# Robust Self-Testing of Quantum Systems via Noncontextuality Inequalities 

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#### Abstract

Characterizing unknown quantum states and measurements is a fundamental problem in quantum information processing. In this Letter, we provide a novel scheme to self-test local quantum systems using noncontextuality inequalities. Our work leverages the graph-theoretic framework for contextuality introduced by Cabello, Severini, and Winter, combined with tools from mathematical optimization that guarantee the unicity of optimal solutions. As an application, we show that the celebrated Klyachko-Can-Binicioğlu-Shumovsky inequality and its generalization to contextuality scenarios with odd $n$-cycle compatibility relations admit robust self-testing.


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Introduction.-The deployment and analysis of mathematical models have been crucial tools to advance our scientific understanding of the physical world. Nevertheless, complex mathematical models often admit a multitude of possible solutions, a phenomenon that can lead to ambiguity and erroneous predictions when the solution of the model is used to study some real-life problem. Models with no uniquely identifiable solutions manifest themselves across most fields of science and mathematics, typical examples being the nonuniqueness of solutions to partial differential equations and the existence of multiple Nash equilibria in noncooperative games. More pertinent to this work, the uniqueness of the ground state of a Hamiltonian is a problem with important engineering applications. Indeed, quantum annealing crucially relies on the uniqueness of the ground state of the underlying Hamiltonian, which is used to encode the solution of an optimization problem [1].

From a practical standpoint, the noisy nature of the collected data governing the model selection process suggests we should employ "robust" models, i.e., models that have a unique solution that is moreover stable under perturbations of the input data. Notwithstanding the ubiquitousness and importance of problems related to the unicity and robustness of the solutions of a given model, there is no general framework allowing us to address these questions in a unified manner.

One of the most extensively used modeling tools in science and engineering is mathematical optimization. In this setting, the model is specified by a family of decision variables that satisfy certain feasibility constraints. The goal is then to find the value of the decision variables that maximizes an appropriate measure of performance.

Undoubtedly, one of the most important optimization models is linear programming (LP), where the decision variables are scalar variables subject to affine constraints. An equally important optimization model is semidefinite programming (SDP), constituting a wide generalization of linear programming with extensive modeling power and efficient algorithms for solving them. Unlike linear programs, the decision variables in a SDP are vectors, and the constraints are defined in terms of the inner products of the vectors. SDPs have many important applications in physics, e.g., in quantum foundations (Bell nonlocality, contextuality, steering) [2-4], quantum information theory (entanglement witnesses, tomography, quantum state discrimination) [5-7], quantum cryptography [8], and quantum complexity [9], just to mention a few. Most importantly, the aspect of SDPs that is crucial to this work is that, like LPs, they offer a general framework for studying uniqueness and robustness of model solutions.

In this Letter, we employ the paradigm of identifiable robust models to characterize untrusted devices via contextuality. Contextuality refers to the impossibility of reproducing a set of probability distributions, each of them for a context (defined as a set of compatible and mutually nondisturbing observables) that share some marginal probabilities with a joint probability distribution in a single probability space. Quantum theory is an example of a contextual theory [10]. In this work we appropriately extend the paradigm of Bell self-testing to the framework of contextuality. In terms of techniques, our work leverages the well-known link between contextuality and semidefinite programming identified in the seminal work by Cabello, Severini, and Winter [3], combined with some
lesser-known results concerning the unicity and robustness of optimal solutions to semidefinite programs. Roughly speaking, we show that the nearness-of-optimality of the CSW semidefinite program bounds the distance in the SDP-solution space, which in turn translates into a bound on the distance from the ideal quantum realization. We believe that the tools employed in this Letter will have value outside of the domain of contextuality, e.g., see Ref. [11] for a recent application in Bell nonlocality. Our results render new insights into the foundations of quantum contextuality and a proof-of-principle approach to characterize the underlying quantum states and measurements manifesting quantum contextuality via experimental statistics. We provide an innovative scheme to attest robust self-testing for any noncontextuality inequality and present a concrete illustration for the case of the generalized KCBS inequality, which is defined for any odd number of measurement events $n \geq 5$. Lastly, in terms of applications, our results allows one to verify quantum systems locally under the following three assumptions characteristic of Kochen-Specker contextuality scenarios [10,12,13]. Assumption 1: The measurements are ideal $[14,15]$ (i.e., they give the same outcome when performed consecutive times, they do not disturb compatible measurements, all their coarse grainings admit realizations that satisfy these properties), Assumption 2: The measured system has no more memory than its information carrying capacity, each measurement device is only used once, and there is an unlimited supply of them. Assumption 3: The measurements obey the compatibility relations dictated by the odd cycle graph. In the case of Bell self-testing, it is necessary to assume that the involved parties are spacelike separated and that there is no superluminal communication [16,17], otherwise, the statistics that attain the quantum supremum of a Bell inequality [18] can be simulated using classical resources. In the same spirit, Assumption 2 is necessary in the setting of contextuality, otherwise, contextuality can be simulated by classical systems [19,20].

Self-testing in Bell scenarios.-To motivate our results, it is instructive to survey the relevant results in the setting of Bell nonlocality, a special case of contextuality where the contexts are generated by the spacelike separation of the involved parties [21]. The experimental tests that reveal the nonlocal nature of a physical theory are called Bell inequalities or Bell tests. Geometrically, a Bell inequality corresponds to a half-space that contains the set of local behaviors, i.e.,

$$
\begin{equation*}
\sum_{a, b, x, y} B_{x y}^{a b} p(a b \mid x y) \leq B_{\ell} \tag{1}
\end{equation*}
$$

for all local behaviors $p(a b \mid x y)$. The quantum supremum of the Bell inequality (1), denoted by $B_{q}$, is the largest possible value of the expression $\sum_{a, b, x, y} B_{x y}^{a b} p(a b \mid x y)$, when $p(a b \mid x y)$ ranges over the set of quantum behaviors, i.e.,

$$
p(a b \mid x y)=\langle\psi| A_{x \mid a} \otimes B_{y \mid b}|\psi\rangle
$$

for a quantum state $|\psi\rangle \in \mathcal{H}_{A} \otimes \mathcal{H}_{B}$ and quantum measurements $\left\{A_{x \mid a}\right\},\left\{B_{y \mid b}\right\}$ acting on $\mathcal{H}_{A}$ and $\mathcal{H}_{B}$, respectively. Besides their physical significance, Bell inequality violations witness the existence of certifiable randomness, and have been leveraged to power many other important information-theoretic tasks [22-24].

The feature of Bell inequalities that is most pertinent to this work is that the quantum realizations that achieve the quantum supremum of a Bell inequality are sometimes uniquely determined up to local isometries and ancilla degrees of freedom. Formally, a Bell inequality is a self-test for the realization $\left(\mathcal{H}_{A}, \mathcal{H}_{B}, \psi,\left\{A_{x \mid a}\right\},\left\{B_{y \mid b}\right\}\right)$ if for any other realization $\left(\mathcal{H}_{A^{\prime}}, \mathcal{H}_{B^{\prime}}, \psi^{\prime},\left\{A_{x \mid a}^{\prime}\right\},\left\{B_{y \mid b}^{\prime}\right\}\right)$ that also attains the quantum supremum, there exists a local isometry $V=V_{A} \otimes V_{B}$ and an ancilla state $|\mathrm{junk}\rangle$ such that

$$
\begin{align*}
V\left|\psi^{\prime}\right\rangle & =\mid \text { junk }\rangle \otimes|\psi\rangle, \\
V\left(A_{x \mid a}^{\prime} \otimes B_{y \mid b}^{\prime}\right)\left|\psi^{\prime}\right\rangle & =\mid \text { junk }\rangle\left(A_{x \mid a} \otimes B_{y \mid b}\right)|\psi\rangle \tag{2}
\end{align*}
$$

In practical terms, however, when a Bell experiment is performed in the lab, experimental imperfections will only allow us to achieve a value which is close, but not equal, to the ideal quantum supremum $B_{q}$. These practical considerations naturally lead to the notion of robust self-testing. Specifically, a Bell inequality is an $(\epsilon, r)$-robust self-test for the realization $\left(\mathcal{H}_{A}, \mathcal{H}_{B}, \psi,\left\{A_{x \mid a}\right\},\left\{B_{y \mid b}\right\}\right)$ if it is a self-test as defined above, and furthermore, whenever for some realization $\left(\mathcal{H}_{A^{\prime}}, \mathcal{H}_{B^{\prime}}, \psi^{\prime},\left\{A_{x \mid a}^{\prime}\right\},\left\{B_{y \mid b}^{\prime}\right\}\right)$,

$$
\sum_{a, b, x, y} B_{x y}^{a b}\left\langle\psi^{\prime}\right|\left(A_{x \mid a}^{\prime} \otimes B_{y \mid b}^{\prime}\right)\left|\psi^{\prime}\right\rangle \geq B_{q}-\epsilon
$$

we have that

$$
\left.\| V\left(A_{x \mid a}^{\prime} \otimes B_{y \mid b}^{\prime}\right)\left|\psi^{\prime}\right\rangle-\mid \text { junk }\right\rangle\left(A_{x \mid a} \otimes B_{y \mid b}\right)|\psi\rangle \| \leq \mathcal{O}\left(\epsilon^{r}\right)
$$

As an example, the well-known Clauser-Horne-ShimonyHolt (CHSH) Bell inequality is an $\left(\epsilon, \frac{1}{2}\right)$-robust self-test for the singlet state and appropriate Pauli measurements, e.g., see Refs. [25-28]. The term self-testing was first introduced by Mayers and Yao [26] in the setting of Bell nonlocality [16]. However, the idea underlying self-testing is present in earlier works, for example, in the works of Tsirelson [29], Summers-Werner [30], and PopescuRohrlich [25]. Recent research on self-testing moves in various new directions, e.g., which states can be self-tested [31,32] or how to tighten the robustness results, so that selftesting results have practical applications [33].

Self-testing in contextuality scenarios.-In this section we introduce a natural analogue of the notion of (robust) self-testing for contextuality scenarios, where the
noncontextuality assumption is not enforced via locality. We follow the exclusivity graph approach to contextuality [3].

A contextuality scenario is defined by a family of measurement events $e_{1}, \ldots, e_{n}$. Two events are mutually exclusive when they can be realized by the same measurement but correspond to different outcomes. To the events $\left\{e_{i}\right\}_{i=1}^{n}$ we associate their exclusivity graph, whose vertex set is $\{1, \ldots, n\}$ (denoted by $[n]$ ), and two vertices $i$, $j$ are adjacent (denoted by $i \sim j$ ) if the measurement events $e_{i}$ and $e_{j}$ are exclusive.

For an exclusivity graph $\mathcal{G}_{\mathrm{ex}}$, we consider theories that assign probabilities to the measurement events corresponding to its vertices. A behavior corresponding to $\mathcal{G}_{\text {ex }}$ is a mapping $p:[n] \rightarrow[0,1]$, where $p_{i}+p_{j} \leq 1$, for all $i \sim j$. Here, the nonnegative scalar $p_{i} \in[0,1]$ encodes the probability that measurement event $e_{i}$ occurs. Furthermore, note that the linear constraint $p_{i}+p_{j} \leq 1$ enforces that if measurement event $e_{i}$ takes place [i.e., $p\left(e_{i}\right)=1$ ], the event $e_{i+1}$ cannot take place.

A behavior $p:[n] \rightarrow[0,1]$ is deterministic noncontextual if all events have predetermined values that do not depend on the occurrence of other events. Concretely, a deterministic noncontextual behavior $p$ is a mapping $p$ : $[n] \rightarrow\{0,1\}$, where $p_{i}+p_{j} \leq 1$, for all $i \sim j$. The polytope of noncontextual behaviors, denoted by $\mathcal{P}_{n c}\left(\mathcal{G}_{\text {ex }}\right)$, is the convex hull of all deterministic noncontextual behaviors. Behaviors that do not lie in $\mathcal{P}_{n c}\left(\mathcal{G}_{\text {ex }}\right)$ are contextual. A behavior $p:[n] \rightarrow[0,1]$ is quantum if there exists a quantum state $\rho$ and projectors $\Pi_{1}, \ldots \Pi_{n}$ acting on a Hilbert space $\mathcal{H}$ where
$p_{i}=\operatorname{tr}\left(\rho \Pi_{i}\right), \quad \forall i \in[n]$ and $\operatorname{tr}\left(\Pi_{i} \Pi_{j}\right)=0$, for $i \sim j$.
We refer to the realization $\rho,\{\Pi\}_{i=1}^{n}$ satisfying (3) as a quantum realization of the behavior $p$. The convex set of all quantum behaviors is denoted by $\mathcal{P}_{q}\left(\mathcal{G}_{\text {ex }}\right)$. For the purposes of this manuscript, we will denote a quantum realization by $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$. Furthermore, $p_{i} \equiv\left|\left\langle u_{o} \mid u_{i}\right\rangle\right|^{2}, \forall i \in[n]$ and $p \in \mathcal{P}_{q}\left(\mathcal{G}_{\text {ex }}\right)$. A noncontextuality inequality corresponds to a half-space that contains the set of noncontextual behaviors, i.e.,

$$
\begin{equation*}
\sum_{i \in[n]} w_{i} p_{i} \leq B_{n c}\left(\mathcal{G}_{\mathrm{ex}}, w\right), \tag{4}
\end{equation*}
$$

for all $p \in \mathcal{P}_{n c}\left(\mathcal{G}_{\text {ex }}\right)$, where $w_{1}, \ldots, w_{n} \geq 0$. The quantum supremum of the noncontextuality inequality (4), denoted by $B_{q c}\left(\mathcal{G}_{\text {ex }}, w\right)$, is the largest value of the expression $\sum_{i \in[n]} w_{i} p_{i}$, as $p$ ranges over the set of quantum behaviors $\mathcal{P}_{q}\left(\mathcal{G}_{\text {ex }}\right)$.

Motivated by Bell self-testing, we now introduce a natural notion of "uniqueness" for the quantum realizations $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$ that attain the quantum supremum of a noncontextuality inequality. In this setting, uniqueness
refers to identifying the state and measurement operators that achieve the quantum supremum, up to a global isometry. The notion of uniqueness and robustness appropriate for our work is introduced below.

Definition 1.-(Self-testing) A noncontextuality inequality $\sum_{i \in[n]} w_{i} p_{i} \leq B_{n c}\left(\mathcal{G}_{\mathrm{ex}}, w\right)$ is a self-test for the realization $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$ if (1) $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$ achieves the quantum supremum $B_{q c}\left(\mathcal{G}_{\text {ex }}, w\right)$. (2) For any other realization $\left\{\left|u_{i}^{\prime}\right\rangle\left\langle u_{i}^{\prime}\right|\right\}_{i=0}^{n}$ that also achieves $B_{q c}\left(\mathcal{G}_{\mathrm{ex}}, w\right)$, there exists an isometry $V$ such that

$$
\begin{equation*}
V\left|u_{i}\right\rangle\left\langle u_{i}\right| V^{\dagger}=\left|u_{i}^{\prime}\right\rangle\left\langle u_{i}^{\prime}\right|, \quad 0 \leq i \leq n . \tag{5}
\end{equation*}
$$

Definition 2.-(Robustness) A noncontextuality inequality $\sum_{i \in[n]} w_{i} p_{i} \leq B_{n c}\left(\mathcal{G}_{\mathrm{ex}}, w\right)$ is an $(\epsilon, r)$-robust self-test for $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$ if it is a self-test, and furthermore, for any other realization $\left\{\left|u_{i}^{\prime}\right\rangle\left\langle u_{i}^{\prime}\right|\right\}_{i=0}^{n}$ satisfying

$$
\sum_{i=1}^{n} w_{i}\left|\left\langle u_{i}^{\prime} \mid u_{0}^{\prime}\right\rangle\right|^{2} \geq B_{q c}\left(\mathcal{G}_{\mathrm{ex}}, w\right)-\epsilon
$$

there exists an isometry $V$ such that

$$
\begin{equation*}
\| V\left|u_{i}\right\rangle\left\langle u_{i}\right| V^{\dagger}-\left|u_{i}^{\prime}\right\rangle\left\langle u_{i}^{\prime}\right| \| \leq \mathcal{O}\left(\epsilon^{r}\right), \quad 0 \leq i \leq n \tag{6}
\end{equation*}
$$

This definition of self-testing is in stark contrast to the case of Bell self-testing, where uniqueness is defined up to local isometries [recall Eq. (2)] to account for the physical operational freedom of spacelike separated parties to preprocess their local quantum systems and measurements. Furthermore, unlike the case of Bell self-testing, in contextuality scenarios there is no meaningful sense in which the state can be self-tested in isolation, rather, a state is always self-tested in relation to a measurement. On a side note, it is worth noticing that closeness between a pair of quantum realizations implies closeness of the corresponding pair of quantum behaviors.

How to show self-testing.-To show that a noncontextuality inequality is a self-test we rely on the connection with SDPs established in Ref. [3], where it was shown that the quantum supremum of a noncontextuality inequality

$$
\begin{equation*}
\max \left\{\sum_{i=1}^{n} w_{i} p_{i}: p \in \mathcal{P}_{q}\left(\mathcal{G}_{\mathrm{ex}}\right)\right\}, \tag{7}
\end{equation*}
$$

is equal to the value of the following SDP:

$$
\begin{align*}
\vartheta\left(\mathcal{G}_{\mathrm{ex}}, w\right)=\max \sum_{i=1}^{n} w_{i} X_{i i} & \\
\text { subject to } X_{i i}=X_{0 i}, & 1 \leq i \leq n \\
X_{i j}=0, & i \sim j \\
X_{00}=1, & X \in \mathcal{S}_{+}^{1+n} \tag{8}
\end{align*}
$$

where $\mathcal{S}_{+}^{1+n}$ denotes the cone of positive semidefinite matrices of size $n+1$. The optimization program (8) is known as the Lovász theta number of the vertex-weighted graph $\left(\mathcal{G}_{\text {ex }}, w\right)$ [34], where the vertex-weighted graph refers to a graph where a weight is assigned to each vertex. Moreover, the equivalence between the optimization problems (7) and (8) also induces a correspondence between their optimal solutions. Specifically, if $p \in \mathcal{P}_{q}\left(\mathcal{G}_{\text {ex }}\right)$ is optimal for Eq. (7) and $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$ is a quantum realization of $p$, the Gram matrix of the vectors $\left|u_{0}\right\rangle,\left\langle u_{0} \mid u_{1}\right\rangle\left|u_{1}\right\rangle, \ldots,\left\langle u_{0} \mid u_{n}\right\rangle\left|u_{n}\right\rangle$ corresponds to an optimal solution for Eq. (8). Conversely, for any optimal solution $X=\operatorname{Gram}\left(\left|u_{0}\right\rangle,\left|u_{1}\right\rangle, \ldots,\left|u_{n}\right\rangle\right)$ of the $\operatorname{SDP}$ (8), the realization $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right| \|\left|u_{i}\right\rangle\left\langle u_{i}\right| \|^{-1}\right\}_{i=0}^{n}$ is optimal for Eq. (7). This correspondence leads to the following three-step proof strategy for showing that the noncontextuality inequality (7) is an $\left(\epsilon, \frac{1}{2}\right)$-robust self-test. (i) First, show that the SDP (8) has a unique optimal solution $X^{*}$. (ii) Second, show that any $\epsilon$-suboptimal solution $X$ of Eq. (8), i.e., a feasible $X$ where $\sum_{i} w_{i} X_{i i} \geq \vartheta\left(\mathcal{G}_{\text {ex }}\right)-\epsilon$, satisfies $\left\|\tilde{X}-X^{*}\right\|_{F} \leq \mathcal{O}(\epsilon)$. (iii) Third, show that for two positive semidefinite matrices that are $\epsilon$ close in Frobenius distance, the vectors in their Gram decompositions are $\mathcal{O}(\sqrt{\epsilon})$ close in 2-norm.

Whenever the first step holds, the second step is satisfied for the SDP (8) and the third step is always true. The proofs of the first two steps hinge on the rich duality theory of SDPs. Specifically, the Lagrange dual of the SDP (8) is given by the least scalar $t \geq 0$ for which
$Z \equiv t E_{00}+\sum_{i=1}^{n}\left(\lambda_{i}-w_{i}\right) E_{i i}-\sum_{i=1}^{n} \lambda_{i} E_{0 i}+\sum_{i \sim j} \mu_{i j} E_{i j} \succeq 0$,
where $E_{i j}=\left(e_{i} e_{j}^{\top}+e_{j} e_{i}^{\top} / 2\right)$ and the column vectors $\left\{e_{i}\right\}_{i=0}^{n}$ form the standard basis of $\mathbb{R}^{n+1}$. Furthermore, $\lambda_{i}, w_{i}$, and $\mu_{i j}$ are the Lagrange multipliers corresponding to the constraints of the primal SDP (8). The first tool we use is a sufficient condition for showing that an arbitrary SDP admits a unique optimal solution, in terms of the existence of an appropriate optimal solution for its dual problem; see Theorem 1.2 in the Supplemental Material [35-42]. The second crucial tool are error bounds for SDPs, which allow us to bound the distance of a feasible solution from the set of optimal solutions, in terms of the suboptimality of the objective function; see Theorem 1.4 in the Supplemental Material [35]. Combining these two tools, we arrive at our main technical tool, allowing us to show that a noncontextuality inequality is a self-test:

Main Theorem.-Consider a noncontextuality inequality $\sum_{i=1}^{n} w_{i} p_{i} \leq B_{n c}\left(\mathcal{G}_{\text {ex }}, w\right)$. Assume that (1) There exists an optimal quantum realization $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$ such that

$$
\sum_{i} w_{i}\left|\left\langle u_{i} \mid u_{0}\right\rangle\right|^{2}=B_{q c}\left(\mathcal{G}_{\mathrm{ex}}, w\right)
$$

and $\left\langle u_{0} \mid u_{i}\right\rangle \neq 0$, for all $1 \leq i \leq n$, and (2) There exists a dual optimal solution $Z^{*}$ for the SDP (9) such that the homogeneous linear system

$$
\begin{align*}
M_{0, i} & =M_{i, i}, \quad \text { for all } 1 \leq i \leq n, \\
M_{i, j} & =0, \quad \text { for all } i \sim j \\
M Z^{*} & =0 \tag{10}
\end{align*}
$$

in the symmetric matrix variable $M$ only admits the trivial solution $M=0$.Then, the noncontextuality inequality is an $\left(\epsilon, \frac{1}{2}\right)$-robust self-test for $\left\{\left|u_{i}\right\rangle\left\langle u_{i}\right|\right\}_{i=0}^{n}$.

The proof of the main theorem is deferred to Sec. II in the Supplemental Material [35]. In the next section we shift our focus to a particular instance of the main theorem, namely, the KCBS noncontextuality inequalities. Specifically, we show that for the KCBS inequalities, condition (10) is satisfied and therefore, such inequalities are robust self-tests.

An application: The KCBS inequalities.-A celebrated noncontextuality inequality is the Klyachko-Can-Binicioğlu-Shumovsky (KCBS) inequality, first introduced for $n=5$ in Ref. [12] and subsequently generalized to general odd values of $n$ [43,44]. The KCBS inequality corresponds to an odd number of measurement events $e_{1}, \ldots, e_{n}$ with the property that $e_{i}$ and $e_{i+1}$ are exclusive, where indices are taken modulo $n$. The corresponding exclusivity graph is the $n$ cycle and the set of noncontextual behaviors is $\mathcal{P}_{n c}\left(C_{n}\right)$. Concretely, for any odd $n$, the $\mathrm{KCBS}_{n}$ noncontextuality inequality is given by

$$
\begin{equation*}
\max \left\{\sum_{i=1}^{n} p_{i}: p \in \mathcal{P}_{n c}\left(C_{n}\right)\right\}=\frac{(n-1)}{2} \tag{11}
\end{equation*}
$$

The $\mathrm{KCBS}_{n}$ inequality witnesses quantum contextuality, as quantum behaviors can achieve values greater than $(n-1) / 2$. Specifically, for any odd $n$, we have that

$$
\begin{equation*}
\max \left\{\sum_{i=1}^{n} p_{i}: p \in \mathcal{P}_{n c}\left(C_{n}\right)\right\}=\frac{n \cos \pi / n}{1+\cos \pi / n} \tag{12}
\end{equation*}
$$

and a quantum behavior in $\mathcal{P}_{q}\left(C_{n}\right)$ that achieves the quantum supremum of the $\mathrm{KCBS}_{n}$ inequality is

$$
\begin{equation*}
p_{i}^{(n)}=\frac{\cos \pi / n}{1+\cos \pi / n}, \quad 1 \leq i \leq n . \tag{13}
\end{equation*}
$$

A quantum realization that achieves the quantum supremum corresponds to

$$
\begin{align*}
& \left|u_{0}\right\rangle=(1,0,0)^{T} \quad \text { and } \\
& \left|u_{j}\right\rangle=\left(\cos (\theta), \sin (\theta) \sin \left(\phi_{j}\right), \sin (\theta) \cos \left(\phi_{j}\right)\right)^{T} \tag{14}
\end{align*}
$$

where $\cos ^{2}(\theta)=\{[\cos (\pi / n)] /[1+\cos (\pi / n)]\}$ and $\phi_{j}=$ $[j \pi(n-1) / n]$ for $1 \leq j \leq n$. As it turns out, the generalised

KCBS inequality satisfies the assumptions of the main theorem, and the resulting self-testing statement is formally stated as follows:

Corollary.-For any odd integer $n$, the $\mathrm{KCBS}_{n}$ inequality is an $\left(\epsilon, \frac{1}{2}\right)$-robust self-test for the realization corresponding to Eq. (14).

By the main theorem, the proof of the corollary boils down to finding a dual optimal solution satisfying Eq. (10). In Sec. III of the Supplemental Material [35], we show that for any odd integer $n$, the following matrix has the desired properties:

$$
Z_{n}^{*}=\left[\begin{array}{c|c}
\vartheta\left(C_{n}\right) & -e_{n}^{\top}  \tag{15}\\
\hline-e_{n} & I_{n}+\frac{n-\vartheta\left(C_{n}\right)}{2 \vartheta\left(C_{n}\right)} A_{C_{n}}
\end{array}\right] \in \mathbb{R}^{(1+n) \times(1+n)},
$$

where $e_{n}$ is the all-ones column vector of length $n$, and $A_{C_{n}}$ is the adjacency matrix of the cycle graph $C_{n}$.

Concretely, for $n=5$, the dual optimal solution is

$$
Z_{5}^{\star}=\left(\begin{array}{c|ccccc}
\sqrt{5} & -1 & -1 & -1 & -1 & -1  \tag{16}\\
\hline-1 & 1 & c & 0 & 0 & c \\
-1 & c & 1 & c & 0 & 0 \\
-1 & 0 & c & 1 & c & 0 \\
-1 & 0 & 0 & c & 1 & c \\
-1 & c & 0 & 0 & c & 1
\end{array}\right)
$$

where $c=(5-\sqrt{5} / 2 \sqrt{5})$. Robust self-testing for the five cycle KCBS inequality corresponds to showing that the only solution to the linear system $M_{5} Z_{5}^{\star}=0$ of the form

$$
M_{5}=\left(\begin{array}{c|ccccc}
0 & m_{1} & m_{2} & m_{3} & m_{4} & m_{5}  \tag{17}\\
\hline m_{1} & m_{1} & 0 & m_{6} & m_{9} & 0 \\
m_{2} & 0 & m_{2} & 0 & m_{7} & m_{10} \\
m_{3} & m_{6} & 0 & m_{3} & 0 & m_{8} \\
m_{4} & m_{9} & m_{7} & 0 & m_{4} & 0 \\
m_{5} & 0 & m_{10} & m_{8} & 0 & m_{5}
\end{array}\right)
$$

is the matrix of all zeros.
Conclusions.-In this work we introduced an appropriate extension of the notion of Bell self-testing to the framework of contextuality, where the noncontextuality assumption is not enforced via locality. In our main technical result, we identified a sufficient condition for showing that an arbitrary noncontextuality inequality is a robust self-test. As an application of our main theorem, we showed that the celebrated KCBS noncontextuality inequalities are robust self-tests. Our main theorem is not restricted to KCBS inequalities and can be used to self-test other noncontextuality inequalities, given they satisfy the necessary conditions; this will be the topic of future investigations. Equally important, our proof techniques leverage a largely
unnoticed connection between unicity problems in physics with uniqueness properties of optimization problems, which we believe will be of independent interest to the physics community.

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