From the Kochen-Specker Theorem to Noncontextuality Inequalities without Assuming Determinism

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The Kochen-Specker theorem demonstrates that it is not possible to reproduce the predictions of quantum theory in terms of a hidden variable model where the hidden variables assign a value to every projector deterministically and noncontextually. A noncontextual value assignment to a projector is one that does not depend on which other projectors—the context—are measured together with it. Using a generalization of the notion of noncontextuality that applies to both measurements and preparations, we propose a scheme for deriving inequalities that test whether a given set of experimental statistics is consistent with a noncontextual model. Unlike previous inequalities inspired by the Kochen-Specker theorem, we do not assume that the value assignments are deterministic and therefore in the face of a violation of our inequality, the possibility of salvaging noncontextuality by abandoning determinism is no longer an option. Our approach is operational in the sense that it does not presume quantum theory: a violation of our inequality implies the impossibility of a noncontextual model for *any* operational theory that can account for the experimental observations, including any successor to quantum theory.

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An ontological model of operational quantum theory [1] associates to each quantum system a set of physical or "ontic" states, to each preparation procedure a probability distribution over such ontic states, and to each measurement procedure a conditional probability distribution over its outcomes for each ontic state. Contrary to naïve impressions, such models have no difficulty reproducing quantum predictions *unless* additional assumptions are made. The Kochen-Specker theorem [2] derives a contradiction from an assumption we term KS noncontextuality. Consider a set of measurements, each represented by an orthonormal basis, where some rays are common to more than one basis. Every ontic state assigns a definite value to each ray, 0 or 1, regardless of the basis (i.e., context) in which the ray appears. If a ray is assigned value 1 (0) by an ontic state λ, the measurement outcome associated with that ray occurs with probability 1 (0) when any measurement including the ray is implemented on the system in ontic state λ. Hence, for every basis, precisely one ray must be assigned the value 1 and the others 0.

Unlike the Kochen-Specker theorem, determinism is not an assumption of Bell's theorem [3,4], as is evident from derivations of the CHSH inequality [5]. Even in Bell's 1964 article [3], where deterministic assignments are used, determinism is not assumed but rather *derived* from local causality and the fact that quantum theory predicts perfect correlations if the same observable is measured on two parts of a maximally entangled state (an argument from EPR [6] that Bell recycled [7]). Similarly, rather than assuming determinism in noncontextual models, one can derive it [11] from a generalized notion of noncontextuality and from two facts about quantum theory: (i) the outcome of a measurement of some observable is perfectly predictable whenever the preceding preparation is of an eigenstate of that observable, and (ii) the indistinguishability, relative to all quantum measurements, of different convex decompositions of the completely mixed state into pure states.

Hence, in the Kochen-Specker theorem one can replace the assumption of determinism with the generalized notion of noncontextuality and the quantum prediction of perfect predictability. If perfect predictability is observed, then in the face of the resulting contradiction, one must abandon noncontextuality: one cannot salvage it by abandoning determinism.

Of course, no real experiment ever yields *perfect* predictability, so this manner of ruling out noncontextuality is not robust to experimental error. Following ideas introduced in recent work [12], we show how to contend with the lack of perfect predictability of measurements and how to derive an experimentally robust noncontextuality inequality for any uncolorability proof of the Kochen-Specker theorem.

Review of the Kochen-Specker theorem.—The original proof of the KS theorem required 117 rays in a 3d Hilbert space [2]. We use the simpler proof in Ref. [13], requiring a 4d Hilbert space and 18 rays that appear in 9 orthonormal bases, each ray appearing in two bases [Fig. 1(a)]. There is no 0-1 assignment to these rays that respects KS

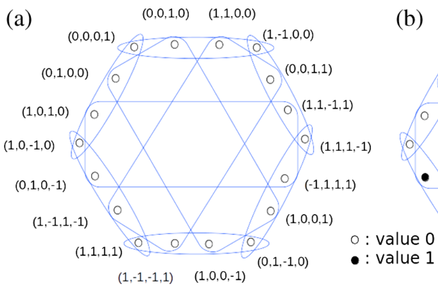

FIG. 1 (color online). Each of the 18 rays is depicted by a node, and the 9 orthonormal bases are depicted by 9 edges, each enclosing 4 nodes. There is no KS-noncontextual assignment to these nodes. For instance, a noncontextual assignment of 0*s* and 1*s* to 17 of the nodes cannot be completed to an assignment to all 18 because neither 0 nor 1 can be assigned to the remaining node (marked X): one edge enclosing it requires it to be 0, the other 1.

noncontextuality: the hypergraph is uncolorable [Fig. 1(b)]. Of course, if the value assigned to a ray were allowed to be 0 in one basis and 1 in the other (KS contextuality) then there is no contradiction.

Can the possibility of a KS-noncontextual ontological model be tested experimentally? One view is that it cannot, that the KS theorem merely constrains the possibilities for *interpreting* the quantum formalism [14,15]. This answer, however, is inadequate. One *can* and *should* ask, what is the minimal set of operational predictions of quantum theory that need to be experimentally verified in order to show that it does not admit of a noncontextual model?

We show that this minimal set is a far cry from the whole of quantum theory and is therefore consistent with other possible operational theories. As such, our no-go result shows that none of these theories admits of a noncontextual model. Therefore, if corroborated by experiment, it implies that any future theory of physics that might replace quantum theory also fails to admit of a noncontextual model.

An operational theory is a triple $(\mathcal{P}, \mathcal{M}, p)$ where $\mathcal{P}$ is a set of preparations, $\mathcal{M}$ is a set of measurements, and p specifies, for every pair of preparation and measurement, the probability distribution over outcomes for that measurement if it is implemented on that preparation. Denoting the set of outcomes of measurement M by $\mathcal{K}_M$, we have $\forall\ P \in \mathcal{P}$, $\forall\ M \in \mathcal{M}$, $p(\cdot|P, M) : \mathcal{K}_M \to [0, 1]$.

An ontological model of an operational theory $(\mathcal{P}, \mathcal{M}, p)$ is a triple (Λ, μ, ξ), where Λ denotes a space of possible ontic states for the physical system, μ specifies a probability distribution over the ontic states for every preparation procedure, that is, $\forall\ P \in \mathcal{P}, \mu(\cdot|P) : \Lambda \to [0, 1]$, such that $\sum_{\lambda\in\Lambda} \mu(\lambda|P) = 1$, and ξ specifies, for every measurement, the conditional probability of obtaining a given outcome if the system is in a particular ontic state, that is, $\forall\ M \in \mathcal{M}, \xi(k|M, \cdot) : \Lambda \to [0, 1]$, such that $\sum_{k\in\mathcal{K}_M} \xi(k|M, \lambda) = 1$. The ontological model should reproduce the statistical predictions of the operational theory:

$$p(k|P, M) = \sum_{\lambda\in\Lambda} \xi(k|M, \lambda)\mu(\lambda|P) \tag{1}$$

for all $P \in \mathcal{P}$, and $M \in \mathcal{M}$.

We denote the event of obtaining outcome k of measurement M by $[k|M]$. If M is assigned a deterministic outcome by every ontic state in the ontological model, i.e., if $\xi(k|M, \cdot) : \Lambda \to \{0, 1\}$, then it is said to be outcome-deterministic in that model.

We explain how to derive an experimental test of noncontextuality using a sequence of four refinements on the standard account of the KS theorem.

Operationalizing KS noncontextuality.—In a KS-noncontextual model of operational quantum theory, the value (0 or 1) assigned to the event $[k|M]$ by λ is the same as the value assigned to $[k'|M']$ whenever these two events correspond to the same ray of Hilbert space (here, M and M' are assumed to be maximal projective measurements). We get to the crux of KS noncontextuality, therefore, by describing the operational grounds for associating the same ray to $[k|M]$ as is associated to $[k'|M']$. Letting $\Pi_{k|M}$ and $\Pi_{k'|M'}$ represent the corresponding rank-1 projectors, the grounds for concluding that $\Pi_{k|M} = \Pi_{k'|M'}$ are that $\mathrm{tr}(\rho\Pi_{k|M}) = \mathrm{tr}(\rho\Pi_{k'|M'})$ for an appropriate set of density operators ρ. It is clearly sufficient for the equality to hold for the set of *all* density operators, but it is also sufficient to have equality for certain smaller sets of density operators, namely, those complete for measurement tomography.

What then should the operational grounds be for assigning the same value to $[k|M]$ and $[k'|M']$ in a general operational theory, where preparations are not represented by density operators? The answer, clearly, is that the event $[k|M]$ *occurs with the same probability* as the event $[k'|M']$ for *all* preparation procedures of the system,

$$p(k|M, P) = p(k'|M', P) \quad \text{for all } P \in \mathcal{P}, \tag{2}$$

or equivalently, if this holds for a subset of $\mathcal{P}$ that is tomographically complete. In this case, we shall say that $[k|M]$ and $[k'|M']$ are operationally equivalent, and denote this as $[k|M] \simeq [k'|M']$. We can therefore define a notion of KS noncontextuality for any operational theory as follows: an ontological model (Λ, μ, ξ) of an operational theory $(\mathcal{P}, \mathcal{M}, p)$ is KS noncontextual if (i) operational equivalence of events implies equivalent representations in the model, i.e., $[k|M] \simeq [k'|M'] \Rightarrow \xi(k|M, \lambda) = \xi(k'|M', \lambda)$ for all $\lambda \in \Lambda$, and (ii) the model is outcome-deterministic, $\xi(k|M, \cdot) : \Lambda \to \{0, 1\}$.

The operational equivalences among measurements required for the KS construction in Fig. 1(a) are made explicit in Fig. 2(a), where every measurement event $[k|M]$ is represented by a distinct node, and a novel type of edge between nodes specifies operational equivalence between events. This affords a nice depiction of contextual value assignments, as in Fig. 2(b). It follows that *any* operational

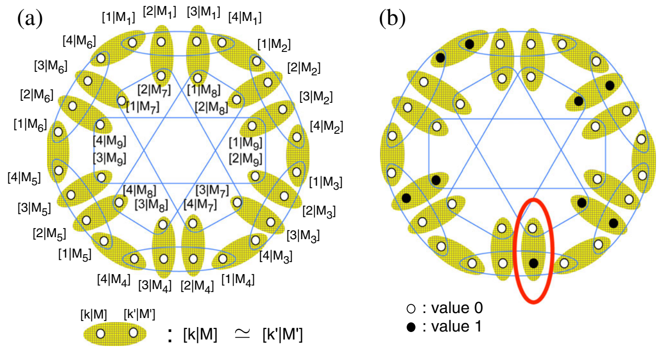

FIG. 2 (color online). (a) Nine four-outcome measurements, each depicted by a set of four nodes encircled by a blue loop. A yellow hashed region enclosing a set of nodes implies that the corresponding events are operationally equivalent. (b) An illustration of the fact that there is no outcome-deterministic noncontextual assignment to the measurement events. The depicted outcome-deterministic assignment breaks the assumption of noncontextuality for the highlighted pair.

theory with 9 four-outcome measurements satisfying the operational equivalences depicted in Fig. 2(a) fails to admit of a KS-noncontextual model.

Defining noncontextuality without outcome determinism.—The essence of noncontextuality is that context independence at the operational level should imply context independence at the ontological level. The operationalized version of KS noncontextuality, however, makes an additional assumption about what sort of thing should be context independent at the ontological level, namely, a deterministic assignment of an outcome. However, one can equally well assume that the ontic state merely assigns a probability distribution over outcomes, and take *this distribution* to be the thing that is context independent. In Ref. [11], this revised notion of noncontextuality was termed "measurement noncontextuality." Measurement noncontextuality is satisfied by an ontological model (Λ, μ, ξ) of an operational theory $(\mathcal{P}, \mathcal{M}, p)$ if $[k|M] \simeq [k'|M']$ implies $\xi(k|M, \lambda) = \xi(k'|M', \lambda)$ for all $\lambda \in \Lambda$. Here, $\xi(k|M, \cdot) \in [0, 1]$, so that outcome determinism is not assumed.

Justifying outcome determinism for perfectly predictable measurements.—Outcome determinism can, however, be justified sometimes if one assumes a notion of noncontextuality for *preparations* [11]. First, a definition: P and P' are said to be operationally equivalent, denoted $P \simeq P'$, if for every measurement event $[k|M]$, P assigns the same probability to this event as P' does, that is,

$$p(k|M, P) = p(k|M, P') \text{ for all } k \in \mathcal{K}_M, \text{ for all } M \in \mathcal{M}. \tag{3}$$

A preparation-noncontextual ontological model is then defined as follows. Preparation noncontextuality is satisfied by an ontological model (Λ, μ, ξ) of an operational theory $(\mathcal{P}, \mathcal{M}, p)$ if $P \simeq P'$ implies $\mu(\lambda|P) = \mu(\lambda|P')$ for all $\lambda \in \Lambda$.

Insofar as both measurement and preparation noncontextuality are inferences from operational equivalence to ontological equivalence, it is most natural to assume *both*, that is, to assume universal noncontextuality [17].

Reference [11] showed that in a preparation-noncontextual model of quantum theory, all projective measurements must be represented outcome-deterministically. Here, we provide a version of this argument for the 18 ray construction.

Suppose that one has experimentally identified 36 preparation procedures organized into 9 ensembles of 4 each, $\{P_{i,k} : i \in \{1, \ldots, 9\}, k \in \{1, \ldots, 4\}\}$, such that for all i, measurement M_i on preparation $P_{i,k}$ yields the kth outcome with certainty,

$$\forall\ i, \forall\ k : p(k|M_i, P_{i,k}) = 1. \tag{4}$$

We call this property "perfect predictability." In quantum theory, it suffices to let $P_{i,k}$ be the preparation associated with the pure state corresponding to the kth element of the ith measurement basis.

Define the effective preparation $P_i^{(\mathrm{ave})}$ as the procedure obtained by sampling k uniformly at random and then implementing $P_{i,k}$. Suppose one has experimentally verified the operational equivalences (Fig. 3)

$$P_i^{(\mathrm{ave})} \simeq P_{i'}^{(\mathrm{ave})} \quad \text{for all } i, i' \in \{1, \ldots, 9\}. \tag{5}$$

They hold in our quantum example because each $P_i^{(\mathrm{ave})}$ corresponds to the completely mixed state.

Given Eq. (5) and the assumption of preparation noncontextuality, there is a single distribution over Λ, denoted $\nu(\lambda)$, such that

$$\mu(\lambda|P_i^{(\mathrm{ave})}) = \nu(\lambda) \quad \text{for all } i \in \{1, \ldots, 9\}. \tag{6}$$

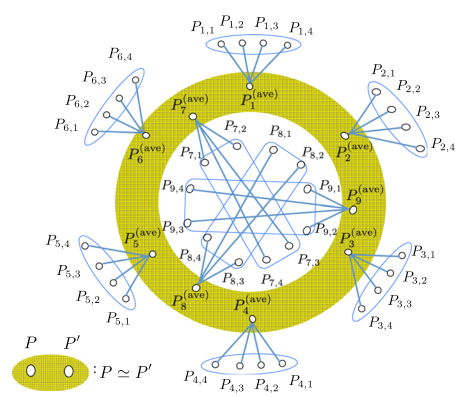

FIG. 3 (color online). Thirty-six preparation procedures, 9 ensembles of 4 each. A node connected to the elements of an ensemble represents the effective preparation procedure achieved by sampling uniformly from the ensemble.

Given the definition of $P_i^{(\mathrm{ave})}$, it follows that

$$\frac{1}{4}\sum_k \mu(\lambda|P_{i,k}) = \nu(\lambda) \quad \text{for all } i \in \{1, \ldots, 9\}. \tag{7}$$

Furthermore, recalling Eq. (1), for the ontological model to reproduce Eq. (4), we must have

$$\forall\ i, \forall\ k\ :\ \sum_\lambda \xi(k|M_i,\lambda)\mu(\lambda|P_{i,k}) = 1. \tag{8}$$

Because every λ in the support of $\nu(\lambda)$ appears in the support of $\mu(\lambda|P_{i,k})$ for some k, it follows that if $\xi(k|M_i,\lambda)$ had an indeterministic response on any such λ, we would have a contradiction with Eq. (8). Consequently, for all i and k, the measurement event $[k|M_i]$ must be outcome-deterministic for all λ in the support of $\nu(\lambda)$.

To summarize then, if one has experimentally verified the operational equivalences depicted in Figs. 2(a) and 3 and the measurement statistics described in Eq. (4), then universal noncontextuality implies that the value assignments to measurement events should be deterministic and noncontextual, hence KS noncontextual, and we obtain a contradiction:

$$\text{universal noncontextuality} + \text{operational equivalences} \\ + \text{perfect predictability} \rightarrow \text{contradiction}. \tag{9}$$

Contending with imperfect predictability in real experiments.—In real experiments, the ideal of perfect predictability described by Eq. (4) is never achieved, so we cannot derive a contradiction from it. However, Eq. (9) is logically equivalent to the following inference:

$$\text{universal noncontextuality} + \text{operational equivalences} \\ \rightarrow \text{failure of perfect predictability}. \tag{10}$$

That is, the degree of predictability, averaged over all i and k, will necessarily be bounded away from 1. It is this bound that is the operational noncontextuality inequality. For the 18 ray example, we prove that

$$A \equiv \frac{1}{36}\sum_{i=1}^{9}\sum_{k=1}^{4} p(k|M_i,P_{i,k}) \le \frac{5}{6}. \tag{11}$$

We now outline how the bound in Eq. (11) is obtained. First, we use Eq. (1) to express A in terms of $\xi(k|M_i,\lambda)$ and $\mu(\lambda|P_{i,k})$. Defining the max predictability of a measurement M given an ontic state λ by

$$\zeta(M,\lambda) \equiv \max_{k'\in\mathcal{K}_M} \xi(k'|M,\lambda), \tag{12}$$

we deduce that

$$\begin{aligned} A &\le \sum_\lambda \left(\frac{1}{9}\sum_i \zeta(M_i,\lambda)\left[\frac{1}{4}\sum_k \mu(\lambda|P_{i,k})\right]\right) \\ &= \sum_\lambda \left(\frac{1}{9}\sum_i \zeta(M_i,\lambda)\right)\nu(\lambda) \\ &\le \max_\lambda \left(\frac{1}{9}\sum_i \zeta(M_i,\lambda)\right), \end{aligned} \tag{13}$$

where we have used Eq. (7).

The measurements can have indeterministic responses, $\xi(k|M,\cdot): \Lambda \rightarrow [0,1]$, but measurement noncontextuality implies that $\xi(k|M_i,\lambda) = \xi(k'|M_{i'},\lambda)$ for the operationally equivalent pairs $\{[k|M_i],[k'|M_{i'}]\}$. There are many such assignments. Every unit-trace positive operator, for instance, specifies an indeterministic noncontextual assignment via the Born rule, and there are other, nonquantum assignments as well, such as the one depicted in Fig. 4.

Consider the average max predictability achieved by the assignment of Fig 4. Here, six measurements have max predictability of 1, three of $\frac{1}{2}$, implying that $\frac{1}{9}\sum_i \zeta(M_i,\lambda) = \frac{1}{9}(6\times 1 + 3\times\frac{1}{2}) = \frac{5}{6}$. As we demonstrate in the Supplemental Material [18], no ontic state can do better, so that $\max_\lambda[\frac{1}{9}\sum_i \zeta(M_i,\lambda)] \le \frac{5}{6}$, thereby establishing the noncontextual bound on A. The logical limit for the value of A is 1, so the noncontextual bound of $\frac{5}{6}$ is nontrivial. The quantum realization of the 18 ray construction achieves $A = 1$.

In the Supplemental Material [18], we discuss the noise tolerance of our inequality, and we criticize a previous proposal for a noncontextuality inequality [24] on two main grounds: (i) that logic alone rules out the possibility of satisfying it, and (ii) that all operational theories supporting the measurement equivalences of Fig. 2(a) necessarily violate it, regardless of whether or not they admit of a noncontextual model.

Although we have used the proof of Ref. [13] for illustration, our scheme can turn any proof of the Kochen-Specker theorem based on an uncolorable set

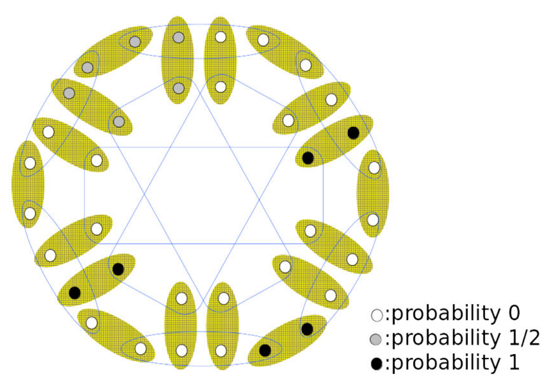

FIG. 4 (color online). A noncontextual outcome-indeterministic assignment.

into an experimental inequality, as we describe in the Supplemental Material [18].

An issue we have not addressed is that in practice no two measurement events are assigned *exactly* the same probability by each of a tomographically complete set of preparations, nor do any two preparations assign *exactly* the same probability distribution over outcomes to each of a tomographically complete set of measurements. The solution to this problem is described in related work [12,25]. A remaining question is how one accumulates evidence that a given set of measurements or preparations is indeed tomographically complete. This question represents the new frontier in the project of devising strict experimental tests of the assumption of noncontextuality.

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[18] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.115.110403, which includes Refs. [19–23], for a proof of the noncontextuality inequality, a recipe for deriving such an inequality for any KS construction based on an uncolorable hypergraph, an analysis of our noncontextuality inequality's robustness to noise, and a criticism of a previous proposal [24] for deriving a noncontextuality inequalty for the 18 ray construction.

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