Noncontextuality inequalities for Specker's compatibility scenario

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We derive operational noncontextuality inequalities for the simplest compatibility scenario capable of exhibiting contextuality: Specker's scenario. In doing this, we show how to rehabilitate the so-called "state-dependent" proofs of *quantum* contextuality to tests of contextuality for *arbitrary operational theories*. We explicitly take into account the lack of perfect predictability of measurement outcomes in realistic experiments. Too much noise would render these inequalities impossible to violate, unlike the case of Kochen-Specker type inequalities which fail to take noise into account. We also construct a quantum realization of Specker's scenario and demonstrate a violation of our theory-independent inequality. Specker's scenario involves three two-outcome measurements that are pairwise jointly measurable but need not be triplewise jointly measurable. It is the minimal scenario in which contextuality with respect to joint measurement contexts can be expected to manifest itself and our analysis provides a robust noncontextuality inequality for this scenario. We also generalize our analysis to arbitrary n-cycle scenarios.

I. MOTIVATION

Traditionally, whenever the word "contextuality" appears in the quantum foundations literature, it has referred to context-dependence for a particular kind of context that is specific to projective measurements in quantum theory (in the spirit of the Kochen-Specker theorem): this kind of context refers to Hermitian operators (say, B and C) that commute with a given Hermitian operator in question (say A) but do not commute with each other. That is, $[A, B] = [A, C] = 0$ and $[B, C] \neq 0$. Since commutativity is equivalent to joint measurability in the case of projective measurements, B and C provide two different contexts for the measurement of A. The quantum statistics of A is seen to be independent of whether it is marginalized from the joint measurement statistics of A and B or of A and C. This motivates the Kochen-Specker assumption of noncontextuality that any ontic state λ assigns values to A independently of whether it is measured with B or with C, an assumption we term KS-noncontextuality. We will refer to the particular kind of contexts involving joint measurements as *compatibility contexts*.

To be able to talk about whether the value assignment to a measurement depends on the context in which it is measured, it is necessary that the measurement be implementable in more than one context. Consequently, one must have at minimum *three* measurements to study contextuality. It turns out that three measurements is also sufficient to derive interesting examples of contextuality. The simplest scenario in which contextuality with respect to compatiblity contexts has been manifested is this: *three two-outcome measurements such that every pair of them is jointly measurable but the triple need not be so.* In other words, joint measurability holds pairwise but not necessarily triplewise. In fact this was the first contextualtiy scenario ever to have been studied, by Specker in 1960 [1]. We shall refer to it as the *Specker scenario.*

Significantly, the compatibility relations of Specker's scenario (when triplewise joint measurability is forbidden) cannot be achieved using projective measurements (PVMs) in quantum theory. This is because for projective measurements, joint measurability implies commutativity of the associated observables. Consequently, if one has three binary-outcome measurements that are pairwise jointly measurable, then every pair of observables is a commuting pair and it then follows that all three observables are jointly diagonalizable and therefore that all three measurements can be implemented jointly. Indeed, the minimal scenario achievable with PVMs that shows KS-contextuality is the 5-cycle scenario of Klyachko et al.[2].

On the other hand, the compatibility relations of Specker's scenario *can* be achieved using generalized quantum measurements, that is, positive operator-valued measures (POVMs) which are not projective. This is because for a pair of POVMs, although commutativity of all of the elements of one with all of the elements of the other implies that they can be measured jointly, the converse is not true—a pair of POVMs can be jointly measurable even if this commutativity property fails [3]. It follows that there is scope for proofs of the failure of noncontextuality in quantum theory within the Specker scenario as long as one considers POVM measurements. [1]

Such an investigation, however, requires a notion of noncontextuality for POVM measurements. The notion of measurement noncontextuality, proposed in Ref. [5] provides such a notion, and in subsequent work [6] it was shown that, unlike the case of projective measurements, one must allow that the outcome assigned to a

[1] See Ref. [4] for a discussion of these issues.

POVM measurement is not fixed deterministically by the ontic state. Ref. [3] posed the question of whether one could identify a quantum experiment—using some triple of binary-outcome POVM measurements having the compatibility relations of Specker's scenario—for which one could prove that there was no possibility of a noncontextual model in the sense of Ref. [5]. The question was answered in the affirmative in Ref. [7].

We are here interested in leveraging this new proof of the impossibility of a noncontextual model of quantum theory to derive noncontextuality inequalities.

Noncontextuality inequalities are inequalities evaluated on experimental statistics which have the feature that if the experimental statistics can be explained by a noncontextual ontological model, then the inequalities are satisfied. As such, they stand to the principle of noncontextuality as Bell inequalities stand to Bell's notion of local causality. And like Bell inequalities, noncontextuality inequalities can be derived and tested independently of the truth of quantum theory. In particular, a violation of a noncontextuality inequality by some experiment attests to the impossibility of a noncontextual model of that experiment and hence of any physical theory that can account for the results of that experiment, including physical theories that might be successors to quantum theory.

Techniques have recently been developed for deriving noncontextuality inequalities from so-called "state independent" proofs of the impossibility of a noncontextual model of quantum theory [8]. This contribution (see accompanying paper [9]) shows how to extend such techniques to the case of so-called "state dependent" proofs. We focus on the proof based on the compatibility relations in Specker's scenario because this is the simplest scenario. Also, this scenario is not realizable with projective measurements, unlike the case of higher n-cycle scenarios ($n > 3$).

II. DEFINITIONS

A. Operational theory and its ontological model

An operational theory is specified by $(\mathcal{P}, \mathcal{M}, p)$, where $\mathcal{P}$ is the set of preparation procedures, $\mathcal{M}$ is the set of measurement procedures, and $p(k|M,P) \in [0,1]$ denotes the probability that outcome $k \in \mathcal{K}$ occurs on implementing measurement procedure $M \in \mathcal{M}$ following a preparation procedure $P \in \mathcal{P}$ on a system.

An ontological model (Λ, μ, ξ) of an operational theory $(\mathcal{P}, \mathcal{M}, p)$ posits an ontic state space Λ such that a preparation procedure P is represented by a normalized distribution over Λ, $\mu(\lambda|P) \in [0,1]$ ($\lambda \in \Lambda$) such that $\sum_{\lambda\in\Lambda} \mu(\lambda|P) = 1$ for all $P \in \mathcal{P}$, and the probability of occurrence of a measurement outcome $[k|M]$ for a given $\lambda \in \Lambda$ is specified by $\xi(k|M,\lambda) \in [0,1]$, where the measurement outcomes are assumed to be discrete. The following condition of empirical adequacy prescribes how the operational theory and its ontological model fit together:

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

B. Operational equivalence

Two preparation procedures, P and P', are said to be operationally equivalent (denoted $P \simeq P'$) if no succeeding measurement procedure $M \in \mathcal{M}$ (with outcome set $\mathcal{K}$) yields different statistics for them, that is, if

$$\forall M \in \mathcal{M}, \forall k \in \mathcal{K} : p(k|M,P) = p(k|M,P'). \tag{2}$$

Two measurement events, $[k|M]$ and $[k|M']$ (where M and M' are measurement procedures with outcome set $\mathcal{K}$ each, $k \in \mathcal{K}$), are said to be operationally equivalent (denoted $[k|M] \simeq [k|M']$) if no preceding preparation procedure yields different statistics for them, that is, if

$$\forall P \in \mathcal{P} : p(k|M,P) = p(k|M',P). \tag{3}$$

C. Noncontextuality

Preparation noncontextuality is the following assumption on the ontological model of an operational theory:

$$P \simeq P' \Rightarrow \mu(\lambda|P) = \mu(\lambda|P') \quad \forall\lambda \in \Lambda. \tag{4}$$

Measurement noncontextuality is the assumption that

$$[k|M] \simeq [k|M'] \Rightarrow \xi(k|M,\lambda) = \xi(k|M',\lambda) \quad \forall\lambda \in \Lambda. \tag{5}$$

III. RESULTS

A. Noncontextuality inequalities for Specker's scenario

We consider three two-outcome measurements, $\{M_1, M_2, M_3\}$, each M_i with outcomes labelled by $X_i \in \{0,1\}$, such that every pair, that is, $\{M_i, M_j\}$ for $(ij) \in \{(12),(23),(31)\}$, admits of a joint measurement, denoted by M_{ij}. M_{ij} is a measurement procedure—with four outcomes denoted by (X_i, X_j)—whose measurement statistics can be coarse-grained to obtain the measurement statistics of both M_i and M_j for any preparation $P \in \mathcal{P}$:

$$p(X_i|M_i,P) \equiv \sum_{X_j} p(X_i,X_j|M_{ij},P),$$
$$p(X_j|M_j,P) \equiv \sum_{X_i} p(X_i,X_j|M_{ij},P). \tag{6}$$

Denoting by $M_i^{(j)}$ ($M_j^{(i)}$) the coarse-graining over X_j (X_i) of M_{ij}, pairwise joint measurability of M_1, M_2 and M_3 implies these operational equivalences:

$$\begin{aligned} M_1^{(2)} &\simeq M_1^{(3)} \simeq M_1, \\ M_2^{(1)} &\simeq M_2^{(3)} \simeq M_2, \\ M_3^{(1)} &\simeq M_3^{(2)} \simeq M_3. \end{aligned} \tag{7}$$

We now define a measurement M_* as follows: sample $(ij) \in \{(12),(23),(31)\}$ with probability 1/3 each and then implement M_{ij} and record (X_i, X_j). We are interested in the probability of recording anticorrelated outcomes,

$$p(\text{anti}|M_*, P) \equiv \frac{1}{3}\sum_{(ij)} p(X_i \neq X_j|M_{ij}, P). \tag{8}$$

Similarly, we consider another set of measurements, $\{M'_{12}, M'_{23}, M'_{31}\}$, which also achieve a joint measurement of the respective pairs:

$$\begin{aligned} M_1'^{(2)} &\simeq M_1'^{(3)} \simeq M_1, \\ M_2'^{(1)} &\simeq M_2'^{(3)} \simeq M_2, \\ M_3'^{(1)} &\simeq M_3'^{(2)} \simeq M_3. \end{aligned} \tag{9}$$

We also define a measurement procedure M'_* implementing M'_{12}, M'_{23}, or M'_{31} with equal probabilities such that $p(\text{anti}|M'_*, P)$ is the probability of obtaining anticorrelated outcomes for M'_*.

We define *predictability of* (M,P) *as*:

$$\eta(M,P) \equiv 2 \max_{X\in\{0,1\}} p(X|M,P) - 1, \tag{10}$$

where $\eta(M,P)$ is a measure of how *predictable*, or far away from uniformly random, the distribution over outcomes is for a two-outcome measurement M performed following a preparation P on a system.

Let P_*, $P_*^\perp$, P_1, $P_1^\perp$, P_2, $P_2^\perp$, P_3, $P_3^\perp$ be preparation procedures, and let $P_x^{(\text{ave})}$ be the preparation procedure obtained by implementing P_x with probability 1/2 and $P_x^\perp$ with probability 1/2 for $x \in \{1,2,3,*\}$. We suppose that the following operational equivalences among the preparations hold:

$$P_*^{(\text{ave})} \simeq P_1^{(\text{ave})} \simeq P_2^{(\text{ave})} \simeq P_3^{(\text{ave})}, \tag{11}$$

We can now state our noncontextuality inequalities for Specker's scenario:

Theorem 1. *An operational theory which satisfies the operational equivalences of Eqs. (7,9,11) and admits a noncontextual ontological model must necessarily satisfy the following noncontextuality inequality in Specker's scenario:*

$$\begin{aligned} &p(\text{anti}|M_*, P_*) + p(\text{anti}|M'_*, P_*^\perp) \\ &\leq 2\left(1 - \frac{1}{3}\eta_{\text{ave}}\right), \end{aligned} \tag{12}$$

where

$$\eta_{\text{ave}} \equiv \frac{1}{6}\sum_{i=1}^{3}\left(\eta(M_i,P_i) + \eta(M_i,P_i^\perp)\right). \tag{13}$$

On the other hand, using only the operational equivalences of Eqs. (7,11), such an operational theory must also satisfy:

$$p(\text{anti}|M_*, P_*) + p(\text{anti}|M_*, P_*^\perp) \leq 2\left(1 - \frac{1}{3}\eta_{\text{ave}}\right), \tag{14}$$

and

$$\begin{aligned} &p(\text{anti}|M_*, P_*) \\ &\leq \frac{2}{3}\left(2 - \eta_{\text{ave}}\right). \end{aligned} \tag{15}$$

A KS-noncontextual analysis of Specker's scenario would require that the probability of anticorrelation is bounded above by 2/3 for both M_* and M'_*, so that $p(\text{anti}|M_*, P) + p(\text{anti}|M'_*, P^\perp) \leq 4/3$. Similarly, in such an analysis, $p(\text{anti}|M_*, P_*) + p(\text{anti}|M_*, P_*^\perp) \leq 4/3$. But from Theorem 1 it is clear that these inequalities are not warranted by the assumption of noncontextuality alone. The noncontextual bound of 4/3 will hold if and only if one has verified that $\eta(M_i,P_i) = \eta(M_i,P_i^\perp) = 1$ for all $M_i, P_i, P_i^\perp$, $i \in \{1,2,3\}$. That is, when each measurement M_i produces deterministic outcomes on both preparations P_i and $P_i^\perp$. In this case, $\eta_{\text{ave}} = 1$. At the other extreme, if each M_i has no dependence on the corresponding preparation procedures P_i and $P_i^\perp$, so that $\eta(M_i,P_i) = \eta(M_i,P_i^\perp) = 0$, and therefore $\eta_{\text{ave}} = 0$, then a noncontextual model can achieve perfect anticorrelation. A mere observation of perfect anticorrelation on its own, therefore, is not enough to demonstrate contextuality: one also needs to check that the average predictability is sufficiently large: $\eta_{\text{ave}} > 0$ for Eqs. (12,14) and $\eta_{\text{ave}} > \frac{1}{2}$ for Eq. (15).

Our noncontextuality inequalities in Eqs. (12,14,15) imply a quantitative *tradeoff* between operational quantities: the *anticorrelation* achievable in an operational theory admitting a noncontextual ontological model and the *predictabilities* of the measurements involved.

In our contribution [9], we show that in operational quantum theory Specker's compatibility scenario can be realized by providing an explicit construction and then use this construction to demonstrate violation of the noncontextuality inequality of Eq. (12). The largest violation of the inequality for our choice of preparations and measurements occurs when $\eta_{\text{ave}} \approx 0.4566$ so that the violation is 0.1793: in this case the noncontextual bound on the anticorrelation is 1.6956 and the quantum value is 1.8749.

It follows that if operational quantum theory correctly describes our experiments and one can devise an experiment that is sufficiently precise that it can approach the violation predicted by quantum theory, then this experiment should yield a violation of the noncontextuality inequality. Moreover, if such an experiment is performed and the violation is observed, then this observation rules out the existence of a noncontextual ontological model *regardless of the truth of operational quantum theory.* Hence the result is theory-independent.

B. Generalization to arbitrary n-cycle scenarios

In our contribution [9], we go beyond Specker's scenario and derive noncontextuality inequalities for all n-cycle scenarios in a similar fashion. We also exhibit quantum violations of these inequalities. Our derivation of these inequalities is the first of its kind, as are the obtained quantum violations which are all given by POVMs on a *qubit* for *any* $n \geq 3$.

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