Proof of the Peres conjecture for contextuality

Zhen-Peng Xu,1,∗ Jing-Ling Chen,2,† and Otfried Gühne1,‡

1Naturwissenschaftlich-Technische Fakultät, Universität Siegen, Walter-Flex-Straße 3, 57068 Siegen, Germany
2Theoretical Physics Division, Chern Institute of Mathematics, Nankai University, Tianjin 300071, China

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A central result in the foundations of quantum mechanics is the Kochen-Specker theorem. In short, it states that quantum mechanics cannot be reconciled with classical models that are noncontextual for compatible observables. The first explicit derivation by Kochen and Specker was rather complex, but considerable simplifications have been achieved thereafter. We propose a systematic approach to find Hardy-type and Greenberger-Horne-Zeilinger-type (GHZ-type) proofs of the Kochen-Specker theorem, these are characterized by the fact that the predictions of classical models are opposite to the predictions of quantum mechanics. With this approach, we find the provably minimal GHZ-type proof. Based on our results, we show that the Kochen-Specker set with 18 vectors from Cabello et al. [A. Cabello et al., Phys. Lett. A 212, 183 (1996)] is the minimal set for any dimension, verifying a long-standing conjecture by Peres. Our results allow to identify minimal contextuality scenarios and to study their usefulness for information processing.

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Introduction.— The fact that quantum mechanics cannot be described by noncontextual hidden variable models is known as the Kochen-Specker (KS) theorem. Since the derivation of experimentally testable inequalities [1,2], plenty of theoretical [3,6] and experimental [7,11] works have been carried out. Consequently, contextuality has been linked to tasks in quantum computation [5] and randomness generation [12], see also [13] for a review.

Bell nonlocality can be seen as a form of noncontextuality, where the locality assumption on separated observers enforces the measurements to behave in a non-contextual manner. Bell’s theorem was originally proved by the derivation of Bell inequalities [14], which hold for classical theories, but are violated in quantum mechanics. After that, however, other proofs have emerged. For instance, Hardy’s proof [15] of nonlocality without inequalities is sometimes considered to be of “the simplest form” [15]. In Hardy’s proof, one shows that certain events can never happen in a classical hidden variable model, while they can happen with a non-vanishing probability in the quantum case. An even stronger version is due to Greenberger, Horne and Zeilinger (GHZ) [16], where some events are excluded in a classical model, but they occur with certainty in the quantum case. Such examples are not only considered for mathematical clarity or beauty; in practice they give strong tests for various forms of multiparticle entanglement [18–20] and the resulting arguments are relevant for information processing. For instance, it has been shown that the building block for the original GHZ argument can be seen as a resource, enabling new computations. More precisely, GHZ correlations are the minimal resource to promote the parity computer to classical universality [21].

A key point of the Kochen-Specker theorem is that its proof can be viewed as a finite version Gleason’s theorem [22], in the sense that it shows that already for a finite collection of measurements, dispersion-free states are impossible. This raises the question for the simplest possible proof. The original proof by Kochen and Specker (KS) [23] is a proof by contradiction, where a set of 117 vectors in a three-dimensional space was used. If viewed as measurements in quantum mechanics, these vectors obey certain conditions of mutual exclusivity, which cannot be reproduced in a classical model; a set of vectors with this property is also called a KS set. In the last 30 years, a march to find simpler KS proofs has been carried out [24–26], see also [27] for an overview. In this respect, the proof of Cabello, Estebaran, and Garcia-Alcaine (CEG) using 18 vectors in a four-dimensional space is the simplest one known, and is often used as the basic explanation of theorem [28]. It was then conjectured by Peres [29] that this is indeed the optimal one, but the proof of this conjecture is still missing [30]. Besides these works, which follow the logic of the original article and construct KS sets, also Hardy-type proofs and GHZ-type proofs have been introduced [26,31], and minimal inequalities for state-independent contextuality have been derived [3,22,33].

In this paper we present a systematic method based on graph theory to construct Hardy-type and GHZ-type arguments for quantum contextuality with the minimal number of measurements. With this, we find the minimal GHZ-type proof, which needs 10 measurement events. The key observation of our approach is a connection between KS sets of vectors and GHZ-type proofs that use a subset of the vectors. Using this, we then can go on and show that 18-vector proof by CEG is indeed the optimal one in any dimension, putting the Peres conjecture at rest. The minimal GHZ-type proof and the 18-vector proof by CEG are therefore the basic building blocks of contextuality and the key to understand the role of it.
in information processing. We add that the GHZ-type argument with 10 events was noted before \cite{29} and similar graph-theoretical calculations were carried out \cite{31}, but only the connection between GHZ-type proofs and KS sets allows to draw far-ranging consequences for the Peres conjecture.

**Kochen-Specker sets of vectors.**— First, recall the notion of ideal (i.e., repeatable) measurements and events, which are a combination of an ideal measurement and one of its outcomes. In quantum theory, ideal events are represented by vectors, corresponding to a measurement outcome. Two events are said to be exclusive if, for any state, one event cannot happen if the other happens. In the quantum mechanical description, two orthogonal vectors represent a pair of exclusive events. A context is a set of compatible (i.e., non-disturbing) measurements, building a set of mutually exclusive events, and a context is said to be complete if always one event happens, whatever the input state is. For instance, in quantum mechanics the eigenvectors of an observable form a complete context, they can all be measured at the same time and exactly one result occurs.

Given these notions, one can ask whether the quantum mechanical predictions can be reproduced by a classical hidden variable model. For a given hidden variable, such a model needs to assign to any ideal event the values 1 or 0, depending on whether the event takes place or not. Here, it is natural to make the constraint of non-contextuality: The assignment should be independent of the contexts where a single event belongs to. Such a model is called a noncontextual hidden variable (NCHV) model.

The key observation of Kochen and Specker was that there are sets of vectors with given exclusivity relations, where such an NCHV assignment can not be made, these sets are then called KS sets. In the original work, a set of 117 vectors was considered \cite{23}, a simpler set was derived by Cabello and coworkers \cite{20} (see Table I and Fig. 1). The CEG set \{\ket{\psi_i}\}\sub{i=1}{18} forms 9 complete contexts, as nine orthogonal bases can be found. Consequently, any NCHV model should assign to one and only one vector the value 1 in each context, and the total number of 1-assignments is 9, an odd number. On the other hand, each vector appears twice which implies that the total number of 1-assignments should be even. Thus, we have a logical contradiction and the CEG set is a special case of a KS set.

**Different proofs of contextuality.**— In general, we call a set of vectors \{\ket{\psi_i}\} in d-dimensional space a Kochen-Specker set (KS set) if there is no 0/1-assignment (denoted by \vec{v}) that satisfies the following two conditions: (a) Two mutually exclusive events cannot both have the value 1. This means that \vec{v}_i \cdot \vec{v}_j = 0 if \ket{\psi_i} and \ket{\psi_j} are orthogonal. (b) In a complete context exactly one assignment has the value 1. This means that \sum_{i \in C} \vec{v}_i = 1, if \{|\psi_i\rangle\}_{i \in C} is a set of mutually orthogonal vectors spanning the whole space, \sum_{i \in C} |\psi_i\rangle\langle\psi_i| = 1.

The proof of quantum contextuality with a KS set is based on the structure of quantum measurements and does not rely on any quantum state. For Hardy-type and GHZ-type proofs, however, also the predictions for some quantum states become important. For a given set of events with specific exclusivity relations, we denote by \{C_k\}\sub{k=0}{K} a subset of all contexts and by \vec{p} a probability assignment to all events (coming from a classical model or quantum theory). We also write \vec{p}_{C_i} := \sum_{i \in C} p_i. Then, if for an NCHV model, \vec{p}_{C_k} = 1, \forall k = 1,2,\ldots,K \Rightarrow \vec{p}_{C_0} = 0, \tag{1}

while, under the same conditions, \vec{p}_{\bar{C}_k} can be non-zero in the quantum case, one has a Hardy-type proof of contextuality. If one can reach \vec{p}_{\bar{C}_0} = 1 in the quantum case, the Hardy-type proof is called a GHZ-type proof.

Note that in this definition \bar{C}_k’s do not need to be complete contexts. In the Bell scenario, the conditions for Hardy-type proofs are often formulated as \vec{p}_{\bar{C}_k} = 0 \cite{32}. This is no real difference, however. Since each context \bar{C}_k can be embedded in a complete context \bar{C}_k, these conditions are equivalent to \vec{p}_{\bar{C}_k \Delta \bar{C}_0} = 1. The latter form of conditions are more suitable for contextuality, where we do not embed any context in a complete one. Below, we will also recover the original Hardy-type proof in the form of Eq. (1).

**GHZ-type proofs from KS sets.**— The key observation for our approach is that any KS proof can be converted for our approach is that any KS proof can be converted.
to a GHZ-type proof with less events. Let us explain this procedure with the CEG set as an example, the detailed discussion is given in Appendix A.

If we take $\rho = |\psi_0\rangle\langle\psi_0|$ as the quantum state, then the probabilities $p_i = |\langle\psi_i|\psi_j\rangle|^2$ for the events are

$$p_0 = 1, \quad p_1 = p_2 = p_3 = p_6 = p_9 = p_{15} = p_{16} = p_{17} = 0, \quad (2)$$

where $p_9$ is due to the incomplete context $\{\emptyset, \emptyset\}$, and

$$p_4 + p_5 + p_6 = 1, \quad p_{10} + p_{11} + p_{12} = 1, \quad p_6 + p_7 + p_8 = 1, \quad p_{12} + p_{13} + p_{14} = 1, \quad p_5 + p_7 + p_{14} = 1, \quad p_4 + p_{11} + p_{13} = 1, \quad (3)$$

If an NCHV model satisfies Eq. (3), then the deterministic probability assignment with $p_k \in \{0, 1\}$ for any given hidden variable should also satisfy it. Summing over the equations, one has

$$(p_8 + p_{10}) = 6 - 2(p_4 + p_5 + p_6 + p_7 + p_{11} + p_{12} + p_{13} + p_{14}),$$

which is an even number. Since $p_8 + p_{10} \leq 1$ by exclusivity, $p_8 + p_{10} = 0$ must hold for any hidden variable. In the quantum case, however, $p_8 + p_{10} = 1$, as can be directly calculated for the state $\rho = |\psi_0\rangle\langle\psi_0|$. Thus, a GHZ-type proof has been constructed from CEG set. This GHZ-type proof consists of 10 events and 7 contexts, these are shown in Fig. 2.

Proof of optimality.— Our method of proving optimality makes use of the graph-theoretic approach to contextuality [...], where any contextuality scenario corresponds to a graph. More precisely, for a given set of events $\{e_i\}_{i \in V}$, their exclusivity relations can be represented by an exclusivity graph $G$. This consists of vertices, where two vertices $i, j$ are connected (also written as $i \bullet \bullet j$) if and only if $e_i, e_j$ are exclusive events in $V$. For example, the exclusivity graph of events in the GHZ-type proof in Fig. 2 is given in Appendix A. In this way, a probability assignment for events is automatically a value assignment for vertices in the exclusivity graph.

It’s known that the set of probability assignments for a set of events $\{e_i\}_{i \in V}$ in the NCHV model is the so-called stable set polytope $STAB(G)$ [4, 36], given by

$$STAB(G) := \text{conv} \{ v | v \in \{0, 1\}^{|V|}, v_i v_j = 0 \text{ if } i \bullet \bullet j \} ,$$

where $|V|$ is the size of $V$ and conv$\{\cdot\}$ denotes the convex hull. Similarly, the set of probability assignments in quantum mechanics is the so-called theta body $TH(G)$,

$$TH(G) := \{ v | v_i = (\bar{u}_i, 0)^2/\|\bar{u}_i\|^2, \bar{u}_i \bar{u}_j^T = 0 \text{ if } i \bullet \bullet j \} ,$$

where the $\bar{u}_i$ are real vectors of arbitrary dimension with coefficients $\bar{u}_{i,k}$ and $\|\bar{u}_i\|^2 = \bar{u}_i \bar{u}_j^T$. Physically, this means that any probability assignment can always be obtained with rank-1 projectors and a pure state, both can chosen to be real.

For an arbitrary graph, a clique is a set of pairwise connected vertices. By definition, a context just corresponds to a clique in the exclusivity graph. So, Hardy-type proofs and GHZ-type proofs can be phrased in the language of graph theory in the following way:

For a given exclusivity graph, we denote by $\{C_i\}_{i=0}^k$ a subset of all cliques. For a given value assignment $\bar{v}$, we define as above $\bar{v}|_{C_i} := \sum_{k \in C_i} v_k$. We define $Y = \{ v | v|_{C_i} = 1, \forall i = 1, 2, \ldots \}$ as the set of value assignments which satisfies all the conditions of the Hardy-type proof to be constructed, see also Eq. (1). If $\bar{v}|_{C_0} \equiv 0$ in the intersection of $Y$ and $STAB(G)$, but $\max \bar{v}|_{C_0} > 0$ in the intersection of $Y$ and $TH(G)$, then we have a Hardy-type proof. If $\max \bar{v}|_{C_0} = 1$ in the latter case, then we have a GHZ-type proof.

In fact, one only needs linear programming and semi-definite programming to check whether or not $\{C_i\}_{i=0}^k$ in a given graph provides a Hardy-type or GHZ-type proof. By exhausting all the 288266 graphs with less than 10 vertices, we find no GHZ-type proof [37]. More details about the calculations are given in Appendix C. Thus, the ten vectors in Fig. 2 constitute the minimal GHZ-type proof of contextuality.

Let’s explain details of our systematical approach using as example the exclusivity graph coming from the original
Hardy proof in a bipartite Bell scenario. We denote by $A_i$’s and $B_j$’s the measurements with two outputs $\{0,1\}$ for Alice and Bob. Then, the original Hardy proof can be phrased as

$$p(A_1 \geq B_1) = p(B_1 \geq A_2) = p(A_2 \geq B_2) = 1, \quad \implies p(A_1 < B_2) \leq \text{HV},$$

where LHV stands for local hidden variable model. While, under the same conditions, $\max p(A_1 < B_2) = (5\sqrt{5} - 11)/2 \approx 0.09$ can be achieved for entangled quantum states. Traditionally, the conditions in Eq. 6 are formulated as $p(A_1 < B_1) = 0$ etc., which is equivalent to our notation.

There are 10 events in the Hardy proof, which can be written as,

\[
\{[0,0,1,1],[0,1,0,1],[1,1,1,1], [0,0,1,1],[0,1,0,1],[1,1,1,1],
[0,0,2,1],[0,1,2,1],[1,1,2,1],
[0,0,2,2],[0,1,2,2],[1,1,2,2], \text{ and } [0,1,1,2], \tag{7}\n\]

where $[a,b,i,j]$ represents the event that the outcomes are $a, b$ for the measurements $A_i, B_j$. Then the exclusivity relations of these 10 events can be represented by the graph $G_{\text{Hardy}}$ as in Fig. 3, see also Fig. 5 in Appendix B.

Starting from $G_{\text{Hardy}}$, we only need to consider Hardy-type proofs with all vertices included, this means that the size of the minimal KS set is 18. The key idea is that to show that any KS set with 17 vectors would imply that the size of the minimal KS set is 18. The key idea is that to show that any KS set with 17 vectors would imply that

\[
\{C_i\}_{i=0}^3 = \{(9),(0,1,2),(3,4,5),(6,7,8)\}, \tag{8}\n\]

\[
\{C_i\}_{i=0}^3 = \{(9),(0,1,2),(5,6),(3,4,7,8)\}, \tag{9}\n\]

\[
\{C_i\}_{i=0}^4 = \{(9),(0,1,4,5),(2,3),(5,6),(3,4,7,8)\}. \tag{10}\n\]

In the quantum case, $0.11111 \leq \max(p_{09}) \leq 0.11112$ for all these proofs. If we assume that the vertices just represent the 10 events in Eq. 7, then Eq. 8 recovers the original Hardy proof. Its quantum bound $(5\sqrt{5} - 11)/2 \approx 0.09017$ can be found with the NPA hierarchy [36]. This value differs from our value, due to the additional constraint of locality in the NPA hierarchy.

**The proof of the Peres conjecture.**— Based on the fact the size of the minimal GHZ-type proof is 10, we prove that the size of the minimal KS set is 18. The key idea is that to show that any KS set with 17 vectors would result in a GHZ-type proof with 9 events. First, we need one technical Lemma.

**Lemma.** For a given KS set of vectors, if each vector is contained in exactly one complete context, then there should be at least four complete contexts in the whole set.

The idea of the proof is that if there are three or less complete contexts, then a classical assignment can be directly written down, details are given in Appendix B. Now we can prove the final result of this paper:

**Theorem [Peres conjecture].** The size of the minimal Kochen-Specker vector set is 18. So, the construction by Cabello, Estebaranz, and Garcia-Alcaine is optimal.

It was proven already that in three-dimensional space, any KS set should contain no less than 22 vectors, and for $d = 4$ it should contain no less than 18 vectors [39, 40]. Here we only need to consider the dimensions $d \geq 5$. The Lemma implies that we only need to consider the case where there are at least two contexts sharing at least one common vector. Because otherwise, we would have four complete contexts, meaning that the size of the KS set is at least $4d \geq 20$.

Let us say that the $d$-dimensional minimal KS set contains $n$ vectors and there are two complete contexts $C_1, C_2$ with non-empty intersection and $|\psi_0\rangle \in C_1 \cap C_2$. Since $C_1$ must contain at least two vectors which are not in $C_2$, we have $|C_1 \cap C_2| \leq d - 2$. This implies that $|C_1 \cup C_2| \geq d + 2$. Now, as above (see also Appendix A), we can assume that a system is in the quantum state $|\psi_0\rangle$, the common vector. Because otherwise, we would have four complete contexts, meaning that the size of the KS set is at least $4d \geq 20$.

For the case $d = 5$, some extra considerations are needed, details are given in Appendix B. So, the Peres conjecture is proved.

**Conclusion and Discussion.**— By proposing a systematical approach to find Hardy-type and GHZ-type proofs, we showed that the minimal size of a GHZ-type proof of contextuality is 10. Based on this, we proved the Peres conjecture for contextuality, stating that the minimal KS set consist of 18 vectors. There are several directions to extend our results. First, it would be interesting to characterize the minimal GHZ-type proofs in fixed dimensions, e.g., for $d = 3$. Here the techniques of [41, 43] may be useful. Furthermore, while we considered only KS sets of vectors (or one-dimensional projectors), one may define KS sets also using projectors of higher rank.

From the viewpoint of quantum information theory, it
would be highly desirable to study the usefulness of the minimal KS scenarios for information processing. For instance, given the quantum state $|\psi_0\rangle$ and the measurements from Fig. 2 are there any computations that can be carried out better than in a classical model? Similar questions have been discussed for measurement-based quantum computation [21, 44], and the answer may shed light on the role of contextuality in quantum computing.

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Appendix A: From KS sets to GHZ-type proofs

In this section we will explain in detail how any KS set of vectors can be converted into a GHZ-type proof. Let us recall the strategy. Starting from an KS set (as in Fig. 1) we take one arbitrary vector (here, the vector $|\psi_0\rangle$) from the set, and assume this as a quantum state. Then, we remove the vector $|\psi_0\rangle$ and all the vectors orthogonal to it from the set. This, of course, transforms some of the complete contexts in the original KS set into incomplete ones, as also happens in Fig. 2. It remains to show that the reduced graph gives rise to a GHZ-type proof. This was explicitly calculated for the CEG set in Eqs. (3), but for a general initial KS set a more general argument is required.

In the language of graph theory, a KS proof can be expressed as follows. For a given graph $G$ and a set $\{C_k\}_{k=0}^K$ of maximal cliques in $G$, we have a set of conditions for a probability assignment $\vec{p}$ of $G$

- completeness: $\vec{p}|C_k = 1, \forall k = 0, \ldots, K$,
- exclusivity: $p_i p_j = 0$, if $i \cdot \cdot \cdot j, \forall i, j$. (A1)

If all conditions in Eq. (A1) cannot be fulfilled simultaneously in an NCHV model, while they are satisfied by the probability assignment $\vec{p}$ induced by $p_i := \langle \psi_i|\rho|\psi_i\rangle$ for a given set $\{|\psi_i\rangle\}$ of vectors and any state quantum $\rho$, then we have a KS proof.

Such a KS proof is said to be tight if all the conditions can be satisfied simultaneously by an NCHV model after removing a single (but arbitrary) completeness condition. Any KS proof can always be transformed into a tight KS proof by removing the redundant completeness conditions step by step from the original set. So, we can assume without loosing generality that the KS proof is tight.

Let us take from an NCHV model the probabilities $\vec{p} = \sum_{\lambda \in \Lambda} h(\lambda)\vec{p}_\lambda$, given as the convex decomposition of $\vec{p}$ into the deterministic probability assignments $\vec{p}_\lambda$ associated with fixed hidden variables, where $\mu(\lambda) > 0$ and $\sum_{\lambda \in \Lambda} \mu(\lambda) = 1$. Then, for any complete context

$$1 = \vec{p}|C_k = \sum_{\lambda \in \Lambda} \mu(\lambda)\vec{p}_\lambda|C_k \implies \vec{p}_\lambda|C_k = 1, \forall \lambda. \quad (A2)$$

If we assume that all the exclusivity conditions are satisfied, then we can take for the $K+1$ complete contexts an arbitrary ordering $\{C_{k_i}\}_{i=0}^K$, and, since the proof is tight, the relations $\vec{p}|C_{k_i} = 1, \forall i = 1, \ldots, t$ are possible in an NCHV model, but then it’s not possible anymore to obey the condition $\vec{p}|C_{k_0} = 1$. In fact,

$$\vec{p}|C_{k_i} = 1, \forall i = 1, \ldots, K \implies \vec{p}|C_{k_i} = 1, \forall i = 1, \ldots, t \implies \vec{p}|C_{k_0} = 0 \implies \vec{p}|C_{k_0} = 0. \quad (A3)$$

Thus, we have a GHZ-type proof, as $\vec{p}|C_{k_0} = 1$ holds for any quantum state. But this proof is state-independent and still has the same number of events as the KS set.

If we take any state $|\psi_i\rangle$ where $i \notin C_{k_0}$ as a quantum state, we have

$$p_i = 1, p_j = 0, \text{ if } i \cdot \cdot \cdot j, \forall j. \quad (A4)$$

Hence, by assuming the additional exclusivity conditions in Eq. (A4), we can simplify the GHZ-type proof in Eq. (A3). Events related with vertices $\{i\} \cup \{j\} \cdot \cdot \cdot j, \forall j\}$ can be removed from the GHZ-type proof in Eq. (A3). This implies that all vectors in the contexts where $|\psi_i\rangle$ belongs to, disappear. Other contexts $C_{k_j}$ with $\ell = 0, \ldots, K$ are not complete anymore, but this does not change the logic from Eq. (A3). So we arrive at the desired state-dependent GHZ-type proof. Finally, since the choice of the set $C_{k_0}$ is arbitrary, the choice of $|\psi_i\rangle$ also is.

Appendix B: Examples of exclusivity graphs

In this section we present in detail the exclusivity graphs for two important examples in the main text. Fig. 3 shows the exclusivity graph of events used in the GHZ-type proof in Fig. 2 in the main text. Fig. 5 presents the exclusivity graph of events used in the original Hardy-type proof, see Fig. 3 in the main text.
For any set of probabilities $\vec{v}$ is said to be maximal if it is not a subset of any other set of probabilities $\vec{v}'$. An independent set $I$ of $G$ is a set of vertices, in which any two vertices are not connected. An independent set $I$ is said to be maximal if it is not a subset of any other independent set. By definition, $STAB(G) = \text{conv}\{I | I \in \mathcal{I}\}$.

For a set of probabilities $\vec{v} \in STAB(G)$ and any clique $C$, one has $\vec{v}|_C \leq 1$. If we write $\vec{v} = \sum_{i=1}^t x_i \mathbb{I}_{I_i}$ with $x_i > 0$, then $\vec{v} \in \mathcal{V} \implies x_i \mathbb{I}_{I_i} \in \mathcal{V}, \forall i = 1, \ldots, t$.

For two independent sets $I_1$ and $I_2$ with $I_1 \subseteq I_2$ we have $\mathbb{I}_{I_1} \in \mathcal{V} \implies \mathbb{I}_{I_2} \in \mathcal{V}$. By definition, $\mathbb{I}_I \in \mathcal{V} \cap STAB(G)$ means that the independent set $I$ has non-empty intersection with each $C_i$ for $i = 1, \ldots, k$. On the other hand, $\mathbb{I}_I|C_0 = 0$ is equivalent to $I \cap C_0 = \emptyset$. Hence, to check whether $\vec{v}|_{C_0} = 0$ for any $\vec{v}$ in the intersection of $\mathcal{V} \cap STAB(G)$, we can just calculate

$$I_{\text{pre}} := \{I | I \cap C_i \neq \emptyset, \forall i = 1, \ldots, k\} \cap I_{\text{max}},$$

where $I_{\text{max}}$ is the set of all maximal independent sets. Then we check whether the sets $I_{\text{pre}}$ and $\cup_{i \in I_{\text{pre}}} I \cap C_0$ are empty or not.

If $\cup_{i \in I_{\text{pre}}} I \cap C_0 = \emptyset$, we have $\vec{v}|_{C_0} \equiv 0, \forall \vec{v} \in \mathcal{V} \cap STAB(G)$. If $I_{\text{pre}}$ is empty, then it implies that we already have an candidate of Hardy-type proof by choosing one $C_i$ as the new $C_0$ while keeping the rest $C_i$’s as conditions.

2. Quantum mechanics: $\mathcal{V} \cap TH(G)$

In quantum theory, we have to calculate

$$\max : \vec{v}|_{C_0}$$

subject to: $\vec{v}|_C = 1, \forall i = 1, \ldots, k$

$$\vec{v} \in TH(G)$$

For a set of probabilities $\vec{v} \in TH(G)$ in the theta body we have by definition $v_i = (\hat{u}_{i,0})^2/\|\hat{u}_i\|^2$ where $\hat{u}_i\hat{u}_j = 0$ if $i \bullet \bullet j$. This implies that

$$T := \begin{bmatrix} 1 & \vec{v}^T \\ \vec{v} & A \end{bmatrix} \succeq 0$$

where the entries of the matrix $A = (A_{ij})$ are given by $A_{ij} = (\bar{s}\hat{u}_i^T \hat{u}_j \hat{u}_j^T \bar{s}^T)/\|\hat{u}_i\|^2\|\hat{u}_j\|^2$ and $\bar{s} = (1, 0, \ldots, 0)$. Hence, $A_{ii} = v_i$ and $A_{ij} = 0$ if $i \bullet \bullet j$. The positivity of $T$ follows from the fact $T = P^T P$, where the columns of $P$ are

$$P = [\bar{s}^T \ (\hat{u}_1^T \hat{u}_1 \bar{s}^T)/\|\hat{u}_1\|^2 \cdots (\hat{u}_n^T \hat{u}_n \bar{s}^T)/\|\hat{u}_n\|^2].$$

Conversely, consider that we have a positive definite semidefinite matrix $T$ as in Eq. (C7), where $\text{diag}(A) = \vec{v}$ and $A_{ij} = 0$ if $i \bullet \bullet j$. Then, using the Cholesky decomposition, $T$ can always be decomposed as $T = P^T P$ where the columns of $P$ can be written as $P = [\bar{s}^T \ \tilde{s}^T \ \ldots \ \tilde{s}^T]$. The fact that $\text{diag}(A) = \vec{v}$ and the structure of the matrix in Eq. (C7) implies that $v_i = \|\tilde{s}_i\|^2 = \tilde{s}_i \bar{s}^T$. So we have $v_i = (\tilde{s}_i \bar{s}^T)^2/\|\tilde{s}_i\|^2$. If $i \bullet \bullet j$, then $A_{ij} = 0 = \tilde{\mu}_i \tilde{\mu}_j^T$. Hence, $\vec{v} \in TH(G)$ if the quantum state is described by the vector $\bar{s}$.

Thus, the condition $\vec{v} \in TH(G)$ is equivalent to

$$\begin{bmatrix} 1 & \vec{v}^T \\ \vec{v} & A \end{bmatrix} \succeq 0, \ \text{diag}(A) = \vec{v}, \ A_{ij} = 0, \ \text{if} \ i \bullet \bullet j.$$
The whole semi-definite program for the quantum case is
\[
\begin{aligned}
&\max : \vec{\alpha}_i^0 \\
&\text{subject to : } \vec{\alpha}_i^0 = 1, \forall i = 1, \ldots, k, \\
&\begin{bmatrix} 1 & \vec{\alpha} \\ \vec{\alpha}^T & A \end{bmatrix} \succeq 0, \\
&\text{diag}(A) = \vec{\alpha}, \\
&A_{ij} = 0, \text{ if } i \neq j. \\
\end{aligned}
\tag{C10}
\]

Appendix D: Proofs of the Lemma and the Theorem

In this section, we give the detailed proofs of the Lemma and the Theorem in the main text. We repeat the statements here for better readability.

**Lemma.** For a given KS set of vectors, if each vector is contained in exactly one complete context, then there should be at least four complete contexts in the whole set.

**Proof.** Assume that there are only three different complete contexts $C_1, C_2, C_3$ without any intersection. We can always pick $|\psi_1\rangle \in C_1$ and $|\psi_2\rangle \in C_2$ such that $\langle \psi_1 | \psi_2 \rangle \neq 0$. Let us denote by $C_3^{i} := \{|\psi\rangle \mid |\psi\rangle \in C_3, \langle \psi | \psi_i \rangle \neq 0\}$ for $i = 1, 2$ the vectors in $C_3$ which are not orthogonal to $|\psi_1\rangle$ or $|\psi_2\rangle$. The sets $C_3^{i}$ contain each at least two vectors, and the subspace corresponding to $|\psi_i\rangle$ is included in the one spanned by vectors in $C_3^{i}$ for $i = 1, 2$. Since $\langle \psi_1 | \psi_2 \rangle \neq 0$ we must have $C_3^{1} \cap C_3^{2} \neq \emptyset$ and we take a vector $|\psi_3\rangle$ in it. By assigning $1$'s to $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle$, and $0$'s to all the remaining vectors, we have an invalid $0$-$1$ assignment. So, there is no KS proof in this case. \hfill \Box

**Theorem [Peres conjecture].** The size of the minimal Kochen-Specker vector set is $18$. So, the construction by Cabello, Estebaranz, and Garcìa-Alcaine is optimal.

**Proof.** It was proven already that in three-dimensional space, any KS set should contain no less than $22$ vectors, and for $d = 4$ it should contain no less than $18$ vectors. Here we only need to consider the dimensions $d \geq 5$. The Lemma implies that we only need to consider the case where there are at least two contexts sharing at least one common vector. Because otherwise, we would have four complete contexts, meaning that the size of the KS set is at least $4d \geq 20$.

Let us say that the $d$-dimensional minimal KS set contains $n$ vectors and there are two complete contexts $C_1, C_2$ with non-empty intersection and $|\psi_0\rangle \in C_1 \cap C_2$. Since $C_1$ must contain at least two vectors which are not in $C_2$, we have $|C_1 \cap C_2| \leq d - 2$. This implies that $|C_1 \cup C_2| \geq d + 2$. Now, as above (see also Appendix A) we can assume that a system is in the quantum state $|\psi_0\rangle$, remove the vectors in $|C_1 \cup C_2|$ and arrive at a GHZ-type proof. This GHZ-type proof would have maximally $n - (d + 2)$ vectors, but as we know, it must contain $10$ vectors. This proves that $n \geq 18$ if $d \geq 6$.

It remains to consider the dimension $d = 5$ and here two conditions on possible KS sets with less than $18$ vectors can be derived. First, if there are two complete contexts $C_1, C_2$ in the KS set such that they share one or two vectors, then we have that $|C_1 \cup C_2| \geq 8$. This implies, as before, $n \geq 8 + 10 = 18$. Since in $d = 5$ two different contexts have maximally three vectors in common, it follows that for all $i, j$ we have $|C_i \cap C_j| \in \{0, 3\}$ (first condition).

Second, consider the case that a vector is in two complete contexts, $|\psi_0\rangle \in C_1 \cap C_2$ and there is a vector $|\psi_1\rangle$ in the KS set that is orthogonal to $|\psi_0\rangle$, but $|\psi_1\rangle \notin C_1 \cap C_2$. Then we may choose $|\psi_0\rangle$ as a quantum state and remove the 7 vectors in $C_1 \cup C_2$ as well as $|\psi_1\rangle$ and arrive at a GHZ-type proof. So also in this case $n \geq 18$, and it follows that a vector like $|\psi_1\rangle$ cannot exist (second condition).

We now show that there must be three overlapping contexts. If this were not the case, we would have a given complete context, say $C_1$, such there is at most one other complete context $C_2$ that has non-empty intersection with it, and $C_2$ has no intersection with further complete contexts. If there is a feasible $0$-$1$ value assignment to the vectors which are not in $C_1 \cup C_2$, then we can just assign the value $1$ to one vector $|\psi_0\rangle$ in $C_1 \cap C_2$ and $0$ to the remaining vectors in $C_1 \cup C_2$. This will result in a valid global $0$-$1$ value assignment, satisfying the completeness relations and the exclusivity relations for the original KS set, due to the second condition. But such a global assignment is not possible, as we have a KS set. It follows that already an assignment for the vectors which are not in $C_1 \cup C_2$ is not possible, this implies that we can have a simplified KS set by removing the vectors in $C_1 \cup C_2$. But this in contradiction to the optimality of the KS set.

So, we are left with the situation that there is a complete context $C_1$ which has intersection with two different complete contexts $C_2$ and $C_3$. Since $|C_1 \cap C_2| = |C_1 \cap C_3| = 3$ we must have $|C_1 \cap C_2 \cap C_3| \geq 1$. So we can take $|\psi_0\rangle \in C_1 \cap C_2 \cap C_3$. Let us consider the set $C_1 \cup C_2 \cup C_3$. If this consists of eight or more vectors, we can take as usual $|\psi_0\rangle$ as a quantum state and remove the vectors in $C_1 \cup C_2 \cup C_3$, arriving at a GHZ-type proof. So, in this case we have $n \geq 18$.

It may be, however, that $C_1 \cup C_2 \cup C_3$ consists of seven vectors only. Then, up to some permutations, we can assume that these vectors are given by $I = \{|\psi_0\rangle, \ldots, |\psi_7\rangle\}$ and we have $C_1 = \{|\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle\}$, $C_2 = \{|\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle\}$, and $C_3 = \{|\psi_0\rangle, |\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle\}$. Now, there must be a fourth context $C_4$, containing a vector from the set $I$. Otherwise, due to the second condition, any proper $0$-$1$ assignment to the vectors outside of $I$ can be extended to an assignment of the full KS set (by assigning $1$ to $|\psi_0\rangle$ and $0$ to the rest in $I$), and the KS set cannot be minimal.
Since $C_4$ contains a vector from $\mathcal{I}$, it has overlap with two $C_i$, so let us assume that $C_4 \cap C_i \neq \emptyset \neq C_4 \cap C_j$. But then, considering the contexts $C_1, C_2, C_4$, an argument as above shows that either $n \geq 18$ or $|C_1 \cup C_2 \cup C_4| = 7$, implying that $C_4 \subset \mathcal{I}$. But the latter is not possible, one cannot find four different complete contexts in the seven element set $\mathcal{I}$ such that the first condition holds. So, the Peres conjecture is proved.

□

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