Certifying Sets of Quantum Observables with Any Full-Rank State

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We show that some sets of quantum observables are unique up to an isometry and have a contextuality witness that attains the same value for any initial state. We prove that these two properties make it possible to certify any of these sets by looking at the statistics of experiments with sequential measurements and using any initial state of full rank, including thermal and maximally mixed states. We prove that this "certification with any full-rank state" (CFR) is possible for any quantum system of finite dimension $d \geq 3$ and is robust and experimentally useful in dimensions 3 and 4. In addition, we prove that complete Kochen-Specker sets can be Bell self-tested if and only if they enable CFR. This establishes a fundamental connection between these two methods of certification, shows that both methods can be combined in the same experiment, and opens new possibilities for certifying quantum devices.

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Introduction.—Nonlocality [1] and contextuality [2] are two fundamental predictions of quantum theory. Quantum theory also predicts that, in certain cases, there is an essentially unique way to achieve some specific nonlocal [3–5] or contextual [6–8] correlation. Consequently, the observation of this specific correlation allows us to infer which quantum state has been prepared and which quantum observables have been measured, without making assumptions about the functioning of the devices used in the experiment [3–8].

However, none of the existing "device-independent" (DI) certification methods work if the fidelity of the prepared state with respect to a *specific pure state* is below a certain threshold. It is this specific pure state that guarantees the uniqueness of the quantum realization in the noiseless (ideal) case. In particular, none of the methods works if the prepared state is maximally mixed. This leads to the question of whether it would be possible to certify quantum observables using correlations produced by measurements on *unspecified mixed states*, including the maximally mixed state.

That, in quantum theory, this question may have an affirmative answer is suggested by the observation that, for any quantum system of finite dimension $d \geq 3$, there exist finite sets of observables that produce contextual correlations for any quantum state [9–12]. These sets of observables are called state-independent contextuality (SI-C) sets [2,13,14]. SI-C sets have fundamental applications in quantum information [15–28] and have been experimentally tested [29–34].

But the existence of SI-C sets itself leads to another question: are there SI-C sets that are unique up to an isometry? This question is particularly relevant for understanding the mathematical structure of the set of quantum observables. Interestingly, if the answer to this question is positive, then there may be a connection to the question of whether there are quantum observables that can be certified with arbitrary mixed states.

In this Letter, we first show that there are SI-C sets that (i) are unique up to an isometry, and (ii) have a SI-C witness $\mathcal{W}$ that achieves the same value for every initial quantum state. These SI-C sets have therefore a characteristic signature that can be experimentally tested: the relations of compatibility between the observables (which are encoded in the expression of $\mathcal{W}$) and the state-independent value of $\mathcal{W}$.

Next, we will show that SI-C sets with properties (i) and (ii) can be certified from the correlations of experiments with sequential measurements performed on *any full-rank mixed state*, including thermal and maximally mixed states. As soon as a mixed state of full rank gives the characteristic value for $\mathcal{W}$, any other state will do so. This leads to a method for certifying quantum observables from correlations that is fundamentally different than self-testing based on Bell inequalities [3–5], state-dependent contextuality [6–8], prepare-and-measure [35,36], and steering [37–39]. There are two fundamental differences: (a) The initial state required for the certification is not determined by the set of observables to be certified; any state of full rank can be used. (b) The certification guarantees the state-independent uniqueness (up to an isometry) of the set of observables.

In addition, we show that this new method, named certification with any full-rank state (CFR), is possible in every finite dimension $d \geq 3$, and provide a way to obtain sets of observables that enable CFR in any $d \geq 3$. We also prove that CFR is robust against experimental imperfections using examples in $d = 3$ and 4, and show how to test the robustness in any other case.

Finally, we show that, for a fundamental class of SI-C sets, CFR is a necessary condition for Bell self-testing. This points out a connection between two different forms of certification and shows that these two forms can be applied simultaneously in Bell experiments with sequential measurements. This opens up some interesting possibilities which are discussed.

Certification with any full-rank state.—Unless otherwise indicated, hereafter we will focus on SI-C sets of projectors (rather than general self-adjoint operators) and on a special type of contextuality witness that can be defined from them using the following result, which is a generalization of a result in [40], whose proof is in [13].

Lemma 1.—Given a finite set of observables $\{\Pi_i\}$, with possible results 0 or 1, and graph of compatibility G (in which each Π_i is represented by a vertex $i \in V$ and there is an edge $(i, j) \in E$ if Π_i and Π_j are compatible), the following inequality holds for any noncontextual hidden-variable (NCHV) theory:

$$\mathcal{W} \coloneqq \sum_{i \in V} w_i P_i - \sum_{(i,j) \in E} w_{ij} P_{ij} \overset{\text{NCHV}}{\leq} \alpha(G, \vec{w}), \tag{1}$$

where $\vec{w} = \{w_i\}_{i \in V}$ is a set of positive weights for the vertices of G, $w_{ij} \geq \max(w_i, w_j)$, $P_i = P(\Pi_i = 1)$ is the probability of obtaining outcome 1 when measuring observable Π_i, $P_{ij} = P(\Pi_i = 1, \Pi_j = 1)$ is the probability of obtaining outcomes 1 and 1 when measuring Π_i and Π_j, and $\alpha(G, \vec{w})$ is the weighted independence number of G with vertex weight vector $\vec{w}$ (see Ref. [13] for the definition).

Our first result is the following.

Result 1.—For any quantum system of any finite dimension $d \geq 3$, there is a finite set of observables $S = \{\Pi_i\}_{i=1}^n$ and a functional $\mathcal{W}$ such that, for any quantum state ρ, $\mathcal{W}(S, \rho) = Q$, and, if $\mathcal{W}(S', \rho') = Q$ for a set of observables $S' = \{\Pi'_i\}_{i=1}^n$ and a state ρ' of full rank in dimension D, then S' and S are equivalent in the sense that there is a unitary transformation U that, for all i,

$$\Pi_i \otimes \mathbb{1}^{d_1} \oplus \Pi_i^* \otimes \mathbb{1}^{d_2} = U \Pi'_i U^\dagger, \tag{2}$$

where $\mathbb{1}^{d_1}$ is the identity in dimension d_1, with $d_1 + d_2 = D/d$, Π_i^* is the conjugate of Π_i, $\otimes$ denotes tensor product, $\oplus$ denotes direct sum, and $U^\dagger$ is the conjugate transpose of U. Moreover, $\mathcal{W}$ is a SI-C witness since $Q > C$ and

$$\mathcal{W} \leq C \tag{3}$$

is a state-independent noncontextuality inequality.

For the witnesses $\mathcal{W}$ of the form (1), $C = \alpha(G, \vec{w})$. If those d-dimensional Π_i are real (rather than complex), then Eq. (2) becomes

$$\Pi_i \otimes \mathbb{1}^{(D/d)} = U \Pi'_i U^\dagger. \tag{4}$$

The practical consequence of Result 1 is that if, in an ideal experiment with sequential measurements, a set of n measurement devices (one for each observable), combined in sequences as dictated by the form of $\mathcal{W}$, yields $\mathcal{W} = Q$ for a state of full rank, then we can be sure that these devices implement S [or an equivalent set in the sense of Eqs. (2) or (4)]. Then, we will say that S enables CFR. The case of nonideal experiments will be discussed later.

Proof.—The proof is based on identifying sets enabling CFR in any dimension $d \geq 3$. We will name the SI-C sets using the initials of the authors and the number of projectors in the set. For example, BBC-21 [41], CEG-18 [42], and YO-13 [11]. In other cases, we use the full name rather than the initial, as in Peres-24 [43]. In other cases, we use the standard name, as in the Peres-Mermin square [44,45]. While the details of the proof are specific for each SI-C set, a common step in all proofs is showing that the violation of a full-rank state ρ' implies the same violation for any state.

The proof starts by showing that, in $d = 3$, the set of 21 rank-one projectors in Table I enables CFR. This set, hereafter called BBC-21, was introduced in [41] and is the smallest SI-C set of rank-one projectors requiring complex numbers known. The proof that BBC-21 is unique up to unitary transformations, which guarantees that condition (i) for CFR holds, is in [13]. Using the weights in the last row of Table I, the noncontextual bound of the witness $\mathcal{W}$ defined in Eq. (1) is $\alpha(G, \vec{w}) = 36$, while, for any initial quantum state, the value of $\mathcal{W}$ is $\vartheta(G, \vec{w}) = 40$. This proves that BBC-21 also satisfies condition (ii) for CFR.

In $d = 4$, we show that three related fundamental SI-C sets enable CFR: (I) CEG-18 [42], which is the smallest KS set [13] of rank-one projectors in any dimension (as proven in [46]), (II) Peres-24 [43], which is the smallest complete KS set (see Definition 4) of rank-one projectors known, and (III) the Peres-Mermin square [44,45], which is the smallest SI-C set of arbitrary self-adjoint operators (rather than projectors) known. The proofs that these sets are unique up to unitary transformations and the corresponding optimal state-independent contextuality witnesses yielding the same value for any state are in [13].

TABLE I. *BBC-21*. Each column v_i corresponds to one observable represented by the projector $|v_i\rangle\langle v_i|$. The column v_{ij} gives the components of $|v_i\rangle$ (unnormalized). $\bar{x} = -x$, $q = e^{2\pi \mathrm{i}/3}$, and $g = q^2$. Compatible observables correspond to orthogonal vectors. The last row contains optimal weights w_i for a SI-C witness $\mathcal{W}$ of the form (1). The weights w_{ij} in (1) can be chosen in any way that satisfies $w_{ij} \geq \max\{w_i, w_j\}$.

	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9	v_{10}	v_{11}	v_{12}	v_{13}	v_{14}	v_{15}	v_{16}	v_{17}	v_{18}	v_{19}	v_{20}	v_{21}
v_{i1}	0	0	0	1	1	1	1	1	1	1	0	0	1	1	1	1	1	1	1	1	1
v_{i2}	1	1	1	0	0	0	$\bar{1}$	$\bar{q}$	$\bar{g}$	0	1	0	1	q	g	1	q	g	1	q	g
v_{i3}	$\bar{1}$	$\bar{q}$	$\bar{g}$	$\bar{1}$	$\bar{q}$	$\bar{g}$	0	0	0	0	0	1	1	g	q	q	1	g	g	q	1
w_i	4	4	4	4	4	4	4	4	4	7	7	7	7	7	7	7	7	7	7	7	7

Finally, for any finite dimension $d \geq 5$, we prove (see Ref. [13]) that each of the members of a family of SI-C sets of rank-one projectors generated from Peres-24 using a method introduced in [47] is unique up to unitary transformations and has a SI-C witness producing the same value for any initial state. ■

While existing correlation-based certification methods require preparing a state with a high overlap with a target pure state, the SI-C sets that enable CFR can be certified using any unspecified full-rank state, something that is easier to prepare. A simple strategy is to let an arbitrary state go through randomly chosen measurements [34], resulting in a maximally mixed state. Another strategy is to let the system interact with the environment, resulting in a thermal state. Both types of states are of full rank.

Not all SI-C sets enable CFR. For example, Peres-33 [43], which is the KS set of rank-one projectors in $d = 3$ with the smallest number of bases known, is not unique up to unitary transformations. Interestingly, YO-13 [11], which is the SI-C set with smallest number of rank-one projectors in any dimension (as proven in [48]) and is a subset of Peres-33, enables CFR if two additional conditions are satisfied: (I') The relations of orthogonality between the elements S' are the same as the relations of orthogonality between the elements S, and (II') for ρ', the probabilities are normalized for every set of mutually orthogonal projectors summing up to the identity. This is shown in [13]. Both (I') and (II') can be experimentally tested (as in [34]).

Robustness.—The possibility of CFR of SI-C sets is a prediction of quantum theory. Now the question is whether this prediction can be tested in actual experiments or it requires idealizations that cannot be achieved in realistic experiments such as the requirement of perfectly sharp and compatible measurements for all pairs of compatible observables in the SI-C set. In other words, the question is whether CFR is robust against experimental imperfections.

Answering this question requires an additional analysis based on semidefinite programming whose size is related to the size of the SI-C sets. Here, we have performed this analysis for three of the SI-C sets, in dimensions 3 and 4, that we have proven that enable CFR. In all cases, the analysis was performed on a laptop computer and the computational execution time was less than 1 h. The analysis of the robustness of the CFR of the other SI-C sets can be carried out using higher computational power.

Our result here is that the CFRs based on BBC-21, CEG-18, and Peres-24 are robust. We will also show that the CFR of YO-13 is robust under an extra assumption. Our result requires introducing some definitions.

Definition 1.—A set of projectors $\{\Pi_i\}$ is said to be a (θ, ϵ) realization of a SI-C set with respect to a contextuality witness $\mathcal{W}$ of type (1) if, for all states $|\psi\rangle$,

$$\sum_{i=1}^{n} w_i \langle\psi|\Pi_i|\psi\rangle \geq \theta > \alpha(G, w), \tag{5a}$$

$$\langle\psi|\Pi_i \Pi_j \Pi_i|\psi\rangle \leqslant \epsilon, \tag{5b}$$

whenever i and j are adjacent in G (i.e., whenever the corresponding projectors are orthogonal).

The conditions in Eqs. (5a) and (5b) are related to the sum of probabilities $\sum_i w_i P_i$ and joint probability P_{ij} in Eq. (1). In the ideal case, $\theta = Q$ (defined in Result 1), and $\epsilon = 0$, which implies that the quantum value of $\mathcal{W}$ is Q. As θ is close enough to Q and ϵ is close enough to 0, the projectors $\{\Pi_i\}$ have the same rank. See Ref. [13] for details.

Definition 2.—A noncontextuality inequality of the form (1) provides an (ϵ, r)-robust CFR of a $(Q, 0)$ realization $\{\Pi_i\}$ of a SI-C set, if, for any $(Q - \epsilon,\ \epsilon)$ realization $\{\Pi'_i\}$ of the SI-C set, there is an isometry Φ such that

$$|\Phi(\Pi_i) - \Pi'_i| \leq \mathcal{O}(\epsilon^r). \tag{6}$$

Result 2.—The contextuality witnesses $\mathcal{W}$ of the form (1) for BBC-21, CEG-18, Peres-24, and YO-13 used in Result 1 provide $(\epsilon, 1/2)$ robustness when ϵ is smaller than 0.132, 0.134, 0.177, and 0.208, respectively. For YO-13, the proof requires the extra assumption that the probabilities of every three mutually orthogonal projectors sum 1.

For more details on the proof, see Ref. [13].

Any witness $\mathcal{W}$ of the form (1) can be expressed with the joint probabilities of the outcomes of two sequential measurements from $\{A_j\}$. From the observed values satisfying conditions related to the ideality and the orthogonality relations of the projectors, one can certify the projectors and the measurements A_i. Moreover, when the experimental value of $\mathcal{W}$ is close enough to the quantum value, the robustness of the CFR is also ensured. See Ref. [13] for more details.

Bell self-testing and CFR.—Bell self-testing [3] is the task of certifying quantum states and measurements using only the statistics of Bell experiments. One advantage of Bell self-testing with respect to CFR is that the former does not require projective measurements. One disadvantage, however, is that Bell self-testing requires spacelike separation between the tests. Therefore, an interesting question is whether SI-C sets that allow for CFR can be Bell self-tested and, if so, what is the relation between Bell self-testing and CFR. To address these questions, the following definitions will be useful.

Definition 3.—(Generalized KS set) A generalized Kochen-Specker (KS) set is a set of projectors of arbitrary rank (not necessarily of rank-one as it is the case in a KS set [49]) which does not admit an assignment of 0 or 1 satisfying that: (I) two orthogonal projectors cannot both be assigned 1, (II) for every set of mutually orthogonal projectors summing up to the identity, one and only one of them must be assigned 1.

Definition 4.—(Complete KS set) The complete KS set associated to a generalized KS set S is the set obtained by adding to S the projectors $\mathbb{1} - \Pi_i - \Pi_j$ for every pair of orthogonal projectors (Π_i, Π_j) in S that does not belong to a complete basis.

For example, Peres-24 is a complete KS set, but CEG-18 and Peres-33 are not (BBC-21 and YO-13 are not KS sets). A complete KS set enables CFR if it satisfies properties (i) and (ii).

Now we need a way to produce Bell nonlocality using a complete KS set. For that aim, we will define the following nonlocal game.

Definition 5.—(Context-projector KS game [16,17,21]) In each round of the game, a referee gives to one of the players, Alice, one of the contexts (i.e., a set of commuting projectors summing up the identity) of a complete KS set S and asks her to output one of the projectors of this context. In the same round, the referee gives to one spatially separated player, Bob, one of the projectors of the same context and asks him to output 1 or 0. Alice and Bob win the round either if Alice outputs the projector given to Bob and Bob outputs 1, or if Alice outputs a projector different than the one given to Bob and Bob outputs 0.

This is a game that cannot be won with probability 1 with classical resources and no communication, but that can be won with probability 1 if the parties share copies of a qudit-qudit maximally entangled state with $d \geq 3$ and measure a complete KS set in dimension d.

Now, we can address the question of whether the SI-C sets that allow for CFR can be Bell self-tested.

Result 3.—The projectors of a complete KS set can be Bell self-tested if and only if the KS set enables CFR.

The proof is in [13]. Here, we will focus on some implications of this result. One is that Bell self-testing and CFR can be accomplished simultaneously in an experiment that combines Bell and sequential tests [50–52]. Consider two spatially separated parties, Alice and Bob 1, sharing copies of a qudit-qudit maximally entangled state and performing local measurements of the projectors of a complete KS set S. In addition, consider a third party, Bob 2, that receives the system that Bob 1 has measured (we assume that Bob 1's measurements are nondemolition measurements [34,53]). Suppose that Bob 2 measures elements of S on this system. Then: (a) The Alice-Bob 1 statistics can Bell self-test S in Alice's and Bob 1's sides. (b) The Bob 1-Bob 2 statistics enable CFR of S in Bob 1's and Bob 2's sides (and the Alice-Bob 1 Bell self-test can guarantee that Bob 1's input state is of full rank). (c) The Alice-Bob 2 statistics conditioned to that Bob 2's measurement is compatible to Bob 1's can Bell self-test S in Alice's and Bob 2's sides. This allows for the simultaneous certification of Bob 1's S by two different methods and opens new possibilities.

Conclusions and future directions.—In this Letter, we have presented three results that push the field of certification of quantum processes based only on correlations beyond its established limits. Results 1 and 2 allow us to circumvent a conceptual limitation of existing methods, namely, the need of targeting specific pure states. We have proven that this is not necessary: for any quantum system of any finite dimension $d \geq 3$, there are sets of quantum observables that can be certified using any full-rank quantum state. This "certification with any full rank state" offers interesting possibilities. For example, suppose that the same preparation is used to certify via CFR two sets of observables: one of them in dimension d_1 and the other in dimension d_2. This automatically certifies via CFR that the dimension of the system is lower bounded by the lowest common denominator of d_1 and d_2. This provides a method to certify quantum systems of high dimensions, something that is difficult in a DI way [54,55]. Moreover, in principle, CFR becomes more useful as the dimension grows, since preparing a full-rank mixed state is easier than preparing a state with a high overlap with a pure target state.

Result 3 pushes the field in a different sense. It shows that, for a general class of sets of observables, CFR is possible if and only if Bell self-testing is possible. This indicates that there may be a general unified framework for certification based solely on correlations, so that all existing methods can be viewed as particular cases. The precise characterization of this framework constitutes an interesting challenge. On the other hand, Result 3 shows that there are sets of observables that can be simultaneously Bell self tested (using Alice-Bob 1 correlations) and certified via CFR (using Bob 1–Bob 2 correlations). This is interesting as it may lead to a robust method for self-testing Lüders processes [56,57] in any finite dimension $d \geq 3$ (which is where observables represented by rank-one projectors have one outcome whose quantum post-measurement state depends on the input state). In the framework of general probabilistic theories, Lüders processes correspond to "ideal (or sharp) measurements" [58]: processes that yield the same outcome when repeated and are minimally disturbing (only disturb incompatible observables). The existence of ideal measurements is "one of the fundamental predictions of quantum mechanics" [57]. The DI certification of ideal measurements in arbitrary (finite) dimension would require the DI certification of the corresponding quantum instruments (which capture both the classical outputs and the corresponding quantum post-measurement states [59–61]). Previous works have explored the DI [62] and semi-DI [63] certification of instruments corresponding to nonideal qubit measurements. The DI certification of ideal measurements would operationally "bridge the gap between general probabilistic theories and the DI framework" [64], blurring the boundaries between three different approaches for understanding quantum theory: DI, general probabilistic theories, and general Bayesian theories [65], where ideal measurements are central. Future research should go in these directions. Additional Refs. [66–70] are cited in the Supplemental Material [13].

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