamma + C_2 + C_3 + 2\bar{C}_2 + 2\bar{C}_6$.

Proof. From Lemma 8, we have $\| \{A_1, A_5\} \| \leq 4C_\gamma \sqrt{\epsilon}$, which implies that there exists a unitary \mathcal{U}_1 acting on V such that

$$\hat{A}_1^{(1)} = X \otimes \mathbb{1}, \quad \text{and} \quad \hat{A}_5^{(1)} = \mathbb{1} \otimes M_1 + X \otimes M_x + Y \otimes M_y + Z \otimes M_z, \quad (\text{A19})$$

where action of \mathcal{U}_k on the operator \mathcal{O} is denoted as $\mathcal{U}_k^\dagger \mathcal{O} \mathcal{U}_k = \mathcal{O}^{(k)}$ for our convenience. Substituting the above form in the bound $\| \{\hat{A}_1, \hat{A}_5\} \| \leq 4C_\gamma \sqrt{\epsilon}$, we get that $\| \{\hat{A}_1^{(1)}, \hat{A}_5^{(1)}\} \| = \| \{X \otimes \mathbb{1}, \hat{A}_5^{(1)}\} \| \leq 4C_\gamma \sqrt{\epsilon}$, which further implies that

$$\| \mathbb{1} \otimes M_1 + X \otimes M_x \| = \| \hat{A}_5^{(1)} - Y \otimes M_y - Z \otimes M_z \| \leq 2C_\gamma \sqrt{\epsilon}. \quad (\text{A20})$$

Therefore, it holds that $\| (Y \otimes M_y + Z \otimes M_z)^2 \| \geq (1 - 2C_\gamma \sqrt{\epsilon})^2$. From this approximate unitary, we can deduce the following:

$$\begin{aligned} \| \mathbb{1} \otimes (M_y^2 + M_z^2) + YZ \otimes [M_y, M_z] \| &\geq (1 - 2C_\gamma \sqrt{\epsilon})^2 \\ \Rightarrow (1 - 2C_\gamma \sqrt{\epsilon})^2 &\leq \| M_y^2 + M_z^2 \| \leq 1, \quad \text{and} \quad \| [M_y, M_z] \| \leq 4C_\gamma \sqrt{\epsilon} - 16C_\gamma \epsilon \leq 4C_\gamma \sqrt{\epsilon}. \end{aligned} \quad (\text{A21})$$

It is known that for such almost commuting Hermitian matrices we can find another pair of commuting Hermitian matrices M'_y, M'_z arbitrarily close to M_y, M_z respectively [34,35], which in our case can be stated as

$$[M'_y, M'_z] = 0, \quad \text{s.t.} \quad \{ \| M_y - M'_y \|, \| M_z - M'_z \| \} \leq C\epsilon^{1/4}, \quad (\text{A22})$$

where C is a constant independent of M_y, M_z ; however, it is function of ϵ and grows slower than any power of ϵ . From (A21) it can also be seen that $\| M_y - \cos \alpha \mathbb{1} \| \leq 2C_\gamma \sqrt{\epsilon}$ and $\| M_z - \sin \alpha \mathbb{1} \| \leq 2C_\gamma \sqrt{\epsilon}, \forall \alpha \in [0, 2\pi]$, which further implies the following:

$$\| M'_y - \cos \alpha \mathbb{1} \| \leq \| M'_y - M_y \| + \| M_y - \cos \alpha \mathbb{1} \| \leq 2C_\gamma \sqrt{\epsilon} + C\epsilon^{1/4}.$$

And similarly, we have $\| M'_z - \sin \alpha \mathbb{1} \| \leq 2C_\gamma \sqrt{\epsilon} + C\epsilon^{1/4}$. Now by substituting these bounds in (A20) we get the following by using triangle inequalities:

$$\begin{aligned} \| \hat{A}_5^{(1)} - \cos \alpha Y \otimes \mathbb{1} - \sin \alpha Z \otimes \mathbb{1} \| - \| Y \otimes (M'_y - \cos \alpha \mathbb{1}) \| - \| Z \otimes (M'_z - \sin \alpha \mathbb{1}) \| &\leq 2C_\gamma \sqrt{\epsilon} \\ \Rightarrow \| \hat{A}_5^{(1)} - \cos \alpha Y \otimes \mathbb{1} - \sin \alpha Z \otimes \mathbb{1} \| &\leq 6C_\gamma \sqrt{\epsilon} + 2C\epsilon^{1/4}. \end{aligned} \quad (\text{A23})$$

Therefore, we can proceed further by applying another unitary \mathcal{U}_2 such that $\mathcal{U}_2^\dagger (\cos \alpha Y \otimes \mathbb{1} + \sin \alpha Z \otimes \mathbb{1}) \mathcal{U}_2 \rightarrow Z \otimes \mathbb{1}$ and keep $\hat{A}_1^{(1)} = X \otimes \mathbb{1}$ unchanged as the rotation is in the y - z plane. Therefore we have a unitary $U_1 = \mathcal{U}_1 \mathcal{U}_2$ such that

$$U_1^\dagger \hat{A}_1 U_1 = X \otimes \mathbb{1}, \quad \| U_1^\dagger \hat{A}_5 U_1 - Z \otimes \mathbb{1} \| \leq 6C_\gamma \sqrt{\epsilon} + 2C\epsilon^{1/4}. \quad (\text{A24})$$

Now that we have the above form of \hat{A}_1 and \hat{A}_5 , we can write the remaining operators in the same basis as following by using Lemmas 7 and 8:

$$\begin{aligned} \| U_1^\dagger \hat{A}_2 U_1 - \mathbb{1} \otimes N \| &\leq 2\bar{C}_2 \sqrt{\epsilon} + 4C\epsilon^{1/4}, \quad \| U_1^\dagger \hat{A}_3 U_1 - X \otimes O \| \leq 2\bar{C}_3 \sqrt{\epsilon} + 4C\epsilon^{1/4}, \\ \| U_1^\dagger \hat{A}_4 U_1 - \mathbb{1} \otimes P \| &\leq 2\bar{C}_4 \sqrt{\epsilon} + 4C\epsilon^{1/4}, \quad \| U_1^\dagger \hat{A}_6 U_1 - Z \otimes Q \| \leq 2\bar{C}_6 \sqrt{\epsilon} + 4C\epsilon^{1/4}, \end{aligned} \quad (\text{A25})$$

where $\bar{C}_2 = (4 + \sqrt{2})C_2 + \sqrt{2}C_3 + 4C_5$, $\bar{C}_3 = 4C_\gamma + \sqrt{2}(C_2 + C_3)$, $\bar{C}_4 = (4 + \sqrt{2})C_4 + 4(C_5 + C_6)$, $\bar{C}_6 = \sqrt{C_\gamma^2 + C_6^2} + 4(C_4 + C_5 + C_6)$, and N, O, P , and Q are Hermitian operators acting on the subspace of dimension $k \leq 2$. We will show explicitly how to obtain the relation for \hat{A}_2 and the remaining operators can be obtained similarly: first, by expanding \hat{A}_2 in the Pauli basis as follows:

$$\hat{A}_2 = \mathbb{1} \otimes N + X \otimes N_x + Y \otimes N_y + Z \otimes N_z. \quad (\text{A26})$$

Substituting this form in the bounds on commutation relations of \hat{A}_2 with \hat{A}_1 and \hat{A}_5 from Lemma 7, we will get the following relations respectively:

$$\begin{aligned} \| Y \otimes N_y + Z \otimes N_z \| &= \| \hat{A}_2 - \mathbb{1} \otimes N - X \otimes N_x \| \leq 2(C_2 + C_3)\sqrt{\epsilon}, \\ \| Y \otimes N_y + X \otimes N_x \| &= \| \hat{A}_2 - \mathbb{1} \otimes N - Z \otimes N_z \| \leq 8(C_2 + C_5)\sqrt{\epsilon} + 4C\epsilon^{1/4}. \end{aligned} \quad (\text{A27})$$

Now notice that since \hat{A}_2 is almost a unitary matrix, the operators N_x, N_y , and N_z approximately commute with each other. We can further show by manipulating the above expression that

$$\begin{aligned} \| (Y \otimes N_y + Z \otimes N_z)^2 \| &= \| \mathbb{1} \otimes N_y^2 + \mathbb{1} \otimes N_z^2 + YZ[\mathbb{1} \otimes N_y, \mathbb{1} \otimes N_z] \| \leq 4(C_2 + C_3)^2 \epsilon \\ &\Rightarrow \| \mathbb{1} \otimes N_y^2 + \mathbb{1} \otimes N_z^2 \| \leq 4(C_2 + C_3)^2 \epsilon + \| YZ[\mathbb{1} \otimes N_y, \mathbb{1} \otimes N_z] \| \leq 8(C_2 + C_3)^2 \epsilon \\ &\Rightarrow \| N_y \|, \| N_z \| \leq (C_2 + C_3)\sqrt{8\epsilon}, \end{aligned}$$

where we have expanded using the triangle inequality and then upper bounded $\| YZ[\mathbb{1} \otimes N_y, \mathbb{1} \otimes N_z] \|$ by $[2(C_2 + C_3)\sqrt{\epsilon}]^2$, using the fact that $1 - 2C_2\sqrt{\epsilon} \leq |a_2| \leq 1$ from (A17). Substituting these in the second relation of (A27), we will get the bound

$\|\hat{A}_2 - \mathbb{1} \otimes N\| \leq 2\bar{C}_2\sqrt{\epsilon} + 4C\epsilon^{1/4}$, with $\bar{C}_2 = (4 + \sqrt{2})C_2 + \sqrt{2}C_3 + 4C_5$. In a similar way we can get the relations for the remaining operators in \hat{A}_3, \hat{A}_4 , and \hat{A}_6 in (A25).

Now, using the bounds on \hat{A}_2 and \hat{A}_4 (A25) and the bound on $\{\hat{A}_2, \hat{A}_4\}$ from Lemma 8 we can show that

$$\begin{aligned} \|\{\mathbb{1} \otimes N, \mathbb{1} \otimes P\}\| &\leq \|(\mathbb{1} \otimes N - A_2)\mathbb{1} \otimes P\| + \|A_2(\mathbb{1} \otimes P - A_4)\| + \|\mathbb{1} \otimes P(\mathbb{1} \otimes N - A_2)\| + \|(\mathbb{1} \otimes P - A_4)A_2\| \\ &\quad + \|\{A_2, A_4\}\| \leq 4(C_\gamma + \bar{C}_2 + \bar{C}_4)\sqrt{\epsilon} + 16C\epsilon^{1/4}. \end{aligned} \quad (\text{A28})$$

We can now find a unitary operator \mathcal{U}_3 such that

$$\|\mathbb{1} \otimes N^{(3)} - \mathbb{1} \otimes Z\| \leq \|\mathbb{1} \otimes N - \hat{A}_2\| + \|\hat{A}_2^{(3)} - \mathbb{1} \otimes Z\| \leq 2(C_2 + \bar{C}_2)\sqrt{\epsilon} + 4C\epsilon^{1/4}, \quad (\text{A29})$$

where we have first used the triangle inequality and then the bounds on $\|\mathbb{1} \otimes N - \hat{A}_2\|$ from (A25), $\|\hat{A}_2 - \mathbb{1} \otimes Z\|$, from the fact that the minimum eigenvalue of \hat{A}_2 is $1 - 2C_2\sqrt{\epsilon}$. Now using the anticommutation bound in (A28) and the inequality in (A29), we can get the following relation:

$$\begin{aligned} \|\{\mathbb{1} \otimes P^{(3)}, \mathbb{1} \otimes Z\}\| &\leq \|\{\mathbb{1} \otimes P, \mathbb{1} \otimes N\}\| + \|\{\mathbb{1} \otimes P^{(3)}, (\mathbb{1} \otimes Z - \mathbb{1} \otimes N^{(3)})\}\| \\ &\leq 4(C_\gamma + C_2 + 2\bar{C}_2 + \bar{C}_4)\sqrt{\epsilon} + 24C\epsilon^{1/4}, \end{aligned}$$

where we first use the triangle inequality and then apply the upper bounds. From the above relation, the form of $\mathbb{1} \otimes P^{(3)} = p_1\mathbb{1} \otimes \mathbb{1} + p_x\mathbb{1} \otimes X + p_y\mathbb{1} \otimes Y + p_z\mathbb{1} \otimes Z$ can be written as

$$\|\mathbb{1} \otimes P^{(3)} - p_x\mathbb{1} \otimes X - p_y\mathbb{1} \otimes Y\| \leq 2(C_\gamma + C_2 + 2\bar{C}_2 + \bar{C}_4)\sqrt{\epsilon} + 12C\epsilon^{1/4}.$$

By finding another unitary \mathcal{U}_4 which rotates the operator $p_xX + p_yY$ to X and leaves $\mathbb{1} \otimes Z$ invariant as it rotates the operators only in the x - y plane, we can get the following by defining $U_2 = \mathcal{U}_4\mathcal{U}_3$:

$$\begin{aligned} \|U_2^\dagger \mathbb{1} \otimes NU_2 - \mathbb{1} \otimes Z\| &\leq 2(C_2 + \bar{C}_2)\sqrt{\epsilon} + 4C\epsilon^{1/4}, \\ \|U_2^\dagger \mathbb{1} \otimes PU_2 - \mathbb{1} \otimes X\| &\leq 2(C_\gamma + C_2 + 2\bar{C}_2 + \bar{C}_4)\sqrt{\epsilon} + 12C\epsilon^{1/4}. \end{aligned} \quad (\text{A30})$$

Thus by defining the effect of these unitaries as $U = U_2U_1$, and then substituting the relations of (A30) further in (A25) for \hat{A}_2 and \hat{A}_4 , we will get

$$\begin{aligned} \|U^\dagger \hat{A}_4U - \mathbb{1} \otimes X\| &\leq \|U^\dagger \hat{A}_4U - U_2^\dagger \mathbb{1} \otimes PU_2\| + \|U_2^\dagger \mathbb{1} \otimes PU_2 - \mathbb{1} \otimes X\| \leq 2(C_2 + 2\bar{C}_2 + 2\bar{C}_4 + C_\gamma)\sqrt{\epsilon} + 16C\epsilon^{1/4}, \\ \|U^\dagger \hat{A}_2U - \mathbb{1} \otimes Z\| &\leq \|U^\dagger \hat{A}_2U - U_2^\dagger \mathbb{1} \otimes NU_2\| + \|U_2^\dagger \mathbb{1} \otimes NU_2 - \mathbb{1} \otimes Z\| \leq 2(C_2 + 2\bar{C}_2)\sqrt{\epsilon} + 8C\epsilon^{1/4}. \end{aligned} \quad (\text{A31})$$

Now to obtain the operators \hat{A}_3 and \hat{A}_6 we need to determine O and Q . To do this, we use the bounds on the commutator and anticommutator of $\hat{A}_3(\hat{A}_6)$ with \hat{A}_2 and \hat{A}_4 from Lemmas 7 and 8. Let us note the following relations for O :

$$\begin{aligned} \|[X \otimes O, \mathbb{1} \otimes Z]\| &\leq \|(X \otimes O - \hat{A}_3)\otimes Z\| + \|\hat{A}_3(\mathbb{1} \otimes Z - \hat{A}_2)\| + \|(\hat{A}_2 - \mathbb{1} \otimes Z)\hat{A}_3\| + \|\mathbb{1} \otimes Z(\hat{A}_3 - X \otimes O)\| \\ &\quad + \|\{\hat{A}_2, \hat{A}_3\}\| \leq 4(C_2 + \bar{C}_2 + C_3 + \bar{C}_3)\sqrt{\epsilon} + 24C\epsilon^{1/4}, \\ \|[X \otimes O, \mathbb{1} \otimes X]\| &\leq \|(X \otimes O - \hat{A}_3)\mathbb{1} \otimes X\| + \|A_3(\mathbb{1} \otimes X - A_4)\| + \|\mathbb{1} \otimes X(X \otimes O - \hat{A}_3)\| + \|(\mathbb{1} \otimes X - A_4)A_3\| \\ &\quad + \|\{A_3, A_4\}\| \leq 4(C_\gamma + \bar{C}_3 + \bar{C}_4)\sqrt{\epsilon} + 24C\epsilon^{1/4}. \end{aligned}$$

Here we have used the triangle inequalities and then the bounds from (A25) and (A31) and then the bounds on $\|[A_2, A_3]\|$ and $\|[A_3, A_4]\|$. From the above two relations, we can deduce that $\|[O, Z]\|$ and $\|[O, X]\|$ also satisfy the same bound. Expanding the operator O as $o_1\mathbb{1} + o_xX + o_yY + o_zZ$, we can conclude the following:

$$\begin{aligned} \|o_xX + o_yY\| &\leq 2(C_2 + \bar{C}_2 + C_3 + \bar{C}_3)\sqrt{\epsilon} + 12C\epsilon^{1/4}, \\ \|o_1\mathbb{1} + o_xX\| &\leq 2(C_\gamma + \bar{C}_3 + \bar{C}_4)\sqrt{\epsilon} + 12C\epsilon^{1/4}, \end{aligned}$$

where from the second relation we can write $|o_1 \pm o_x| \leq 2(C_\gamma + \bar{C}_3 + \bar{C}_4)\sqrt{\epsilon} + 12C\epsilon^{1/4}$, which implies that $|o_1|$ and $|o_x|$ are also bounded by the same number. Substituting this in the first inequality we can bound $\|o_y\|$ and then from there we can show that

$$\begin{aligned} \|O - Z\| &\leq \|O - o_zZ\| + \|o_zZ - Z\| = \|o_1\mathbb{1} + o_xX + o_yY\| + \|o_zZ - Z\| \leq \|o_1\mathbb{1} + o_xX\| + \|o_yY\| + \|o_zZ - Z\| \\ &\leq 2(C_3 + \bar{C}_3 + 2\bar{C}_4 + 2C_\gamma - 2C_2)\sqrt{\epsilon} + 12C\epsilon^{1/4}, \end{aligned}$$

where we have used the triangle inequalities and then the bounds on respective operators proved just above. Also, $|o_z \pm 1| \leq 2C_3\sqrt{\epsilon}$ because the minimum magnitude of \hat{A}_3 eigenvalues is $1 - 2C_3\sqrt{\epsilon}$. In the same way, we can get the following bound on $\|Q - X\|$:

$$\|Q - X\| \leq 2(C_\gamma + C_2 + C_3 + 2\bar{C}_2 + \bar{C}_6)\sqrt{\epsilon} + 12C\epsilon^{1/4}.$$

Substituting these relations in (A25), and by using the triangle inequalities, we get that

$$\begin{aligned} \|U^\dagger \hat{A}_3 U - X \otimes Z\| &\leq \|U^\dagger \hat{A}_3 U - X \otimes O\| + \|X \otimes O - X \otimes Z\| \leq 2(C_3 + 2\bar{C}_3 + 2\bar{C}_4 + 2C_\gamma - 2C_2)\sqrt{\epsilon} + 16C\epsilon^{1/4}, \\ \|U^\dagger \hat{A}_6 U - Z \otimes X\| &\leq \|U^\dagger \hat{A}_6 U - Z \otimes Q\| + \|Z \otimes Q - Z \otimes X\| \leq 2(C_\gamma + C_2 + C_3 + 2\bar{C}_2 + 2\bar{C}_6)\sqrt{\epsilon} + 16C\epsilon^{1/4}. \end{aligned}$$

This completes the proof. ■

Lemma 10. Suppose a nonmaximal quantum violation $5 - \epsilon$ of the inequality (7) is observed. Then, there exists a basis in the subspace V such that

$$|\langle \hat{\psi} | \phi^+ \rangle|^2 \geq 1 - (s_1\epsilon + s_2\epsilon^{3/4} + s_3\sqrt{\epsilon}), \tag{A32}$$

where s_1 and s_2 are positive constants, and $|\phi^+\rangle$ is the two-qubit maximally entangled state and $U(P|\psi\rangle) = |\hat{\psi}\rangle$.

Proof. Let us consider the following expectation value in any arbitrary state from V :

$$\begin{aligned} \langle X \otimes X \rangle &= 1 - \frac{1}{2}\|X \otimes \mathbb{1} - \mathbb{1} \otimes X\|^2 \geq 1 - \frac{1}{2}(\|X \otimes \mathbb{1} - A_1\|^2 + \|A_1 - A_4\|^2 + \|A_4 - \mathbb{1} \otimes X\|^2) \\ &\geq 1 - 2[4C_4^2 + c_4^2]\epsilon - 32c_4C\epsilon^{3/4} - 128C^2\sqrt{\epsilon}, \end{aligned}$$

where we have used triangle inequality in the first line, then used Eq. (A6) and Lemma 9 in the second line. In the same way by using Lemma 9 and Eqs. (A7) and (A8), we can show respectively that

$$\begin{aligned} \langle Z \otimes Z \rangle &\geq 1 - 2[9C_\gamma^2 + C_2^2 + c_2^2 + C_5^2]\epsilon - 4(3C_\gamma + 4c_2)C\epsilon^{3/4} - 34C^2\sqrt{\epsilon}, \\ -\langle Y \otimes Y \rangle &= 1 - \frac{1}{2}\|X \otimes Z - Z \otimes X\|^2 \geq 1 - \frac{1}{2}(\|X \otimes Z - A_3\|^2 + \|A_3 - A_6\|^2 + \|A_6 - Z \otimes X\|^2) \\ &\geq 1 - 2[c_3^2 + c_6^2 + C_3^2 + C_6^2]\epsilon - 32(c_3 + c_6)C\epsilon^{3/4} - 256C^2\sqrt{\epsilon}, \end{aligned} \tag{A33}$$

where we have used $iXZ = -iZX = Y$ with $i = \sqrt{-1}$. From the above three relations, it is straightforward to guess that the state must be of the form $|\hat{\psi}\rangle = \cos(\theta)|\phi^+\rangle + \sin(\theta)|\phi^-\rangle$, where $|\phi^-\rangle$ is orthogonal to $|\phi^+\rangle$. The lowest bound on the fidelity of $|\hat{\psi}\rangle$ with $|\phi^+\rangle$ comes from the last relation (A33). Therefore, we get

$$\cos^2(\theta) - \sin^2(\theta) \geq 1 - 2(s_1\epsilon + s_2\epsilon^{3/4} + s_3\sqrt{\epsilon}),$$

where s_1, s_2 , and s_3 denote the constant factors (divided by 2) in front of $\epsilon, \epsilon^{3/4}$, and $\sqrt{\epsilon}$ respectively in Eq. (A33). This immediately implies the following:

$$|\langle \hat{\psi} | \phi^+ \rangle|^2 = \cos^2(\theta) \geq 1 - (s_1\epsilon + s_2\epsilon^{3/4} + s_3\sqrt{\epsilon}).$$

Hence, we prove the lemma. ■

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