What is Nonclassical about Uncertainty Relations?

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Uncertainty relations express limits on the extent to which the outcomes of distinct measurements on a single state can be made jointly predictable. The existence of nontrivial uncertainty relations in quantum theory is generally considered to be a way in which it entails a departure from the classical worldview. However, this perspective is undermined by the fact that there exist operational theories which exhibit nontrivial uncertainty relations but which are consistent with the classical worldview insofar as they admit of a generalized-noncontextual ontological model. This prompts the question of what aspects of uncertainty relations, if any, *cannot* be realized in this way and so constitute evidence of genuine nonclassicality. We here consider uncertainty relations describing the tradeoff between the predictability of a pair of binary-outcome measurements (e.g., measurements of Pauli X and Pauli Z observables in quantum theory). We show that, for a class of theories satisfying a particular symmetry property, the functional form of this predictability tradeoff is constrained by noncontextuality to be below a linear curve. Because qubit quantum theory has the relevant symmetry property, the fact that its predictability tradeoff describes a section of a circle is a violation of this noncontextual bound, and therefore constitutes an example of how the functional form of an uncertainty relation can witness contextuality. We also deduce the implications for a selected group of operational foils to quantum theory and consider the generalization to three measurements.

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A wide range of phenomena have been viewed as intrinsically quantum, in the sense that they are thought to resist classical explanation—noncommutativity, interference, collapse, no cloning, teleportation, remote steering, and entanglement, to name just a few. However, the aspects of all of these phenomena (and many more) that have traditionally been regarded as relevant to establishing this claim can in fact be reproduced in a noncontextual [1] ontological model [2], as demonstrated in Refs. [4–7]. Therefore, if one takes the possibility of a noncontextual ontological model as a good notion of classical explainability (there are many arguments in favor of doing so; see Sec. V.A.3 of Ref. [7] or the introduction of Ref. [8]), then the possibility of reproducing these aspects undermines the claim that they resist classical explanation. This prompts the question: for each item on the list, are there more nuanced aspects of the full phenomenology that actually *do* resist explanation in terms of a noncontextual ontological model? In other words: what is genuinely nonclassical about its phenomenology? This question has been investigated, for instance, for minimum-error state discrimination [9], unambiguous state discrimination [10,11], state-dependent cloning [12], scenarios with preselection and postselection [13–15], and linear response theory [16].

This Letter undertakes an investigation of what is genuinely nonclassical about uncertainty relations. Many different notions have been termed "uncertainty relations." We are here concerned with the version that asserts that there are pairs of measurements for which there is a nontrivial tradeoff in their predictabilities [17]. Previous works have noted that there are operational theories that admit of a noncontextual ontological model and for which an uncertainty relation holds, such as Gaussian quantum mechanics [5] and the stabilizer theory of qudits where d is an odd prime [21,22]. Thus, although it is conventionally thought that the mere existence of an uncertainty relation is an intrinsically quantum phenomenon, the fact that this happens in theories that admit of a noncontextual ontological model demonstrates that it is not at odds with the classical worldview. The question, therefore, is whether one can identify *other aspects* of uncertainty relations that provably *cannot* arise in a noncontextual ontological model.

We here demonstrate that for a certain class of operational theories, an uncertainty relation describing the predictability tradeoff for a pair of binary-outcome measurements can witness contextuality through its functional form.

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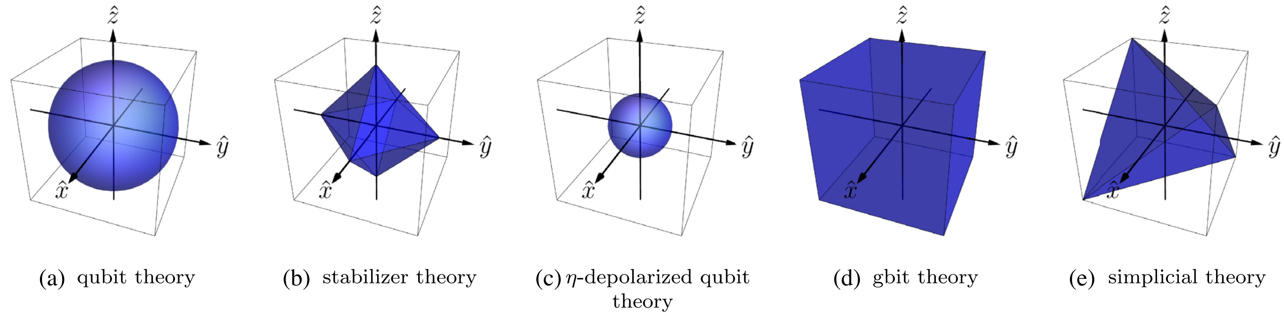

FIG. 1. The state spaces of various operational theories.

A class of uncertainty relations for a qubit.—In the early days of quantum theory, uncertainty relations were formulated in terms of products of standard deviations [23–25]. As has been pointed out by several authors [26,27], these are unsatisfactory for finite-dimensional systems because they involve a bound that depends on the state and which can be trivial for certain states. One solution to this problem is to focus on *sums* of standard deviations rather than *products*, because such sums satisfy a nontrivial bound for *all* states. We will here focus on the Pauli X and Z observables, which are complementary and represent discrete analogs of position and momentum. The strongest uncertainty relation that can be derived for X and Z is $\Delta X^2 + \Delta Z^2 \geq 1$, as we demonstrate in Sec. IV of the Supplemental Material [28]. There, we show that this can be written in several other useful forms, one of which is the form in which it was (to our knowledge) first proposed [39], by building on the work of Ref. [40]. The form that we will prefer for the purposes of this Letter is

$$\langle X\rangle^2 + \langle Z\rangle^2 \leq 1. \tag{1}$$

We will be taking our preferred measure of predictability to be the absolute values of the expectation values, i.e., $|\langle X\rangle|$ and $|\langle Z\rangle|$, so that Eq. (1) expresses a tradeoff relation between the squares of these predictabilities for every state. It is therefore apt to refer to Eq. (1) as the quantum ZX-uncertainty relation.

Note that Eq. (1) follows trivially from

$$\langle X\rangle^2 + \langle Y\rangle^2 + \langle Z\rangle^2 \leq 1, \tag{2}$$

a relation we refer to as the quantum XYZ-*uncertainty relation* and whose validity follows from the fact that it is a description of the Bloch ball of qubit quantum states.

Operational theories.—In prepare-measure scenarios, to which we limit ourselves here, an operational theory stipulates the possible preparations of a system and the possible measurements thereon, as well as an algorithm for computing the probability $\mathbb{P}(y|M,P)$ of obtaining the outcome y of measurement M given preparation P, for all possible measurements and preparations. For the purposes of making predictions, it is possible to represent each preparation P and each effect $[y|M]$ by real-valued vectors $\vec{s}_P$ and $\vec{e}_{y|M}$ respectively, with $\mathbb{P}(y|M,P) = \vec{s}_P \cdot \vec{e}_{y|M}$ [21,41,42].

Quantum theory can be conceptualized as an operational theory, but one can also consider operational theories that make different predictions. These are typically studied because of what they can teach us about quantum theory via the *contrast* they provide with it. For this reason, they are termed *foil theories* [6].

We discuss four examples of operational foils to qubit quantum theory that provide a useful contrast in the domain of uncertainty relations and that have been of independent prior interest (see Fig. 1).

Because the real-valued vector representation of qubit quantum theory is simply the familiar four-dimensional Bloch representation (wherein every qubit operator is represented as a linear combination of elements of a basis of the four-dimensional space of Hermitian operators), we consider foil theories that also have a four-dimensional real-valued vector representation. In discussing these theories, we will reuse the notation X, Y, and Z to refer to a triple of measurements associated with directions in the real-valued representation that are mutually orthogonal to one another and to the unit effect.

The first two foil theories are *subtheories* of the qubit theory, in the sense that they posit that only a *subset* of the preparations and measurements thereof are physically possible. First is the *qubit stabilizer theory*, defined as the subtheory of the full qubit theory arising when the states are restricted to the convex hull of the stabilizer states (an octahedron embedded inside the Bloch sphere) and the effects are restricted to the closure (under both convex mixtures and coarse grainings) of stabilizer effects. It has been of prior interest in quantum information theory [43] and quantum foundations [6,22]. Second is the *η-depolarized qubit theory*, defined by taking the set of effects to be the full set of qubit effects, but taking the states to be restricted to the image of the Bloch ball under the η-depolarizing map $\mathcal{D}_\eta(\rho) \equiv (1-\eta)\rho + \eta\frac{1}{2}I$. The state space in this case corresponds to a contracted Bloch ball of radius $1-\eta$. Note that because this is being considered as a foil theory, the depolarization is imagined to be

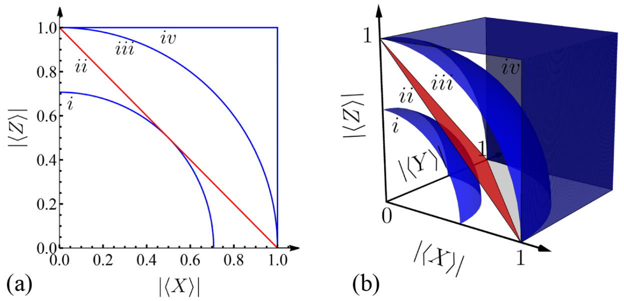

FIG. 2. (a) The ZX-uncertainty relation for (i) η-depolarized qubit theory for $\eta = 1 - (1/\sqrt{2})$, (ii) stabilizer qubit theory, (iii) qubit theory, and (iv) gbit theory and simplicial theory. Curve (ii) also describes the noncontextual bound. (b) The XYZ-uncertainty relation for (i) η-depolarized qubit theory for $\eta = 1 - (1/\sqrt{3})$, (ii) stabilizer qubit theory, (iii) qubit theory, and (iv) gbit theory and simplicial theory. Surface (ii) also describes the noncontextual bound.

fundamental, i.e., the theory is stipulated to have intrinsic decoherence of the type explored in collapse theories [44,45]. Our third example of a foil theory is one that is *postquantum*, in the sense that it predicts statistics in a prepare-measure scenario that are *not* achievable in quantum theory. This is the *gbit theory* [42,46], but defined relative to *three* binary-outcome measurements rather than a pair. We will refer to these three measurements as X, Y, and Z, in analogy with the quantum case. As such, we can describe the states and effects of the gbit theory in the same real vector space as we used for the other foil theories: the effect space of the gbit theory is equivalent to that of the qubit stabilizer theory, while the state space is a cube [47]. The gbit theory has been studied extensively in the context of axiomatizing quantum theory [48,49]. Finally, our fourth example of a foil theory is a strictly classical theory describing a *pair* of binary random variables, which we again denote by X and Z. This *simplicial theory* has a state space which is the convex hull of the four possible joint assignments of values to X and Z, which is a regular tetrahedron, while the effect space is the four-dimensional hypercube that is dual to this simplex [42,50].

The ZX-uncertainty relations of the four foil theories described above are as follows:

$$\text{qubit stabilizer: } |\langle X\rangle| + |\langle Z\rangle| \leq 1, \tag{3}$$

$$\eta\text{-depolarized qubit: } \langle X\rangle^2 + \langle Z\rangle^2 \leq (1-\eta)^2, \tag{4}$$

$$\text{gbit: } |\langle X\rangle| \leq 1, |\langle Z\rangle| \leq 1, \tag{5}$$

$$\text{simplicial: } |\langle X\rangle| \leq 1, |\langle Z\rangle| \leq 1. \tag{6}$$

These are implied by the geometry of the projection of their state spaces into the $\hat{x}\,\hat{z}$ plane, and are plotted in Fig. 2(a) alongside the quantum ZX-uncertainty relation. Note that the relations for the gbit and simplicial theory describe a *lack* of any nontrivial tradeoff, i.e., both X and Z can be made perfectly predictable simultaneously.

Ontological models and noncontextuality.—An ontological model of an operational theory is defined as follows. For each system, the model specifies a set Λ, termed an ontic state space, describing the possible physical states, or *ontic states*, of the system, denoted $\lambda \in \Lambda$. (For our purposes, it suffices to consider Λ finite.) Each preparation procedure P in the operational theory is represented as a probability distribution over the ontic states, denoted $\mu(\lambda|P)$. For each measurement M and outcome y of M, the effect $[y|M]$ is represented by a conditional probability distribution, denoted $\xi(y|M,\lambda)$, that stipulates the probability of obtaining outcome y given that the measurement M was implemented on the system and that the latter was in the ontic state λ. It is often useful to view the probability distribution $\mu(\lambda|P)$ as a vector denoted $\vec{\mu}_P$, and to also view the conditional probability distribution $\xi(y|M,\lambda)$ as a vector denoted $\vec{\xi}_{y|M}$. It follows that the model reproduces the predictions of the operational theory if and only if

$$\mathbb{P}(y|M,P) = \sum_{\lambda\in\Lambda} \xi(y|M,\lambda)\mu(\lambda|P) = \vec{\xi}_{y|M}\cdot\vec{\mu}_P. \tag{7}$$

The principle of generalized noncontextuality, applied to preparation procedures [51], has the following form: two preparation procedures, P and P', that are *operationally equivalent* (defined as leading to the same statistics for all possible measurements, $\forall\, M\colon \mathbb{P}(y|M,P) = \mathbb{P}(y|M,P')$, and denoted $P \simeq P'$) must be represented in the ontological model by the same probability distribution over ontic states:

$$P \simeq P' \Rightarrow \mu(\lambda|P) = \mu(\lambda|P'). \tag{8}$$

The real-valued vector representation $\vec{s}_P$ of a preparation P, described earlier, throws away all information about P besides its operational equivalence class. It follows that a noncontextual ontological model of an operational theory is one wherein all preparation procedures associated to the same vector $\vec{s}$ are represented by the same probability distribution over ontic states. In particular, this implies that if two different mixtures of operational states are equal, the same relation holds among the corresponding probability distributions over ontic states:

$$\sum_i w_i\vec{s}_i = \sum_j w'_j\vec{s}'_j \Rightarrow \sum_i w_i\vec{\mu}_i = \sum_j w'_j\vec{\mu}'_j \tag{9}$$

where $\{w_i\}_i$ and $\{w'_j\}_j$ are probability distributions [2].

Quantum theory, conceived as an operational theory, does not admit of a preparation-noncontextual ontological model even for a single qubit [2]. By contrast, the qubit stabilizer theory, when restricted to a single system in a prepare-measure scenario, admits of a noncontextual ontological model [4]. The η-depolarized qubit theory admits of a noncontextual model for $\eta \geq \frac{2}{3}$ [52]. The gbit theory, like the qubit quantum theory, does not admit of a noncontextual ontological model. Finally, the simplicial theory admits of a noncontextual ontological model where the vertices of the simplex are themselves the ontic states [53].

Main result.—There is an immediate challenge with trying to cast an uncertainty relation as a noncontextuality inequality. An uncertainty relation expresses a predictability tradeoff between two measurements *for any single quantum state*. But the simplest operational scenario in which noncontextuality implies a nontrivial constraint on statistics involves *four* quantum states [54], since this is the smallest number for which there can be a nontrivial operational equivalence.

To see how one solves this problem, consider the case of the qubit theory. Note that for any given quantum state, the values of X predictability and Z predictability that it achieves can *also* be achieved by many other states, and one can find nontrivial operational equivalences among these. In particular, imagine a state with Bloch vector $\vec{s}_1$. Then one can find three other states $\vec{s}_2$, $\vec{s}_3$, and $\vec{s}_4$ that give the same predictabilities, but different signs for the expectation values; that is,

$$\begin{aligned}\langle X\rangle_{\vec{s}_1} &= -\langle X\rangle_{\vec{s}_2} = -\langle X\rangle_{\vec{s}_3} = \langle X\rangle_{\vec{s}_4},\\ \langle Z\rangle_{\vec{s}_1} &= \langle Z\rangle_{\vec{s}_2} = -\langle Z\rangle_{\vec{s}_3} = -\langle Z\rangle_{\vec{s}_4}.\end{aligned} \tag{10}$$

We refer to this as the condition that the state has *equal predictability counterparts*. Moreover, one can always find such quadruples of states which additionally satisfy the operational equivalence relation

$$\frac{1}{2}\vec{s}_1 + \frac{1}{2}\vec{s}_3 = \frac{1}{2}\vec{s}_2 + \frac{1}{2}\vec{s}_4. \tag{11}$$

An example is depicted in Fig. 3. Such a quadruple of states forms the vertices of a rectangle in a plane that is parallel to the $\hat{x}\,\hat{z}$ plane. These vertices are the orbit of the original state under the action of the symmetry group of a rectangle under reflections, the Coxeter group A_1^2, so we refer to the pair of conditions on the state as the condition of A_1^2*-orbit realizability.*

Our main technical result is that, in any operational theory, if one can find a pair of measurements, which we will here denote by X and Z, and a state that satisfies the A_1^2-orbit-realizability condition (where the A_1^2 symmetry is evaluated relative to X and Z), then noncontextuality implies a nontrivial constraint on the X predictability and Z predictability for that state, namely, that they satisfy

$$|\langle X\rangle| + |\langle Z\rangle| \leq 1. \tag{12}$$

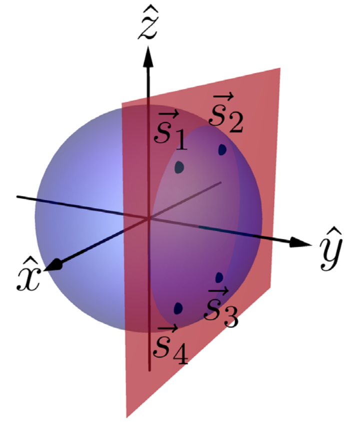

FIG. 3. Depiction of how an arbitrary state $\vec{s}_1$ in qubit quantum theory is part of a quadruple of states that satisfy the A_1^2-orbit-realizability condition.

An analytic and self-contained proof of this claim is given in Sec. I of the Supplemental Material [28]. In Sec. II of the Supplemental Material [28], we show that it also follows as a special case of noncontextuality inequalities that were previously derived using a linear program [55]. Note that the noncontextuality inequality of Eq. (12) is noise-robust, and can therefore be tested experimentally using the techniques described in Refs. [56] and [47].

Equation (12) has an unconventional form for a noncontextuality inequality given that it constrains the predictions associated to a *single* state rather than a set of states. This difference is only cosmetic, however, as the single state is explicitly required to satisfy the A_1^2-orbit-realizability condition, and thus the predictabilities appearing in the inequality in fact refer to the data one can obtain from *any* of the quadruple of states in its A_1^2 orbit.

For any operational theory and choice of X and Z measurements in that theory, one can determine the subset of states that satisfy the A_1^2-orbit-realizability condition relative to that choice. In the case of the simplicial theory, depicted in Fig. 1(e), for instance, it is the strict subset of states defined by the octahedron whose vertices lie at the midpoints of the edges of the tetrahedron [i.e., the octahedron depicted in Fig. 1(b)]. A vertex of the tetrahedron, for example, fails to satisfy the A_1^2-orbit-realizability condition because although it satisfies the condition of having equal predictability counterparts (namely, the three other vertices), these four states do not satisfy the operational equivalence condition. By contrast, there are operational theories wherein *all* states satisfy the A_1^2-orbit-realizability condition. Examples include the qubit theory, the stabilizer qubit theory, the η-depolarized qubit theory, and the gbit theory. We will refer to operational theories of this sort as having A_1^2 symmetry.

Whether or not an operational theory has A_1^2 symmetry, our bound constrains the tradeoff between X predictability and Z predictability for any state within the theory that satisfies the A_1^2-orbit-realizability condition. Consequently, if the theory contains one or more such states that *violate* the inequality, this is a proof of the failure of that theory to admit of a noncontextual ontological model.

For operational theories that *do* have A_1^2 symmetry, our bound has further significance. Because in such theories *all states* satisfy the A_1^2-orbit-realizability condition, our bound is a universal constraint on the predictability tradeoff within such theories; that is, it is a constraint on *the form of the ZX-uncertainty relation* within such theories.

The noncontextual bound [Eq. (12)] is compared with the ZX-uncertainty relation for a qubit [Eq. (1)] in Fig. 2(a), where it is readily seen that there can be quantum violations of the bound. Indeed, only when $|\langle X\rangle| = 1$ or $|\langle Z\rangle| = 1$ does the noncontextual bound intersect the quantum ZX-uncertainty relation. The maximum quantum violation is achieved when $|\langle X\rangle| = |\langle Z\rangle| = (1/\sqrt{2})$ and corresponds to $|\langle X\rangle| + |\langle Z\rangle| = \sqrt{2} \simeq 1.414$.

One can also compare this noncontextual bound with the ZX-uncertainty relation of the three foil theories that are in the A_1^2-symmetry class. The ZX-uncertainty relation for the η-depolarized qubit theory, Eq. (4), satisfies the noncontextual bound if $\eta \geq 1 - (1/\sqrt{2}) \simeq 0.293$. The ZX-uncertainty relation for the qubit stabilizer theory, Eq. (3), has exactly the same form as Eq. (12) and therefore precisely saturates the noncontextual bound. Finally, the uncertainty relation for the gbit theory, Eq. (5), yields the maximum possible violation of the noncontextual bound, namely, $|\langle X\rangle| + |\langle Z\rangle| = 2$.

In contrast, because the simplicial theory is *not* in the A_1^2-symmetry class, our result does not constrain the form of its ZX-uncertainty relation. Therefore, although the ZX-uncertainty relation for the simplicial theory, Eq. (6), is equivalent to that of the gbit theory and thus can violate the bound of Eq. (12), the only states in the theory that achieve this violation (for example, the vertices of the simplex) do not satisfy A_1^2-orbit realizability, and Eq. (12) is not derivable from noncontextuality for them. Meanwhile, the states that *do* satisfy the A_1^2-orbit realizability condition are precisely those inside of the embedded octahedron, namely, the states arising in the qubit stabilizer theory, and these saturate the noncontextual bound. In short, contextuality is not witnessed in the case of the simplicial theory, consistent with the fact that the latter admits of a noncontextual model.

Generalization to three measurements.—The analog of Eq. (12) for *three* measurements (which we denote X, Y, and Z) is

$$|\langle X\rangle| + |\langle Y\rangle| + |\langle Z\rangle| \leq 1. \tag{13}$$

In Sec. III of the Supplemental Material [28], we articulate the condition of A_1^3-orbit realizability under which this bound holds (A_1^3 is the symmetry group of a rectangular prism under reflections) and provide the proof. This constraint is depicted in red in Fig. 2(b), alongside the XYZ-uncertainty relations for the four foil theories discussed above. Note that this inequality admits of a greater quantum violation than Eq. (12) does. The stabilizer qubit theory also saturates this inequality.

Discussion.—It is usually the *lack* of joint predictability of X and Z (or of X, Y, and Z) that is emphasized as a feature of quantum theory that constitutes a departure from the classical worldview. From this perspective, what is striking about our results is that qubit quantum theory contains states that assign *higher* values of the predictabilities of multiple measurements, such as X and Z (or X, Y, and Z) than can occur in any operational theory that is noncontextually realizable (hence classically explainable) and that has A_1^2 symmetry. Similarly, the fact that the gbit theory can achieve *perfect* predictability for X and Z jointly (and even for X, Y, and Z jointly) while having A_1^2 symmetry implies that it is even *further* than the qubit theory from being classically explainable.

The A_1^2-symmetry property is critical to understanding why the degree of nonclassicality increases with the degree of predictability rather than with the degree of *un*predictability. The conventional association of nonclassicality with unpredictability is based on the fact that the simplicial theory—which must surely be included among those that are classically explainable—allows perfect joint predictability of X and Z. However, the states in the simplicial theory that achieve such predictability do not satisfy the A_1^2-orbit-realizability condition, and hence their ontological representations are not constrained by noncontextuality. Moreover, as noted above, if one considers the subset of states within the simplicial theory that *do* satisfy the A_1^2-orbit-realizability condition (namely, the embedded octahedron), they exhibit *less* joint predictability for X and Z than is possible in qubit quantum theory.

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