On the origin of nonclassicality in single systems

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Abstract

In the framework of certain general probability theories of single systems, we identify various nonclassical features such as incompatibility, multiple pure-state decomposability, measurement disturbance, no-cloning and the impossibility of certain universal operations, with the non-simpliciality of the state space. This is shown to naturally suggest an underlying simplex as an ontological model. Contextuality turns out to be an independent nonclassical feature, arising from the intransitivity of compatibility.

Keywords: incompatibility, contextuality, no-cloning, nonsimpliciality

(Some figures may appear in colour only in the online journal)

1. Introduction

It is an interesting question in quantum foundations whether quantum theory can be derived from information theoretic principles, a program that may be traced to [1–3] and which has received considerable attention recently [4–8].

It is well-known that nonclassicality in multipartite systems arises from nonlocal non-signaling correlations [9], an area that has been extensively studied from a foundational and information theoretic perspective [10–16].

In particular, various earlier works have linked nonlocality in the context of multipartite systems to nonclassical properties such as intrinsic randomness [17], non-comeasurability [18–22], uncertainty [23], local quantum mechanical features [24], non-simpliciality of the state space [14]. Yet, there appears to be no systematic study of all these properties solely within the context of single systems. It is this issue that is addressed in the present work.
We call the above-mentioned single-system properties as *base-level nonclassical*. These nonclassical features can be reproduced by an epistemic model over ontic states, as first shown by Spekkens [25]. By contrast, the lack of a joint probability distribution (JD) over measurement outcomes represents the complementary, *‘top-level’ nonclassicality*. Now, contextuality and nonlocality are closely connected. Yet, to our knowledge there are no works that relate contextuality to nonclassical properties like incompatibility or no-cloning. It is this issue that is addressed here. A related but distinct issue is that of identifying a simple principle to derive the quantum bound [26–30] on contextuality [31].

In our approach, we regard a single system as a composite built by aggregating individual *properties*, represented as observables. In practice, we shall regard any given observable as a specific measurement strategy. The basic idea is that a classical system is one where properties coexist peacefully, whereas in a nonclassical system, there is some sort of ‘tension’ prohibiting their peaceful coexistence, or *congruence*. Tension here corresponds to the statement that the state space of a finite-dimensional single-system is not a simplex, manifesting as incompatibility, no-cloning, etc. Our approach employs the framework of generalized probability theories [4, 10, 14, 32–40], with states and measurements as the basic elements of the theory. We identify two levels of nonclassicality: the above mentioned pairwise tension between properties, and a higher level nonclassicality arising from ‘frustration’ in the graph of congruence relations, leading to lack of a joint probability distribution (JD) for the measurements.

In section 2 we formulate our framework to study monopartite systems, identifying the axiomatic requirement for a theory to be classical (section 3) or non-classical (section 4). Nonclassical features that are consequences of the nonsimpliciality assumption are studied in section 5, among them non-comeasurability (section 5.1), measurement disturbance (section 5.2), no-cloning (section 5.3) and the impossibility of jointly distinguishing all pure states (section 5.4). The sense in which uncertainty also follows from nonsimpliciality is explained in section 6.

Section 7 explores certain consequences of nonsimpliciality in conjunction with ontological considerations. The concept of an ontological model as a simplex underlying an operational nonclassical theory is developed in section 7.1. This is then applied to derive a result concerning impossible universal operations (section 7.2) and preparation contextuality (section 7.3). This section thus sets forth what we consider a geometric approach to the ontology of a simple theory of monopartite systems.

The above enumerated sections deal with lower-level nonclassicality arising from pairwise incongruence. This type of nonclassicality will be present even if the pairwise incongruence is transitive. However, when pairwise incongruence is intransitive, the congruence structure associated with the properties of the single system is nontrivial, leading to states that lack a JD and thus correspond to contextuality, as explored in section 8. Section 9 develops the ontological concept of an underlying simplex for contextual correlations. Finally, we conclude in section 10.

### 2. Regular theories for monopartite systems

In the framework of generalized probability theories [4, 10, 14, 32–41], an operational theory $\mathcal{T}$ for monopartite systems is characterized by the state space $\Sigma$, the convex set of all possible states associated to a system governed by the theory. The set of extreme (or, pure) points of $\Sigma$ is denoted $\partial \Sigma$, taken to be a finite number for our purpose (so that $\mathcal{T}$ is discrete).

We shall define a *sharp measurement* as one that does not admit further refinement, i.e. the measurement should not be expressible as a convex combination of any other measurements.
in the theory [42]. In quantum mechanics, sharp measurements correspond to (non-degenerate) projective measurements. Suppose that measuring sharp measurement \( A \) on state \( \sigma \) and post-selecting on outcome \( a \) prepares a pure state \( \psi^A_a \), i.e. identifies some state without any error. This can be operationally verified by repeated measurement of \( A \) on \( \psi^A_a \), which does not alter this state. We call such \( \psi^A_a \) the eigenstate of the sharp measurement \( A \) with ‘eigenvalue’ \( a \) (see [43]). In general, not every measurement has an eigenstate. We call a theory \( T \) regular, if every sharp measurement allowed in \( T \) has an eigenstate \( \psi \in \partial \Sigma \). Thus, a theory is irregular if there are sharp measurements that don’t have eigenstates. A canonical irregular theory is the GDT theory, discussed in section 6.2.

Given a set of ‘fiducial measurements’ \( A_j \), tomographic separability, a state \( \psi \in \Sigma \) is completely specified by the numbers \( P(a_j|A_j) \), i.e. by the conditional probabilities generated by the fiducial measurements individually. Else, the state is tomographically nonseparable for this set. This may be considered as the single-system equivalent of the axiom of ‘local tomography’ [44] or ‘tomographic locality’ [6], encountered in reconstructions of quantum theory. The minimal set of such numbers \( P(a|A) \) to characterize an arbitrary mixed state is the theory’s tomographic dimension \( D \), or simply ‘dimension’. Note that this is the same as the number of degrees of freedom in Hardy’s axiomatic formulation of quantum theory [4].

3. Classical theory

A classical theory \( T \) is a regular theory where all \( m \) fiducial measurements \( X_1, X_2, \cdots, X_m \) coexist peacefully. Mathematically, we express peaceful coexistence as follows. We associate individual state spaces \( \Sigma_1, \Sigma_2, \cdots, \Sigma_m \) with the measurements, where \( \Sigma_j \) is the convex hull of all possible eigenstates of \( X_j \). Clearly, \( \Sigma_j \) is a simplex, meaning that the \( n \) pure points corresponding to definite values (i.e. measurement outcomes) of measurement \( X_j \) are linearly independent.

Peaceful coexistence happens precisely if the full state space \( \Sigma \) is the convex direct product

\[
\Sigma \equiv \Sigma_1 \otimes \Sigma_2 \otimes \cdots \otimes \Sigma_m
\]

of the individual state spaces \( \Sigma_j \), which is defined to be the convex hull of the set of \( n^m \) points:

\[
\partial \Sigma = \partial \Sigma_1 \otimes \partial \Sigma_2 \otimes \cdots \otimes \partial \Sigma_m.
\]

Since these points are linearly independent, \( \Sigma \) is also a simplex and has dimension:

\[
D = |\partial \Sigma| - 1.
\]

Quite generally, we shall identify classicality with the simpliciality of the state space \( \Sigma \).

**Example.** Consider the classical theory \( T \) of two fiducial measurements \( X \) and \( Z \) which take values \( x, z \in \{0, 1\} \). In barycentric coordinates [45], the basis for both \( \Sigma_X \) and \( \Sigma_Z \) is \( \{(1,0), (0,1)\} \). The full state space \( \Sigma_{XZ} \equiv \Sigma_X \otimes \Sigma_Z \) and is given as the convex hull of the points \( \{(1,0), (0,1)\} \otimes \{(1,0), (0,1)\} \):

\[
\begin{align*}
|xz=00 \rangle & \equiv (1,0,0,0), \\
|xz=01 \rangle & \equiv (0,1,0,0), \\
|xz=10 \rangle & \equiv (0,0,1,0), \\
|xz=11 \rangle & \equiv (0,0,0,1).
\end{align*}
\]

The general mixed state is an arbitrary point in \( \Sigma_{XZ} \), and has the unique barycentric coordinate representation given by \( (a,b,c,d) \) with \( a + b + c + d = 1 \) and...
is a regular theory characterized by two fiducial measurements \( q_j \). It is useful to define the following:

- If \( q_j \) is nonclassical, then \( r_j \) is nonclassical, respectively. Here, peaceful coexistence between \( X \) and \( Z \) means that they can assume definite values simultaneously. Thus conjunctive propositions \( (x \land z) \) and \( (x \lor z) \) can be assigned a definite truth value (‘true’ or ‘false’). In the extreme case, only propositions \( 'x \lor z' \) have a definite truth value, even in pure states. This has the following geometric consequence.

We identify nonclassicality with the departure of \( \Sigma \) from a simplicial structure, as discussed below.

### 4. Nonclassicality

Suppose \( T \) is a regular theory characterized by two fiducial \( n \)-output measurements \( X \) and \( Z \), whose outcomes are denoted \( x \) and \( z \), respectively. Here, peaceful coexistence between \( X \) and \( Z \) means that they can assume definite values simultaneously. Thus conjunctive propositions \( ('x \land z') \) can be assigned a definite truth value (‘true’ or ‘false’).

If \( T \) is nonclassical, \( X \) and \( Z \) do not coexist peacefully. Loss of peaceful coexistence means that \( X \) and \( Z \) are linked disjunctively, whereby propositions \( ('x \land z') \) cannot always be assigned a definite truth value. In the extreme case, only propositions \( 'x \lor z' \) have a definite truth value, even in pure states. This has the following geometric consequence.

Denote the \( n \) eigenstates of \( X \) by \( |\psi^k_x \rangle \) and the \( n \) eigenstates of \( Z \) by \( |\psi^k_z \rangle \). Therefore, the state space \( \Sigma \) is the convex hull of these \( |\partial \Sigma| = 2n \) pure points. Any state in \( \Sigma \) is a list of \( (n-1) \) conditional probabilities \( P(x|X) \) and \( (n-1) \) conditional probabilities \( P(z|Z) \). Therefore, the dimension of \( \Sigma \) is \( D = 2(n-1) \). The fact that \( |\partial \Sigma| > D + 1 \) means that not all pure states are linearly independent. Therefore, \( \Sigma \) is non-simplicial.

We shall refer to the relations between the elements of \( \partial \Sigma \), that leads to their linear dependence and hence to the non-simpliciality of \( \Sigma \), as the ‘nonsimpliciality conditions’. Typically, such a condition takes the form:

\[
\sum_j q_j |\psi^j_x \rangle = \sum_k r_k |\psi^k_z \rangle,
\]

with \( \sum_j q_j = \sum_k r_k = 1 \), i.e. in terms of equality of certain \( X \)-mixtures and \( Z \)-mixtures, and so on. Equation (5) has the interpretation that two mixtures on the LHS and RHS are operationally indistinguishable. Thus, the nonsimpliciality conditions have the operational meaning of multiple pure-state decompositions.

Going beyond two measurements, suppose a regular theory has more than two fiducial measurements, namely \( X, Y, Z, \cdots \). It is useful to define the following

**Definition 1.** The associated state space of a pair of measurements (say \( X \) and \( Z \)), denoted \( \Sigma_{XZ} \), is the convex hull of the eigenstates of \( X \) and \( Z \). We describe \( X \) and \( Z \) as pairwise congruent precisely if \( \Sigma_{XZ} \) is a simplex.

A simple nonclassical theory of \( m \)-input-\( n \)-output systems is a noncontextual theory in which all the \( m \) fiducial measurements are pairwise incongruent. To each fiducial measurement we associate a normalized probability distribution of \( (n-1) \) free parameters, and the state space has dimension of \( D = m(n-1) \). Because the property associated with each fiducial measurement fails to peacefully coexist with any other, we associate precisely \( n \) pure states per fiducial measurement, corresponding to states that assigned a definite value under the measurement. Therefore, there will be \( |\partial \Sigma| = mn \) pure states, and:

\[
|\partial \Sigma| - D = m,
\]

from which the nonsimpliciality of \( \Sigma \) follows, for \( m > 1 \).
The idea that incongruence causes properties that are conjunctively connected to become disjunctively linked, is reflected mathematically in the fact that the tensor product structure (1) is replaced by one with tensor sum:

\[ \Sigma = \Sigma_1 \oplus \Sigma_2 \oplus \cdots \oplus \Sigma_m, \]

(7)

which captures the idea that the dimensionalities are added rather than multiplies when composing systems.

**Example.** In the two-input-two-output operational theory \( T \), with two dichotomic measurements \( X \) and \( Z \), suppose the \( X \)- and \( Z \)-eigenstates, which are the pure states of space \( \Sigma \), are:

\[
\begin{align*}
\psi_X^+ & \equiv (1, 0 \mid \frac{1}{2}, \frac{1}{2}) \\
\psi_X^- & \equiv (0, 1 \mid \frac{1}{2}, \frac{1}{2}) \\
\psi_Z^+ & \equiv (\frac{1}{2}, \frac{1}{2} \mid 1, 0) \\
\psi_Z^- & \equiv (\frac{1}{2}, \frac{1}{2} \mid 0, 1),
\end{align*}
\]

(8)

where the vertical bar separates the measurement probabilities of the fiducial measurements \( X \) and \( Z \). The nonsimpliciality condition is:

\[
\frac{1}{2} (\psi_X^+ + \psi_X^-) = \frac{1}{2} (\psi_Z^+ + \psi_Z^-) = (\frac{1}{2}, \frac{1}{2} \mid \frac{1}{2}, \frac{1}{2}).
\]

(9)

The number of pure points is \(|\partial \Sigma_{XZ}| = 4\) whilst the dimension is 2, entailing nonsimpliciality. Clearly, in this case \( \Sigma \neq \Sigma_X \otimes \Sigma_Z \).

We stress that nonsimpliciality does not imply the non-existence of JD in an underlying outcome-deterministic theory. For instance, for each state (8), a JD manifestly exists for \( X \) and \( Z \). For example, corresponding to the state \( |\psi_X^+\rangle \), we have the separable form

\[
P(x, z | X, Z) = P(x|X)P(z|Z),
\]

where \( P(x|X) = (1, 0) \) and \( P(z|Z) = (\frac{1}{2}, \frac{1}{2}) \). And so on for the other three pure states.

Indeed, for \( m = 2 \), one can always find a JD. In section 8, we shall find that only incongruence with a specific structure gives rise to absence of JD. In section 5, we will explore a number of nonclassical consequences of nonsimpliciality in regular theories.

5. **Consequences of nonsimpliciality**

If a regular theory \( T \) has two or more incongruent measurements, then the space \( \Sigma \) characterizing the theory is not a simplex, as noted. Interestingly, a number of nonclassical features follow from the nonsimpliciality of \( \Sigma \), as discussed in the following subsections.

5.1. **Co-measurability**

Two measurements \( X \) and \( Z \) each with \( n \) measurement outcomes are jointly measurable (or, co-measurable) if there exists a joint measurement \( M_{XZ} \) such that the statistics of \( X \) and \( Z \) measurements are obtained under marginalization: \( M_X(x|\psi) = \sum_z M_{XZ}(x,z|\psi) \) and \( M_Z(z|\psi) = \sum_x M_{XZ}(x,z|\psi) \) for any state \( \psi \in \Sigma_{XZ} \) [46]. In the classical world, all
measurements are jointly measurable trivially. Co-measurability roughly corresponds to the commutativity of operators in the Hilbert space formulation of quantum mechanics.

Now consider a nonclassical theory with \( m = 2 \) fiducial measurements, denoted \( X \) and \( Z \). They are taken to be sharp in the sense that there are states (namely, the eigenstates) for which the measurements produce definite values. If these two are jointly measurable, then there are \((n^2 - 1) \times |\partial \Sigma|\) independent terms \( M_{XZ}(x, z|\psi) \) that constitute the putative joint operator, considering each of the possible \(|\partial \Sigma|\) pure states \( \psi \). There are \( 2(n - 1) \times |\partial \Sigma| \) independent constraints on them due to the requirement that \( M_X \) and \( M_Z \) statistics should be reproduced under marginalization.

A nonsimplicity condition, which is of the type equation (5), implies additional \((n^2 - 1)\) independent constraints of the type \( \sum_j q_j M(x, z|\psi) = \sum_k r_k M(x, z|\psi) \), which express the idea that the joint measurement cannot be used to distinguish between the mixtures in the LHS and RHS of (5). These constraints overconstrain \( M \) and thus prohibit joint measurability only if \( 2(n - 1)|\partial \Sigma| + n^2 - 1 > (n^2 - 1)|\partial \Sigma| \), or

\[
|\partial \Sigma| \leq \frac{n + 1}{n - 1} \leq 3, \tag{10}
\]

for \( n \geq 2 \). Clearly, this can never happen for a realistic theory. Therefore, nonsimpliciality by itself does not imply lack of joint measurability. However, for reasons explained, we are only interested in regular theories, and the consequences of nonsimpliciality in them. In this case, the relationship between simpliciality of \( \Sigma \) and joint measurability is tight, as shown below. For a different approach, see [47].

**Theorem 1.** Any pair of measurements \( X \) and \( Z \) in a regular theory are pairwise co-measurable iff their associated state space \( \Sigma_{XZ} \) is a simplex.

**Proof.** ‘Only if’ direction: Let the putative joint measurement be denoted \( M \). Let the ‘eigenvalues’ of \( X \) and \( Z \) be \( x \) and \( z \) taking values from 1 to \( n \). The following argument holds for any one of the \( 2n \) these eigenstates. Without loss of generality, let \( \psi \) be the eigenstate of \( X \) associated with eigenvalue \( x = 1 \). The \( M_X \) marginalization constraints require that:

\[
\begin{align*}
M(1,1|\psi) + M(1,2|\psi) + \cdots + M(1,n|\psi) &= 1 \\
M(2,1|\psi) + M(2,2|\psi) + \cdots + M(2,n|\psi) &= 0 \\
&\vdots \\
M(n,1|\psi) + M(n,2|\psi) + \cdots + M(n,n|\psi) &= 0.
\end{align*}
\]

Note that the signature \((1, 0, 0, \cdots, 0)\) is imposed by the assumption of pure state preparability in a regular theory. The \( M_Z \) marginalization constraints require that:

\[
\begin{align*}
M(1,1|\psi) + M(2,1|\psi) + \cdots + M(n,1|\psi) &= p_1 \\
M(1,2|\psi) + M(2,2|\psi) + \cdots + M(n,2|\psi) &= p_2 \\
&\vdots \\
M(1,n|\psi) + M(2,n|\psi) + \cdots + M(n,n|\psi) &= p,
\end{align*}
\]

where \( p \equiv 1 - \sum_{j=1}^{n-1} p_j \). This implies that all \( M(j,k|\psi) \) vanish for \( j > 1 \) and the \((n - 1)\) independent terms \( p_j \) fix the terms \( M(1,k|\psi) \). Thus, clearly, the \((n - 1)\) independent numbers \( p_j \) completely fix the elements of \( M(j,k|\psi) \). Repeating this argument for each of the \( 2n \) pure
states generating $\Sigma_{XZ}$, we see that the outcome statistics for the pure states fixes all the elements of $M(j, k | \rho)$ for any state, pure or mixed. In general, the $p_j$'s are independent of each other. Therefore, the further $n^2 - 1$ independent constraints due to the nonsimpliciality conditions of the type (9) would overdetermine the elements of $M$. Classical intuition would suggest that no such extra constraints are possible. But nonclassical phenomena show that such constraints can exits and essentially imply that our assumption of existence of the joint measurement, is wrong.

The ‘if’ direction: Intuitively, the challenge to co-measurability happens inside $\Sigma_{XZ}$ rather than outside. Now, if $\Sigma_{XZ}$ is a simplex, then the above operator $M$ can be constructed uniquely with regard to $M$’s action on the states in $\Sigma_{XZ}$. Consider pure states outside this space, of which there are $|\partial \Sigma| - |\partial \Sigma_{XZ}|$, and which are eigenstates of neither $X$ nor $Z$. Assume for simplicity that all systems have $m + 2$ inputs (including $X$ and $Z$) and $n$ outputs. Then, $|\partial \Sigma| - |\partial \Sigma_{XZ}| = mn$ and there are $(n^2 - 1) \times mn$ free variables, whereas the number of constraints are

$$c = 2(n - 1) \times mn + (n^2 - 1) \times \nu$$

(13a)

$$\leq m(n - 1)(3n + 1) - (n^2 - 1),$$

(13b)

where the first term in the RHS of equation (13a) is due to the marginalizations and $\nu \leq m - 1$ is the number of nonsimpliciality conditions of the type (5) in a regular theory. On the number hand, the number of free variables of the type $M_{P,Q}(p, q | \psi)$ given pure state $\psi$, is

$$v = (n^2 - 1) \times mn$$

$$= m(n - 1)(n + 1)n.$$  

(14)

Inasmuch as $c < v$ for $m \geq 1$ and $n \geq 2$, it follows that $M$ does not get overconstrained. ■

In regard to the above proof, we may also show a similar result for the case $m > 2$, by extending the above argument in a straightforward if elaborate way.

Consider the 2-input-2-output case. Comeasurability of $X$ and $Z$ in the classical case is obvious. We illustrate non-comeasurability in a nonclassical theory.

**Example.** Consider two measurements $X$ and $Z$, taking values $\pm 1$, in a 2-dimensional nonclassical theory, whose extreme states are:

$$|\psi_X^+ \rangle \equiv (1, 0 | 0.25, 0.75)$$

(15a)

$$|\psi_X^- \rangle \equiv (0, 1 | 0.75, 0.25)$$

(15b)

$$|\psi_Z^+ \rangle \equiv (0.25, 0.75 | 1, 0)$$

(15c)

$$|\psi_Z^- \rangle \equiv (0.75, 0.25 | 0, 1).$$

(15d)

That the state space $\Sigma_{XZ}$ obtained as the convex hull of the state in (15) is not a simplex is seen by noting that

$$\frac{1}{2}(|\psi_X^+ \rangle + |\psi_X^- \rangle) = \frac{1}{2}(|\psi_Z^+ \rangle + |\psi_Z^- \rangle).$$

(16)
To see that we cannot write down a joint measurement $M_{XZ}$, assume contrariwise that such $M_{XZ}$ exists. To get the right marginalized statistics for $|\psi^+_{XZ})$, we require:

\[
\begin{align*}
M_{XZ}(+,-|\psi^+_X) + M_{XZ}(+,+|\psi^+_X) &= 1 \\
M_{XZ}(+,-|\psi^-_X) + M_{XZ}(+,+|\psi^-_X) &= 0 \\
M_{XZ}(+,-|\psi^+_X) + M_{XZ}(+,+|\psi^-_X) &= 0.25 \\
M_{XZ}(+,-|\psi^-_X) + M_{XZ}(+,+|\psi^-_X) &= 0.75.
\end{align*}
\]

(17)

from which it follows that only $M_{XZ}(−,−|\psi^+_X) = M_{XZ}(−,−|\psi^-_X) = 0$ whereas $M_{XZ}(+,+|\psi^+_X) = 0.25$ and $M_{XZ}(−,−|\psi^+_X) = 0.75$.

Proceeding thus, one finds

\[
\begin{align*}
M_{XZ}(−,−|\psi^+_X) &= 0; \\
M_{XZ}(−,+|\psi^-_X) &= \frac{1}{4}; \\
M_{XZ}(−,+|\psi^+_X) &= \frac{3}{4}.
\end{align*}
\]

(18)

To satisfy the non-simpliciality condition, we must have

\[
M_{XZ}(j,k) \equiv \frac{1}{2}(|\psi^+_X + |\psi^-_X\rangle)
= M_{XZ}(j,k) \equiv \frac{1}{2}(|\psi^+_Z + |\psi^-_Z\rangle),
\]

(19)

which evidently is impossible, as seen for example, setting $(j,k) \equiv (-1, +1)$, since the LHS yields 0.25/2, whereas the RHS yields 0.75/2. □

It is important to stress that lack of comeasurability does not imply an absence of JD in an underlying outcome-deterministic theory. For example, the states (15) have manifestly a separable (indeed, product) form

\[
P(x, z|X, Z) = P(x|X)P(z|Z).
\]

5.2. Measurement disturbance

Measurement disturbance between two measurements refers to the possible random disturbance of a state produced by the measurement of an measurement. We say that $X$ and $Z$ are mutually disturbing if an $X$-eigenstate under $Z$-measurement yields a convex mixture of $Z$-eigenstates and vice versa.

Intuitively, the nonsimpliciality conditions and disturbance are closely connected. If there is no measurement disturbance, all measurements can be performed (infinitely many times if required) without modifying the system, and all pure states can be distinguished. Thus, there would be no indistinguishable mixtures of the type $\sum_{i=1}^{m} p_i |\psi_i\rangle = \sum_{j=1}^{n} q_j |\phi_j\rangle$, and thus no nonsimpliciality conditions. We express this idea formally as following theorem. We observe that without the nonsimplicial conditions, and thereby the lack of corresponding measurement disturbance, the uncertainty of measuring an measurement on a non-eigenstate would be akin to the classical probability, e.g. the color of picked balls in a Polya urn [48].

**Theorem 2.** Any pair of measurements $X$ and $Z$ in a regular theory are mutually non-disturbing iff their associated state space $\Sigma_{XZ}$ is a simplex.

**Proof.** Consider regular theory $\mathcal{T}$ with two fiducial noncomeasurable measurements, $X$ and $Z$. Suppose that $X$ and $Z$ do not produce measurement disturbance for each other. Then for any
state in $\Sigma_{XZ}$, we can perform $M_X$, and later $M_Z$ on the undisturbed state and thereby construct the joint measurement as per the prescription

$$M_{XZ}|\psi\rangle \equiv M_X(\psi)M_Z(\psi),$$

from which simplicity follows per theorem 1. Conversely, if $\Sigma_{XZ}$ is a simplex, then by theorem 1, measurements $X$ and $Z$ are co-measurable. In particular, this means that an unknown state in $\Sigma_{XZ}$ can be determined deterministically, making the joint measurement effectively non-disturbing.

It is not ruled out that there may be states in $\Sigma$ and outside $\Sigma_{XZ}$ that one or both may disturb, even if $X$ and $Z$ are mutually non-disturbing. The following example illustrates how measurement disturbance enforces the indistinguishability of mixtures that are operationally equivalent by virtue of the nonsimpliciality conditions.

**Example.** Suppose Alice prepares (from Bob’s perspective) the unbiased $X$-mixture $\rho \equiv \frac{1}{2}(|\psi_X^+\rangle + |\psi_X^-\rangle)$, where the states $|\psi_X^\pm\rangle$ are as defined in equation (15). This mixture is operationally indistinguishable from the unbiased $Z$-mixture. Under measurement of $X$, the unbiased $X$-mixture returns $\pm 1$ with equal probability and leaves the actual state, and hence the mixture, undisturbed.

If $Z$ is measured, then per (15), both $Z$ values are equiprobable, while the state after disturbance is:

$$\frac{1}{2} \left( \frac{1}{4}|\psi_Z^-\rangle + \frac{3}{4}|\psi_Z^+\rangle \right) + \frac{1}{2} \left( \frac{3}{4}|\psi_Z^-\rangle + \frac{1}{4}|\psi_Z^+\rangle \right) = \rho,$$

meaning that the same mixture is returned. Any POVM in this theory (tossing a loaded coin and measuring $X$ or $Z$ according to the coin’s outcome) also does not help in distinguishing the two mixtures.

In general, the measurement disturbance entailed by nonsimpliciality is not unique. Any prescription for the post-measurement probability distribution that preserves this indistinguishability is admissible.

### 5.3. No-cloning

Cloning is an operation by which, given an unknown pure state $\psi$ in a state space, at least two copies of $\psi$ are produced. We have the following result.

**Theorem 3.** An unknown pure state in the state space $\Sigma_{XZ}$ associated with a pair of measurements $X$ and $Z$ in a regular theory is clonable iff $\Sigma_{XZ}$ is a simplex.

**Proof.** First, we establish the equivalence of measurement disturbance and no-cloning. Suppose in theory $T$, measurements $X$ and $Z$ do not disturb each other. Then each measurement can be measured (repeatedly if required) without disturbing any other. From the resulting classical record, the state of the system is completely determined thus cloned.

For the other direction, we suppose that $T$ permits perfect cloning of an unknown pure state $|\psi\rangle \in \Sigma_{XZ}$. The cloning operation can be used to prepare multiple copies of the same state on any number (say $t$) of other single systems. Now, suppose that $X_1, X_2, \ldots, X_t$ represent measurement trials of a fixed measurement (say $X$) on $t$ clones so made. Thus, $X_j$ represent...
independent and identically distributed random variables each of which takes \( n \) discrete values corresponding to the outcomes.

Let the \( n \) frequencies \( f_j \) obtained by the \( t \) trials be represented by the \( n \)-dimensional vector \( \vec{f} \). Let \( \epsilon \) be a constant in the range \([0, 1]\). We use the notation \( |\vec{a}| \) to denote the vector of component-wise absolute values and the expression \( \vec{a} \geq \vec{b} \) to denote the event that for each component \( j \), \( a_j \geq b_j \).

Since the \( X_j \)'s are independent and identically distributed, the following bound can be shown to hold for the \( t \) trials:

\[
\Pr\left( \left| \vec{f} - \vec{\mu} \right| \geq \epsilon \vec{\mu} \right) \leq 2 \exp\left( -\frac{\epsilon^2 t}{3n} \right),
\]

which implies that for large number of trials \( t \), each observed frequency \( f_j \) converges exponentially fast towards the probability \( \mu_j \).

To prove (22), let \( X = \sum_{j=1}^t X_j \) and \( X \equiv X/t \), where \( X_j \in [0, 1] \). By the two-sided Chernoff bound [49],

\[
\Pr\left( |X - \mu| \geq \epsilon \mu \right) \leq 2 \exp\left( -\frac{\epsilon^2 \mu t}{2 + \epsilon} \right),
\]

where \( \mu \) is the theoretical mean. Now divide \( t \) into \( n \) equal segments. On the \( k \)th segment, define the coarse-grained measurement given by the binary measurement \( X^{(k)} \) which takes the value 1 if \( X^{(k)} = x_k \), and 0 otherwise. Therefore the \( k \)th segment involves \( t/n \) trials of random variable \( X^{(k)}_j \in \{0, 1\} \) with probabilities \( \{\mu_k, 1 - \mu_k\} \).

Applying the Chernoff bound (23) to each segment, we can bound \( \Pr(|\overline{X^{(k)}} - \mu_k| \geq \epsilon \mu_k) \) by the right hand side of (23) with the substitutions \( t \to t/n \) and \( \mu \to \mu_k \). The conjunction of these \( n \) events is the LHS of (22), and the product of these segmental bounds is the RHS of (22), where for simplicity, we have replaced the denominator \( 2 + \epsilon \) by 3 for the considered range \( 0 \leq \epsilon \leq 1 \).

For a sufficiently large number of clones, we can perform a tomography of either measurement according to equation (22) by measuring sufficiently many clones. In this way, the probability vector associated with each measurement can be determined to reconstruct \( |\psi\rangle \) in \( \Sigma_{XZ} \).

This establishes the equivalence of disturbance and no-cloning, which establishes the present theorem in view of theorem 2.

References [17, 10, 14] derive a no-cloning theorem for general probabilistic theories more general than QM in the context of multipartite systems subject to the no-signaling condition.

### 5.4. Joint distinguishability

States \( \psi \) are jointly distinguishable if there is measurement that uniquely identifies the individual states. The measurement dimension \( N \) is the number of pure states that can be distinguished jointly, i.e. by a one-shot measurement by measuring one or more fiducial measurements jointly. Classical intuition suggests \( D + 1 = N \), where the +1 in the LHS is due to normalization. In a general nonclassical theory, the tomographic and measurement dimensions do not match and we have:

\[
N \leq D + 1,
\]

allowing for the possibility that not all pure states are jointly distinguishable.
Theorem 4. All pure states in the state space $\Sigma_{XZ}$ associated with a pair of measurements $X$ and $Z$ in a regular theory are jointly distinguishable iff $\Sigma_{XZ}$ is a simplex.

Proof. If $\Sigma_{XZ}$ is a simplex, then by theorem 2, $X$ and $Z$ are mutually nondisturbing. Therefore, by sufficiently large number of repetitions (and application of the Chernoff bound), any given pure state in $\Sigma_{XZ}$ can be uniquely identified. The entire repetitive process should be considered as a one-shot procedure.

To prove the converse: let $P$ denote the procedure to jointly distinguish all pure states in the state space $\Sigma_{XZ}$ and $Q$ be a classical cloner that can prepare multiple copies of a known state in $\Sigma_{XZ}$. Then, clearly $Q \circ P$ can clone any unknown pure state in $\Sigma_{XZ}$, which per theorem 3 entails the simpliciality of $\Sigma_{XZ}$.

Theorem 4 implies that for a regular theory, a simplicial space $\Sigma$ is necessarily the convex hull of jointly distinguishable states, and the vertices of a nonsimplicial space necessarily lack joint distinguishability. Given regularity, indistinguishability has a purely geometric origin. A theory with $\Sigma$ given as the simplex of states that are not jointly distinguishable must have some other mechanism for preventing joint distinguishment, and would not be regular.

The preceding four theorems imply an equivalence among the nonclassical properties such as measurement incompatibility, measurement disturbance, etc, in the context of regular theories. In particular, theorems 3 and 4 together imply a cloning-discrimination equivalence, essentially using an approach based on state tomography. If instead one uses binary observation tests between pairs of states, then only three clones are sufficient in each pairwise test to establish the simplex structure of the state space [40, theorem 12].

6. Uncertainty from nonsimpliciality in regular theories

Measurement uncertainty refers to the property that two (or more) measurements cannot simultaneously take definite values, as revealed by a measurement. Our definition of a nonclassical regular theory presumes uncertainty. In this section, we shall physically motivate that assumption by showing that a theory with nonsimplicial state space equipped with pure state preparability will necessarily contain measurement uncertainty.

6.1. Uncertainty measure

It is convenient to quantify (measurement) uncertainty in a theory for any two variables $X$ and $Z$, with respective outcomes $x$ and $z$, as follows:

$$U = \max_\psi \left[ 1 - \left( \max_{x,z} \left( \frac{p(x|X, \psi) + p(z|Z, \psi)}{2} \right) \right) \right], \quad (25)$$

where $\psi$ runs over all states of the theory (see [23]). It is straightforward to generalize definition (25) to $m$ ($\geq 2$) measurements, essentially by maximizing the average of the $m$ outcome probabilities over all $m$-outcome strings.

For the classical theory, $U = 0$ for any two properties $X$ and $Z$. For the regular nonclassical theories characterized by states (15) and (8), we find $U = \frac{1}{4}$ and $U = \frac{1}{4}$, respectively.

A theory with uncertainty need not have nonsimplicial state space. This is because the space $\Sigma$ may be the convex hull of linearly independent vertices having uncertainty in the
sense of definition (25). An instance of such a theory is the one whose state space \( \Sigma \) is the convex hull of four linearly independent states:

\[
|\psi_1\rangle \equiv (1, 0 | 1, 0) \\
|\psi_2\rangle \equiv (1, 0 | p, \overline{p}) \\
|\psi_3\rangle \equiv (p, \overline{p} | 1, 0) \\
|\psi_4\rangle \equiv (p, \overline{p} | p, \overline{p}),
\]

(26)

where \( \overline{p} = 1 - p \) and \( 0 \leq p \leq 1 \). Thus, \( \Sigma \) is a simplex. Such a theory has none of the no-go theorems proven in the previous section, and hence the uncertainty in such a theory should properly be regarded as due to classical ignorance. Such a ‘Polya urn theory’ is really a classical theory with some measurement or observation limitations.

6.2. Gdit theories

While uncertainty does not imply nonsimpliciality, conversely nonsimpliciality too does not entail uncertainty. A gdit theory (gdit for ‘generalized dit’) is one with nonsimplicial space \( \Sigma \) and \( \mathcal{U} = 0 \). The pure state in a \( m \)-input-\( n \)-output gdit theory \( T_G \) is one of \( n^m \) boxes represented by an \( m \)-ary vector \((x_1, x_2, \ldots, x_m)\), where \( x_j \in \{1, \ldots, n\} \). Measuring measurement \( X_j \) returns \( x_j \) deterministically. An arbitrary mixed state is described by \( m \) probability distributions with \( n \) outcomes, so that the tomographic dimension of the states space \( \Sigma_G \) is \( m(n - 1) \). Therefore, there are exponentially many relations between the pure states, rendering them linearly non-independent and thereby making \( \Sigma_G \) nonsimplicial. As proven below later, a gdit theory is not regular, because it lacks pure state preparability.

The simplest gdit theory \( T_G^{2,2} \) is the 2-dimensional theory, given by the deterministic version of equation (8). The space \( \Sigma_G^{2,2} \) is the convex hull of

\[
|g_0\rangle \equiv (0, 0) \equiv (1, 0 | 1, 0) \\
|g_1\rangle \equiv (1, 0) \equiv (0, 1 | 1, 0) \\
|g_2\rangle \equiv (0, 1) \equiv (1, 0 | 0, 1) \\
|g_3\rangle \equiv (1, 1) \equiv (0, 1 | 0, 1).
\]

(27)

This satisfies the condition:

\[
\frac{1}{2}(|g_0\rangle + |g_1\rangle) = \frac{1}{2}(|g_1\rangle + |g_2\rangle)
\]

\[
= \left(\frac{1}{2}, \frac{1}{2}\right),
\]

(28)

which, in our framework, means that the mixtures on the LHS and RHS of (28) are indistinguishable.

6.3. Symmetric and asymmetric gdit theories

In a symmetric gdit theory, the prescription for measurement disturbance is that when one of the \( m \) measurements is performed, then the definite value of the performed measurement remains the same but the value assignments to the unmeasured \( m - 1 \) measurements will be equi-probably distributed:
$$(x_1, x_2, \ldots, x_i, \ldots, x_m) \xrightarrow{X_i} d^{1-m} \times \sum_{x_i' \neq x_i} (x_1', x_2', \ldots, x_i', \ldots, x_m').$$

(29)

This corresponds to the concept of a mutually unbiased basis in quantum mechanics. For example, for the states in (27)

$$\begin{align*}
|g_0\rangle &= \frac{1}{\sqrt{2}} (|g_0\rangle + |g_2\rangle), \\
|g_1\rangle &= \frac{1}{\sqrt{2}} (|g_1\rangle + |g_3\rangle),
\end{align*}$$

(30)

whereby the $X$ value is unaltered whilst the $Z$ value is irreversibly replaced by a uniform distribution. This measurement disturbance in the pattern of the measurement uncertainty for states $\psi^{\pm}_X$ in equation (8).

In an asymmetric gdit theory, the prescription for measurement disturbance is similar, except that the post-measurement distribution of values of the unperformed measurements is not necessarily uniform:

$$\begin{align*}
(x_1, x_2, \ldots, x_i, \ldots, x_m) &\xrightarrow{X_i} \sum_{x_i' \neq x_i} p_{x_1', x_2', \ldots, x_i', \ldots, x_m'} \\
&\times (x_1', x_2', \ldots, x_i', \ldots, x_m'),
\end{align*}$$

(31)

where $\sum_{x_i' \neq x_i} p_{x_1', x_2', \ldots, x_i', \ldots, x_m'} = 1$. Such asymmetric disturbance can be shown to leave equivalent mixtures of pure states indistinguishable, as in the symmetric gdit theory.

For example, for the states in (27) an asymmetric prescription for disturbance could be:

$$\begin{align*}
|g_0\rangle &\xrightarrow{X_1} \frac{1}{4} |g_0\rangle + \frac{3}{4} |g_2\rangle, \\
|g_1\rangle &\xrightarrow{X_1} \frac{1}{4} |g_3\rangle + \frac{3}{4} |g_1\rangle,
\end{align*}$$

(32)

which replaces the symmetric disturbance in (30). Here the $X$ value is unaltered $X = \pm 1$, respectively) whilst the $Z$ value is distributed in the pattern of the uncertainty for states $\psi^{\pm}_X$ in equation (15). The following result shows that the nonsimpliciality conditions do not uniquely fix the disturbance.

Generalizing the above argument, in a symmetric or asymmetric $m$-input-$n$-output gdit theory, the measurement disturbance ensures that the indistinguishability implied by the nonsimpliciality conditions is preserved. To see this, suppose that the nonsimpliciality condition in the gdit theory has the form:

$$\frac{1}{2} [(0, 0, x_3, x_4, \ldots) + (1, 1, x_3, x_4, \ldots)] = \frac{1}{2} [(0, 1, x_3, x_4, \ldots) + (1, 0, x_3, x_4, \ldots)].$$

(33)

where $x_j$ ($j = 1, 2, \ldots$) are outcomes that would be obtained when measurement $X_j$ is performed. Given the two mixtures represented by the LHS and RHS of (33), suppose $X_1$ is measured. Then the post-measurement mixture due to the first (resp., second) term in the LHS and the first (resp., second) term in the RHS will be the same. Thus, the post-measurement mixture
is the same for both initial states. Now, if \( X_2 \) is measured, then the post-measurement mixture due to the first (resp., second) term in the LHS and the second (resp., first) term in the RHS will be the same. Clearly, similar arguments can be given for all other \( X_j \)’s. It is straightforward to generalize the above argument from bits to dits, and to relations between pure states more elaborate than equation (33).

An insight that emerges from noting the joint measurability in an arbitrary nonclassical theory versus the non-comeasurability in a regular nonclassical theory (section 5.1) is that the idempotency of the marginal distribution helps ‘kill’ degrees of freedom in the joint measurement, facilitating non-comeasurability. By that yardstick, a gdit theory, in which all pure states are idempotent, should readily lack joint measurability. This is indeed the case, as the following example shows.

**Example.** Consider the 2-input-n-output gdit theory. Proceeding along the lines of equation (11), it is readily observed that the joint measurement should, if it exists, have the form \( M(j, k|\langle r, s \rangle) = \delta j \delta k \). Now a particular nonsimpliciality condition is:

\[
\frac{1}{2}((j, k) + (j', k')) = \frac{1}{2}((j, k') + (j', k)),
\]

where \( j \neq j' \) and \( k \neq k' \). For any state, equation (34) constrains the joint measurement \( M(a, b|\psi) \) such that:

\[
M(j, k|\psi) + M(j', k'|\psi) = M(j, k'|\psi) + M(j', k|\psi).
\]

Suppose such a joint operator \( M(a, b|\psi) \) exists. Let \( \psi = (j, k) \). In equation (35), of the four terms, the first is 1, while the remaining vanish, implying that the equation cannot be satisfied. It is easy to extend this argument to an arbitrary \( m \)-input-\( n \)-output gdit theory. Therefore, no joint measurement exists for gdit theory.

As a canonical irregular theory, no sharp measurement in the theory has an associated eigenstate. Thus, gdit theory lacks preparability. For any state, there is no measurement that leaves it undisturbed. Therefore, a pure state in a gdit theory can never be prepared, and state preparations are always ambiguous. It turns out that the preparation ambiguity in a gdit theory can be matched to the uncertainty of a regular theory, as discussed below.

### 6.4. Uncertainty-disturbance correspondence

An \( m \)-input-\( n \)-output (symmetric or asymmetric) gdit theory \( T_G \), characterized by a disturbance probability distribution \( P_{x_1, x_2, \ldots, x_m} \) given in (31) under measurement of \( X_i \), is said to correspond to a \( m \)-input-\( n \)-output regular theory \( T_U \), if the pure state with definite value \( X_i = x_i \) is given by

\[
|X_i = x_i\rangle_U = \sum_{x'_i \neq x_i} P_{x'_1, x'_2, \ldots, x'_m} x'_1, x'_2, \ldots, x'_m \rangle_G,
\]

where the paranthesized term with subscript \( G \) is a gdit state. This point was already noted in connection with equations (30) and (32).

The number of pure states in theory \( T_G \) is \( n^m \) while it is \( mn \) in the corresponding regular theory \( T_U \). On the other hand, both have the same dimension \( m(n - 1) \), which implies that \( T_G \) will have exponentially more number of nonsimplicial conditions. To determine the nonsimpliciality conditions in \( T_U \) starting from those in \( T_G \), we measure the LHS and RHS of
a gdit nonsimpliciality conditions in the same measurement, and re-interpret the resulting measurement-disturbed states as pure states with uncertainty in the regular theory obtained using the above $\mathcal{T}_G - \mathcal{T}_U$ correspondence.

For example, to get from equation (28) to (16), we measure the LHS of (28) by $X$, which effects according to the above recipe:

$$|g_0\rangle \rightarrow |\psi_X^+\rangle; \quad |g_1\rangle \rightarrow |\psi_X^-\rangle,$$

and we measure RHS of (28) by $Z$, which effects:

$$|g_1\rangle \rightarrow |\psi_Z^+\rangle; \quad |g_2\rangle \rightarrow |\psi_Z^-\rangle,$$

from which (16). The gdit and the corresponding regular theories have the same measurements, though the states that lack measurement uncertainty are different.

Interestingly, a gdit theory and its corresponding regular theory are operationally indistinguishable in our framework, essentially because of the interplay of disturbance and uncertainty, as discussed below.

For our purpose, a theory with tomographic separability can be fully characterized at the operational level in two steps: (1) State preparation: measuring fiducial measurement $A$ and post-selecting on outcome $a$; (2) Measurement: determining the outcome probabilities of a subsequent measurement $B \neq A$ of other measurements. If $B = A$, then the outcome is always assumed $a$ (i.e. repeatability assumed).

Suppose we have two theories $\mathcal{T}_1$ and $\mathcal{T}_2$, and two $n$-dimensional measurements $X$ and $Z$ in $\mathcal{T}_1$, and their analogues in $\mathcal{T}_2$, also referred to as $X$ and $Z$. In either theory, we can prepare a state by measuring one of the measurements (say $X$) and post-selecting on a particular outcome. If a subsequent measurement of the other measurement (say $Z$) yields the same outcome probabilities, and this holds true for every preparation in $\mathcal{T}_1$ and its analogous preparation in $\mathcal{T}_2$, then $\mathcal{T}_1$ and $\mathcal{T}_2$ are operationally indistinguishable. An observer cannot determine whether $\mathcal{T}_1$ or $\mathcal{T}_2$ is applicable in the operational world.

Note that in a gdit theory, because of preparation ambiguity, the first step above does not produce an unambiguous pure state. For example, suppose that in the 2-input-2-output gdit theory, Alice needs to prepare $(X=0, Z=0)$. If she measures $X$ on an unknown state and postselects on 0, $Z$ remains indeterminate. A subsequent measurement on $Z$ disturbs $X$. This ambiguity in preparation mimics the measurement uncertainty of the corresponding regular theory, as the following result shows.

**Theorem 5.** A gdit theory $\mathcal{T}_G$ and its corresponding regular theory $\mathcal{T}_U$ are operationally indistinguishable from each other.

**Proof.** Let us consider a gdit theory $\mathcal{T}_G$ of two measurements $X$ and $Z$ (with straightforward generalization to more measurements). Without loss of generality, suppose we first prepare $X = x$ during the state preparation step. In the gdit theory, if the state preceding measurement was such that $X \neq x$, then it will be ‘post-rejected’, i.e. post-selected out. Thus, a post-selected state necessarily pre-possessed definite value $X = x$. Therefore, no matter what the unknown pure state preceding the measurement, the post-selected state under the subsequent measurement of $Z$ will reflect the same disturbance probability $p_X(z)$, which will be $\frac{1}{2}$ in a symmetric gdit theory.

By definition of the corresponding regular theory, the preparation step above will produce the unique regular state $|X = x\rangle$, whose uncertainty probability distribution will be $p_X(z)$. A $Z$ measurement in step (2) will thus give the outcome statistics for the gdit theory and its corresponding regular theory.

$\blacksquare$
The ability of observers to prepare any pure state is obviously a nice feature and hence an important requirement for any operational theory. Requiring preparability is the reason that a nonclassical regular theory has $\mathcal{U} > 0$. This justifies our inclusion of uncertainty as a basic feature of regularity in section 2.

The uncertainty-disturbance shows that the regular theory corresponding to a gdit theory can be considered as having an *epistemic interpretation* over ontic states supplied by the gdit theory. This observation generalizes to Spekkens’ model for an epistemic model [25], discussed later below.

In figure 1, the outer square represents a two-input-two-output gdit theory, with the two fiducial measurements being $X$ and $Z$. The inner square is the regular theory corresponding to the symmetric gdit theory. The circular disk represents a more general regular theory, with infinitely many pure states (circular rim), generated by the gdit theory considering a continuum of asymmetric measurement disturbances. The antipodal points of the circle will represent eigenstates of rotated fiducial measurements $A$ and $B$, obtained under suitable continuous transformation of $X$ and $Z$.

7. Ontology of noncontextual nonclassical theories

The preceding consequences of nonsimpliciality follow from purely operational considerations. In this section, we take up certain ontological issues. Here our approach is comparable with that of [30, 50, 51], which explore graph theoretic approaches to nonclassicality in quantum mechanics. We return to this matter in section 9, but here we only note that in contrast to the three aforementioned works, which are applicable to contextuality and nonlocality, our combinatoric approach (as explored in this section) works also for nonclassical effects arising in the absence of contextuality and nonlocality, but associated with the nonsimpliciality of the state space.

7.1. Underlying simplex and $\Sigma$-ontology

The idea that an ontological model for a nonclassical theory is itself a classical theory of some kind suggests an underlying simplex $\Sigma_{\mathcal{U}}$ and a corresponding underlying classical theory $\mathcal{T}_{\mathcal{U}}$ as natural representations of an ontological model. Given fiducial measurements $X, Y, Z, \cdots$ in $\mathcal{T}$, we posit underlying versions of these measurements, which will also be referred to as $X, Y, Z, \cdots$. However, unlike in $\mathcal{T}$, these measurements do in the underlying theory peacefully coexist. Therefore, $\Sigma_{\mathcal{U}} \equiv \Sigma_X \otimes \Sigma_Z \otimes \cdots$. Since the individual spaces $\Sigma_j$ are simplexes, so is $\Sigma_{\mathcal{U}}$. So long as an underlying JD exists for the properties, such an underlying theory $\mathcal{T}_{\mathcal{U}}$ exists. The ontological model that it can provide for the overlying operational theory $\mathcal{T}$ is discussed below. In particular, the elements $\partial \Sigma_{\mathcal{U}}$ are taken to constitute the underlying ontic states $\lambda$.

The relationship between the simplex $\Sigma_{\mathcal{U}}$ and the nonsimplex $\Sigma$ of $\mathcal{T}$, represented by the mapping $\varphi: \Sigma_{\mathcal{U}} \to \Sigma$, cannot be linear-injective, since this would preserve the simplex property. It is convenient to think of $\varphi$ as the composition of two maps: $\varphi \equiv \varphi_+ \circ \varphi_-$. The map $\varphi_+ : \Sigma_{\mathcal{U}} \to \Sigma_{\mathcal{U}}$, where $\Sigma_{\mathcal{U}}$ is either an intermediate underlying simplex or an intermediate underlying gdit space such that

$$\dim(\Sigma_{\mathcal{U}}) = \dim(\Sigma).$$

Therefore, for a nonclassical $m$-input-$n$-output regular theory with pairwise incongruent measurements, $\varphi_-$ reduces the dimensionality exponentially from $\dim(\Sigma_{\mathcal{U}}) = n^m - 1$ to $\dim(\Sigma) = m(n - 1)$. It is convenient to call the map $\varphi_-$ as *compression*. 

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Typically, map $\varphi$ does not introduce uncertainty. This introduction happens via the partial function of crumpling, $\varphi_s: \Sigma_{ij} \to \Sigma$, which is such that $\varphi_s^{-1}: \Sigma \to \Sigma_{ij}$ is an embedding. We refer to $\varphi_s$ as a crumpling map because it introduces vertices and faces. We call the map $\varphi$ and the corresponding ontological model as g-type (resp., s-type) if space $\Sigma_{ij}$ is a gdit space (resp., simplex).

The term $\Sigma$-ontology will refer to this general procedure for constructing an ontological model on the basis of the underlying simplex $\Sigma_{ij}$ and the intermediate underlier $\Sigma_{ij}$. An example is given by figure 1, where the regular theory is the inner square. The outer square represents an intermediate underlying theory $\Sigma_{ij}$, while the tetrahedron (not shown) is the underlying simplex $\Sigma_{ij}$.

7.1. G-type ontological model. Here the intermediate space $\Sigma_{ij}$ is the $m$-input-$n$-output gdit theory, which one may call the underlying gdit theory. It preserves the $n^m$ extreme points of $\Sigma_{ij}$ such that $\varphi_\Sigma: \partial \Sigma_{ij} \to \partial \Sigma_{ij}$ is a one-to-one correspondence. If the points in $\Sigma_{ij}$ are represented in a barycentric coordinate system $B$, then those in $\Sigma_{ij}$ can be expressed using a generalized barycentric coordinate system $G$ derived from $B$ using $\varphi_\Sigma$. Owing to the nonsimpliciality of the gdit theory, the representation in $G$ in general will not be unique.

**Example.** Suppose there are two fiducial measurements $X, Z$ taking values $x, z \in \{0, 1\}$ in the operational theory characterized by the pure states in equation (8). Here the underlying simplex $\Sigma_{ij}$ is the 3-simplex generated by four vertices $\lambda_j \equiv x \otimes z$ ($j \in \{1, 2, 3, 4\}$). In the barycentric coordinate system, the $\lambda$’s are the states in equation (4).

Employing the generalized barycentric coordinates for $\Sigma_{ij}$, we can express the action of $\varphi_\Sigma$ on pure states of $\Sigma_{ij}$ by $\varphi_\Sigma(x \otimes z) = (x, z) \in \mathbb{R}^2$. Given a point in $\Sigma_{ij}$ described by the barycentric coordinates $(a_1, a_2, a_3, a_4)$, where $a_j \geq 0$, $\sum_j a_j = 1$, we have

$$
\varphi_\Sigma[(a_1, a_2, a_3, a_4)] = \sum_{j=1}^4 a_j / \varphi_\Sigma(\lambda_j)
= a_1(0, 0) + a_2(0, 1) + a_3(1, 0) + a_4(1, 1)
= (a_1 + a_2, a_2 + a_3, a_3 + a_4)
\equiv (a_1 + a_2, a_3 + a_4 | a_1 + a_3, a_2 + a_4)
$$

(38)

where $(0, 0), (0, 1), (1, 0)$ and $(1, 1)$ are the vertices of the underlying gdit theory. Note that distinct interior points in $\Sigma_{ij}$ may map to the same point in $\Sigma_{ij}$, since the vertices $\varphi_\Sigma(\lambda_j)$ are not linearly independent. For instance, the distinct ontic mixtures $(\frac{1}{2}, 0, 0, \frac{1}{2})$ and $(0, \frac{1}{2}, \frac{1}{2}, 0)$ in the underlying simplex map to the same mixture $(\frac{1}{2}, \frac{1}{2}) \equiv (\frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2})$ in the gdit theory.

In figure 1, space $\Sigma_{ij}$ is represented by the outer square and operational space $\Sigma$ by the circle or the inner square. Map $\varphi_\Sigma^{-1}$ embeds the circle in the outer square $\Sigma_{ij}$. The square is obtained by compressing set $\Sigma_{ij}$ (a 3-simplex, not shown in the figure) via the map $\varphi$. This compresses the tetrahedron to the square.

**Example.** In our approach, Spekkens’ toy theory [25] has the following operational description. There are three pairwise incongruent measurements $X, Y, Z$, with $\Sigma$ given as the convex hull of:
The nonsimpliciality of $\Sigma$ is a consequence of dependences among the extreme states:

$$
\begin{align*}
\psi_X^+ & \equiv (1, 0 | \frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2}) \\
\psi_X^- & \equiv (0, 1 | \frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2}) \\
\psi_Y^+ & \equiv (\frac{1}{2}, \frac{1}{2} | 1, 0 | \frac{1}{2}, \frac{1}{2}) \\
\psi_Y^- & \equiv (\frac{1}{2}, \frac{1}{2} | 0, 1 | \frac{1}{2}, \frac{1}{2}) \\
\psi_Z^+ & \equiv (\frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2} | 0, 1) \\
\psi_Z^- & \equiv (\frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2}).
\end{align*}
$$

The nonsimpliciality of $\Sigma$ is a consequence of dependences among the extreme states:

$$
\begin{align*}
\left(\frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2} | \frac{1}{2}, \frac{1}{2}\right) & = \frac{1}{2}(\psi_X^+ + \psi_X^-) \\
& = \frac{1}{2}(\psi_Y^+ + \psi_Y^-) \\
& = \frac{1}{2}(\psi_Z^+ + \psi_Z^-).
\end{align*}
$$

Therefore the various nonclassical features noted in Spekkens’ toy theory are seen to follow essentially from the nonsimpliciality of $\Sigma$ in that theory.
The underlying simplex is
\[ \Sigma_{\cup} = \Sigma_X \otimes \Sigma_Y \otimes \Sigma_Z, \] (41)
of dimensionality \( \dim(\Sigma_{\cup}) = 7 \). Since for the toy theory \( D = 3 \), therefore \( \Sigma_{\cup} \) is the three-dimensional 3-input-2-output gdit theory, with vertices given by the 8 states \( \gamma_{4i+2j+l+1} \equiv (j,k,l) \) in Cartesian coordinates, and \( j,k,l \in \{0,1\} \). The compression map is given by \( \varphi_\gamma (j \otimes k \otimes l) \equiv (j,k,l) \), where the ontic elements \( \lambda \equiv (j \otimes k \otimes l) \) are the 8 extreme points of the 7-simplex \( \Sigma_{\cup} \) and distinct from Spekkens’ ontic set of 4 points (which are the extreme points of the \( \Sigma_{\cup} \) in the s-type ontology, discussed below).

In the g-type ontology, the Spekkens toy theory corresponds to the octahedron formed as the convex hull of the six face-centers of the 3-input-2-output gdit theory. The ontic representation of the states (39) in terms of the intermediate gdit theory is:

\[
\begin{align*}
\mu_X^+ &= \frac{1}{4} (\gamma_1 + \gamma_2 + \gamma_3 + \gamma_4) \\
\mu_X^- &= \frac{1}{4} (\gamma_5 + \gamma_6 + \gamma_7 + \gamma_8) \\
\mu_Y^+ &= \frac{1}{4} (\gamma_1 + \gamma_2 + \gamma_5 + \gamma_6) \\
\mu_Y^- &= \frac{1}{4} (\gamma_3 + \gamma_4 + \gamma_7 + \gamma_8) \\
\mu_Z^+ &= \frac{1}{4} (\gamma_1 + \gamma_3 + \gamma_5 + \gamma_7) \\
\mu_Z^- &= \frac{1}{4} (\gamma_2 + \gamma_4 + \gamma_6 + \gamma_8),
\end{align*}
\] (42)

which are just the generalized barycentric coordinates in the gdit theory.

A geometrization of Spekkens’ toy theory using precisely four ontic points, based on s-type \( \Sigma \)-ontology, is discussed below.

7.1.2. S-type ontological model. In this type of model, the intermediate space \( \Sigma_{\cup} \) is taken to be the \( D \)-simplex, where \( D \equiv \dim(\Sigma) \). Thus, \( \varphi_\gamma \) is a function that preserves the simplicial property. The crumpling map \( \varphi_\star \) introduces nonsimpliciality, in addition to uncertainty. This idea can be illustrated by giving an s-type model for Spekkens’ toy theory [25], in contrast to the g-type given above.

Example. For the Spekkens toy theory, whose \( \Sigma \) is the convex hull of the states (39), the intermediate underlying simplex \( \Sigma_{\cup} \) is the 3-simplex, or tetrahedron. The compression function \( \varphi_\gamma \) maps the 7-simplex \( \Sigma_{\cup} \) defined in (41), to this. Here \( \Sigma_{\cup} \) is taken to be the convex hull of any four convex independent points \( \gamma_i \) in \( \mathbb{R}^3 \). In particular, we can take \( \gamma_1 \equiv (0,0,0), \gamma_2 \equiv (0,1,1), \gamma_3 \equiv (1,0,1) \) and \( \gamma_4 \equiv (1,1,0) \).

The state space \( \Sigma \) in Spekkens toy theory is the octahedron formed as the convex hull of the six face-centers of the above 3-simplex, which serves as \( \Sigma_{\cup} \), with vertices \( \{\gamma_j\} \) (\( j \in \{1,2,3,4\} \)). The ontic representation in terms of the intermediate underlying simplex is:
\[
\mu^+_X = \frac{1}{2}(\gamma'_1 + \gamma'_2)
\]
\[
\mu^-_X = \frac{1}{2}(\gamma'_1 + \gamma'_4)
\]
\[
\mu^+_Y = \frac{1}{2}(\gamma'_1 + \gamma'_2)
\]
\[
\mu^-_Y = \frac{1}{2}(\gamma'_1 + \gamma'_4)
\]
\[
\mu^+_Z = \frac{1}{2}(\gamma'_1 + \gamma'_4)
\]
\[
\mu^-_Z = \frac{1}{4}(\gamma'_2 + \gamma'_3),
\]
(43)

which may be contrasted with the g-type representation, equation (42).

This geometric containment of state space $\Sigma$ in the above 3-simplex for Spekkens’ toy theory’s was first shown in [52].

7.2. Impossible universal operations

We define a coherent transformation $U$ in an operational $\mathcal{T}$ as one that reversibly maps any pure state to another pure state. An instance of a coherent operation for a theory with $N = 2$ is the inverter, which transforms any state to another which is orthogonal in the sense of being deterministically distinguishable from the initial state. Thus, the inverter is fully specified by

\[
|\psi^+_X\rangle \leftrightarrow |\psi^-_X\rangle,
|\psi^+_Z\rangle \leftrightarrow |\psi^-_Z\rangle,
\]
(44)

for the theory determined by pure states (8). In quantum mechanics, it is known that there exists no universal inverter [53]. Spekkens showed [25] that an analogous non-invertibility result exists is his model. His proof, which employs an ontological argument, proceeds along the following lines.

In the ontic representation (43) of the states (39), to implement $\psi^+_X \leftrightarrow \psi^-_X$ and $\psi^+_Y \leftrightarrow \psi^-_Y$, it is seen that the requisite ontic transformation is

\[
\gamma'_1 \leftrightarrow \gamma'_4
\]
\[
\gamma'_2 \leftrightarrow \gamma'_3.
\]
(45)

Applying this to $\mu^+_Z$, it is clear that this the transformation (45) does not work, implying that the coherent operation (44) is disallowed.

This observation prompts the question of whether an analogous result can be produced for any operational theory $\mathcal{T}$ with non-simplicial space $\Sigma$ in the $\Sigma$-ontology. Here, in the spirit of Spekkens’ argument, it may be assumed that coherent transformations in the operational theory should have a representation in terms of reversible transformations among the ontic states $\lambda$ in the ontological model $\mathcal{T}_\lambda$ or in the intermediate underlying model in the g-type ontology. Then universal coherent operations can be shown not to exist.

To see this we note that Spekkens’ proof, in our terminology, employs the s-type ontology. However, it is readily verified that in the g-type ontology, the following ontic transformation indeed implements the universal inverter (44):
This shows that this nonclassicality is dependent on the ontological model. From the perspective of interpretation, this result says that if certain coherent operations are not observed, then it restricts the class of possible underlying classical explanations.

Mathematically, the result shows that by increasing the number of ontic states for the same operational theory, we can create more ‘space for manoeuvre’. Given a discrete $m$-input-$n$-output theory $T$, with space $\Sigma$, $|\partial \Sigma| = mn$ pure states, and dimension $D_T = m(n-1)$, we have for the underlying simplex, $D_{\Sigma} = n^m - 1$ and $|\partial \Sigma_{\cup}| = n^m$. The cardinality $|\partial \Sigma|$ is exponentially smaller than $|\partial \Sigma_{\cup}|$. More generally, $\partial \Sigma$ could be arbitrarily enlarged within a fixed underlying $\Sigma_{\cup}$. The theory represented by the circular disk in figure 1 is such an example.

There are in all $|\partial \Sigma|!$ permutations and hence distinct coherent transformations in $T$. In the underlying theory, there are $|\partial \Sigma_{\cup}|!$ ontic permutations. If $|\partial \Sigma|! > |\partial \Sigma_{\cup}|!$, and hence $|\partial \Sigma| > |\partial \Sigma_{\cup}|$, then one there will coherent operations that are impossible in the $\Sigma$-ontology, but whether such coherent operations are physically interesting is another matter.

As an illustration, we can show how to include arbitrarily many pure points through the function $\varphi_*$, to create such impossibilities. Given ontic states (4), from equation (38) we obtain the ontic probability distributions for states in (8) to be:

\[
\begin{align*}
\mu^+_{X} &= \left( \frac{1}{2}, \frac{1}{2}, 0, 0 \right), \\
\mu^-_{X} &= \left( 0, 0, \frac{1}{2}, \frac{1}{2} \right), \\
\mu^+_{Z} &= \left( \frac{1}{2}, 0, \frac{1}{2}, 0 \right), \\
\mu^-_{Z} &= \left( 0, \frac{1}{2}, 0, \frac{1}{2} \right),
\end{align*}
\]

(47)

The operational theory characterized by space $\Sigma$ which is the convex hull of the states (8) is a non-simplex geometrically contained within the underlying gdit theory $\Sigma_{\cup}$.

This theory can be described as a nonsimplex in the convex hull of the classical states (4). From equation (47), we see that the ontic operations

\[
\begin{align*}
\gamma_1 &\leftrightarrow \gamma_4, \\
\gamma_2 &\leftrightarrow \gamma_3,
\end{align*}
\]

(48)

indeed implement inversion (44).

Suppose we add to $T$ any state quantumly realizable through a rotation with angle $\theta$ in the $X-Z$ (equatorial) plane. This is seen to be:

\[
\begin{align*}
|\psi^+_Y\rangle &= (\delta, 1 - \delta | v, 1 - v) \\
|\psi^-_Y\rangle &= (1 - \delta, \delta | 1 - v, v)
\end{align*}
\]

(49)

where

\[
\begin{align*}
\delta &= \frac{1}{2} (1 + \sin \theta), \\
v &= \cos^2 \left( \frac{\theta}{2} \right).
\end{align*}
\]

(50)
These can be derived from the corresponding ontic distributions:

\[
\begin{align*}
\mu_Y^+ &= (\delta \nu, \delta(1 - \nu), (1 - \delta)\nu, (1 - \delta)(1 - \nu)), \\
\mu_Y^- &= ((1 - \delta)(1 - \nu), (1 - \delta)\nu, \delta(1 - \nu), \delta \nu),
\end{align*}
\] (51)

where \(0 \leq \delta, \nu \leq 1\). Clearly, if the added pure points have the pattern (51), then \(\mu_Y^+ \leftrightarrow \mu_Y^-\) under ontic transformation (48), making all pure states are invertible.

However, consider the coherent transformation defined by:

\[
\begin{align*}
\psi_X^+ &\leftrightarrow \psi_X^- \\
\psi_Y^+ &\leftrightarrow \psi_Y^-.
\end{align*}
\] (52a)

Equation (52a) requires \(\gamma_1\) to transform to \(\gamma_2\) or \(\gamma_3\), neither of which is congruent with the equation (52b), as seen in equation (51). However, clearly the operation (52) is rather artificial.

On the other hand, the existence of fewer pure states in the overlying theory \(\Sigma\) than extreme points in the underlying \(\Sigma_{\cup}\) does not guarantee that all universal coherent operations are possible. To see this, suppose we replace the last two states in equation (39) by:

\[
\begin{align*}
|\psi_Y^+\rangle &\equiv (\frac{1}{3}, \frac{2}{3}, \frac{1}{2}, \frac{1}{2} | 1, 0) \\
|\psi_Y^-\rangle &\equiv (\frac{1}{3}, \frac{2}{3}, \frac{1}{2}, \frac{1}{2} | 0, 1).
\end{align*}
\] (53)

In this case, the resulting theory remains nonsimplicial, but the \(Z\) eigenstates satisfy \(\frac{1}{2}(\psi_Y^+ + \psi_Y^-) = (\frac{1}{3}, \frac{2}{3}, \frac{1}{2}, \frac{1}{2} | 1, 0)\). It follows that

\[
\begin{align*}
\mu_Y^+ &= \frac{1}{6}(\gamma_1 + \gamma_3) + \frac{2}{6}(\gamma_5 + \gamma_7) \\
\mu_Y^- &= \frac{1}{6}(\gamma_2 + \gamma_4) + \frac{2}{6}(\gamma_6 + \gamma_8),
\end{align*}
\] (54)

instead of the last two equations in (42). It is observed that in this case there is no ontic permutation of the kind (46), implying the lack of existence of a universal inverter.

### 7.3. Preparation contextuality and nonsimpliciality

Suppose there are different preparations \(P, P', \cdots\) that lead to the same outcome statistics in the operational theory \(T\) such that for all measurements \(M\), \(p(k|M, P) = p(k|M, P') = \cdots\). Thus, operationally, these preparations are indistinguishable or equivalent. Consider the ontological model for these preparations, given by the underlying probability distributions \(\mu_P(\lambda), \mu_{P'}(\lambda), \cdots\) over ontic states \(\lambda\). If \(\mu_P(\lambda) = \mu_{P'}(\lambda) = \cdots\), i.e. they are also ontologically indistinguishable, then theory \(T\) is said to be preparation non-contextual; else, the theory is preparation contextual [37].

Consider the regular theory determined by pure states (8). It satisfies the condition (16), in which the LHS and RHS represent distinct mixtures. The pure states are described by the ontological probability distributions \(\mu_X^\pm\) and \(\mu_Z^\pm\) given by (47). Since these ontological distributions satisfy
\[
\frac{1}{2} (\mu_X^+ (\lambda) + \mu_X^- (\lambda)) = \frac{1}{2} (\mu_Z^+ (\lambda) + \mu_Z^- (\lambda)),
\]
\[
= \left( \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right)
\]
\[
\equiv Y,
\]
(55)
the corresponding ontic mixtures also are indistinguishable and therefore preparation contextuality cannot be demonstrated in this case.

If the \(Y\)-outcomes are taken to be given by equation (49), then we have from equations (51) and (50)
\[
\frac{1}{2} (\mu_Y^+ (\lambda) + \mu_Y^- (\lambda)) = \frac{1}{4} (1 + \xi, 1 - \xi, 1 - \xi, 1 + \xi)
\]
\[
\neq Y,
\]
(56)
where \(\xi \equiv \frac{\sin(2\theta)}{2}\), giving a similar argument for preparation contextuality. Thus, only cases \(\theta = 0\) (corresponding to \(X\)) and \(\theta = \frac{\pi}{2}\) (corresponding to \(Z\)) are the two exceptional, preparation noncontextual cases.

The above counterexamples to preparation contextuality illustrate the following general result.

**Theorem 6.** A nonclassical theory \(\mathcal{T}\) is in general preparation contextual in the \(\Sigma\)-ontology.

**Proof.** Quite generally, let \(\mathcal{T}\) be a regular theory embedded in the gdit theory \(\mathcal{T}_{\Sigma}\), which is the convex hull of pure points \(g_j\) \((j \in \{0, 1, 2, \ldots, N\})\).

A nonsimpliciality condition in \(\mathcal{T}_{\Sigma}\) has the form:
\[
\sum_{j=0}^{M} g_j = \sum_{k=M+1}^{N} g_k,
\]
(57)
where \(M + 1 < N\) and the LHS and RHS represent preparation-like contexts, though not proper preparation contexts because gdit theories lack unambiguous preparability of pure states (see section 6.2).

Although map \(\varphi_{\Sigma}\) is non-injective, the map \(\varphi_{\Sigma}^{-1}\) is one-to-one when applied to the pure points \(g_j\)'s and thus well defined for the domain \(\{g_j\}\). However, upon inverting the individual \(g_j\)'s in the LHS and RHS of equation (57), we find by virtue of the simpliciality of the underlying simplex \(\Sigma_{\Sigma}\) that
\[
\sum_{j=0}^{M} \varphi_{\Sigma}^{-1} (g_j) \neq \sum_{k=M+1}^{N} \varphi_{\Sigma}^{-1} (g_k),
\]
(58)
which is a manifestation of the fact that \(\varphi_{\Sigma}\) is non-injective. Inequality (58) implies a preparation-like contextuality, since it demonstrates the two preparation-like contexts in the gdit theory are distinguishable ontologically.

Now consider the nonsimpliciality condition in the regular theory \(\mathcal{T}\):
\[
\sum_{j} \psi_j = \sum_{k} \phi_k,
\]
(59)
where $\psi_j$ and $\phi_k$ are possibly un-normalized basis states from two different bases. Equation (59) would be trivial if both the LHS and RHS independently sum to same quantity, typically $\sum_{j=0}^{N} g_j$, and thus (59) would not make use of the nonsimpliciality (57) of the underlying gdit theory.

Quite generally, the condition (59) can be satisfied by the requirement:

$$
\sum_{i} \psi_i = f \left[ \sum_{j=0}^{M} g_j \right] + (1 - f) \left[ \sum_{k=M+1}^{N} g_k \right],
$$

(60)

$$
\sum_{i} \phi_i = g \left[ \sum_{j=0}^{M} g_j \right] + (1 - g) \left[ \sum_{k=M+1}^{N} g_k \right],
$$

where $0 \leq f, g \leq 1$ and it is not necessary that $f = g$. Then we derive (59) nontrivially because in this case we must make use of equation (57). The trivial case corresponds to $f = g$.

Mapping the two LHS in (60) to the underlying simplex by applying $\varphi_\Psi^{-1}$ to the $g_j$’s we obtain the corresponding mixtures in the underlying simplex $\sum_\Psi$:

$$
\varphi_\Psi^{-1} : \sum_{i} \psi_i \mapsto f \left[ \sum_{j=0}^{M} \varphi_\Psi^{-1}(g_j) \right] + (1 - f) \left[ \sum_{k=M+1}^{M+N} \varphi_\Psi^{-1}(g_k) \right],
$$

$$
\equiv \varphi_\Psi^{-1}(\Psi)
$$

$$
\varphi_\Phi^{-1} : \sum_{i} \phi_i \mapsto g \left[ \sum_{j=0}^{M} \varphi_\Phi^{-1}(g_j) \right] + (1 - g) \left[ \sum_{k=M+1}^{M+N} \varphi_\Phi^{-1}(g_k) \right],
$$

(61)

$$
\equiv \varphi_\Phi^{-1}(\Phi).
$$

However, in view of equation (58), it follows that

$$
\varphi_\Psi^{-1}(\Psi) \neq \varphi_\Phi^{-1}(\Phi),
$$

(62)

entailing that two distinct underlying states map to the same mixture in the overlying theory $\mathcal{T}$, which implies preparation contextuality.

As a simple illustration of preparation contextuality in $\sum$-ontology, note that in the case of the 2-input-2-output gdit theory, the nonsimpliciality condition among the four extreme points $(j,k)$, where $j,k \in \{0,1\}$, is given by:

$$
\frac{1}{2}[(0,0) + (1,1)] = \frac{1}{2}[(0,1) + (1,0)].
$$

(63)

Under $\varphi_\Psi^{-1}$, the LHS maps to the mixture $(1,0,0,1)$ in the underlying simplex $\sum_{\Psi}$ whilst the RHS maps to $(0,1,1,0)$.

According to theorem 6, we obtain preparation contextuality for bases in which the uniform mixture of the eigenstates should correspond to an ontic mixture in $\sum_{\Phi}$ of the form $(a,b,b,a)$ where $2(a+b) = 1$ while $a \neq b$. This explains why we fail to obtain a proof for preparation contextuality using the measurements $X$ and $Z$, as determined by equation (8), in view of (55). On the other hand, by a similar argument, any two measurements $Y$ parametrized by two distinct values of $\theta \in \left[0, \frac{\pi}{2}\right]$ in equation (51) yield an argument for preparation contextuality by virtue of equation (56).
All the above nonclassical features, whether with reference to the ontology or not, require only measurement incongruence, without reference to the question of the transitivity of congruence or its extendability to higher orders. These features correspond to what we call as base level nonclassicality. In the following sections, we shall consider nonclassical phenomena arising when congruence is not transitive or extendable to higher orders, and correspond to so-called ‘higher-level’ nonclassicality.

8. From incongruence to contextuality

If pairwise congruence is transitive in a regular theory $\mathcal{T}$, then the above theorems (discussed in section 5) suffice to characterize the nonclassicality of the theory. Further, the geometro-ontological models discussed previously (in section 7) also apply.

However, if pairwise congruence is intransitive in general in $\mathcal{T}$, then any definite value assignment to all the measurements in question can not be context-independent. Therefore, the above ontological models, which presume a JD for all measurements, cannot be applied without suitable generalization.

Now assume that congruence is extendable, whereby if $A$ and $B$ are congruent and so are $B$ and $C$, then it is assumed that $A$, $B$, and $C$ are jointly measurable, and so on for any number of measurements. Later we will discuss examples of how extendability can break down.

**Theorem 7.** If a regular operational theory $\mathcal{T}$ in which congruence is transitive and extendable, then all states in $\mathcal{T}$ have a joint distribution (JD) in an outcome-deterministic underlying model. However, the converse is not true (i.e. intransitivity does not imply lack of JD).

**Proof.** The classical case, where all measurements are pairwise congruent, is trivial. For the case where no two variables are congruent (and thus congruence is trivially transitive), given measurements $X, Y, Z, \ldots$, one can always construct the JD in an underlying theory, given by

$$P(x, y, z, \ldots) = P(x)P(y)P(z) \cdots$$

For the case where incongruence exists but congruence is transitive, we can partition all measurements into equivalence classes $Q_j$, whereby all measurements $Q_k(j)$ within the class are congruent, and any two measurements in different classes, such as $Q_k(j)$ and $Q_j(m)$ ($m \neq n$) are incongruent. All measurements in a given equivalence class are jointly congruent and therefore jointly measurable, by the assumption of extendability.

We can thus treat each equivalence class as a single ‘class measurement’ $Q_j$ determined by a probability distribution $P^0_j$. Therefore we can always write down a JD in an underlying (outcome deterministic) model for all measurements, given by:

$$P(q_1^{(1)}, q_2^{(2)}, \ldots, q_2^{(1)}, q_2^{(2)}, \ldots) = P^0_1P^0_2 \cdots$$ \hspace{1cm} (64)

where the LHS denotes the probability over all measurements in the theory.

To see that the converse is not true, consider the theory (fragment) $\mathcal{T}_{2,2}$ consisting of four measurements, $\mathcal{A} \equiv \{A_1, A_2\}$ and $\mathcal{B} \equiv \{B_1, B_2\}$, such that any element of $\mathcal{A}$ is congruent with any element of $\mathcal{B}$, i.e. any pair $(A_j, B_k)$ is congruent, which we represent by $R(A_j, B_k)$ where $R$ represents the congruence relation template. Now suppose we have $\neg R(A_1, A_2)$ but $R(B_1, B_2)$, i.e. incongruence on only one side. We then have intransitivity from the chains $R(A_1, B_1), R(B_1, A_2)$ and $R(A_1, B_2), R(B_2, A_2)$. However, this does not lead to lack of JD, because we can construct a JD based on the quantities that can be jointly measured:
\[ P(A_1, A_2, B_1, B_2) = \frac{P(A_1, B_1, B_2)P(A_2, B_1, B_2)}{P(B_1, B_2)}, \]  

(65)

which has been constructed such that tracing out \( A_1 \) or \( A_2 \) or \( A_1 A_2 \) returns the operational probabilities.

In light of this result, the existence of incompatibility is necessary but not sufficient for a Kochen-Specker theorem contextuality [31]. A non-trivial super-transitive structure of congruence is required to thwart JD.

In respect of the above example, note that if we have incongruence among both the \( A_j \)’s and \( B_k \)’s, i.e. \( \neg R(A_1, A_2) \) and \( \neg R(B_1, B_2) \), then it can be shown that JD does not exist. Therefore, in such a \( \{A, B\} \) scenario, we obtain a tight link between congruence and JD, which clarifies such a link studied by various authors [18–22].

8.1. Unextendability of congruence

We now point out how congruence of measurements can fail to be extendable. An example is provided by Specker’s ‘overprotective seer’ (OS) correlations [54]. Here let \( A, B \) and \( C \) be three dichotomic measurements, such that any two are congruent and can be measured, and the outcomes will be anticorrelated with equal probability. However, they can’t be jointly measured because there is no JD over measurements \( A, B, C \) for the state. If it did, it must be probability distribution of the 8 three-bit string \( abc \in \{+1, -1\}^3 \). Anticorrelation on \( AB \) and on \( BC \) implies \( abc \) is of the pattern \( + - + \) or \( - + - \), but in this case \( AC \) will not be anticorrelated. The quantity \( \langle AB \rangle + \langle BC \rangle + \langle AC \rangle \), which is the OS inequality, thus reaches noncontextuality the minimum of -1.

We can now extend Specker’s idea to an ‘extended OS’ (XOS) theory. Consider the state \( \rho \) in an operational theory, which has the property that for any three-way joint-measurement, all three outcomes must be distinct. There is no JD over measurement outcomes \( a, b, c \) and \( d \) that can satisfy this. To see this suppose that we assign 0, 1, 2 to \( A, B, C \). Then to satisfy the distinctness requirement for \( B, C, D \), we should assign 0 to \( D \). However, this assignment scheme will imply that measuring \( A, B, D \) would yield 0, 1, 0, violating the outcome distinctness requirement.

This contextual correlation in the extended OS theory can be experimentally tested via the violation of the inequality:

\[ \langle ABC \rangle + \langle BCD \rangle + \langle CDA \rangle + \langle DAB \rangle \leq 2, \]  

(66)

where each of the four summands is experimentally determined as follows.

For any three jointly measurements (say \( A, B, C \)), in each trial determine the maximum, intermediate and minimum outcomes of the three measurements, which are denoted \( v_{\text{max}}, v_{\text{mid}} \) and \( v_{\text{min}} \), respectively, provided the three are distinct. If the three outcomes are not distinct but one of them is distinct from the other two, then assign \( v_{\text{max}} \) (resp., \( v_{\text{min}} \)) to the larger (resp., smaller) outcome and assign \( v_{\text{mid}} \) to the outcome is majority. (E.g. if measuring \( A, B, C \) produces outcomes 0, 1, 1 then assign 0 to \( v_{\text{min}} \) and 1 to both \( v_{\text{mid}} \) and \( v_{\text{max}} \).) If all three outcomes of a three-way joint measurement are identical, then assign that value uniformly to \( v_{\text{max}}, v_{\text{mid}} \) and \( v_{\text{min}} \).

For any three measurements (say \( A, B, C \)), the quantity

\[ ABC \equiv \langle (v_{\text{max}} - v_{\text{mid}})(v_{\text{mid}} - v_{\text{min}}) \rangle, \]  

(67)
where the angles indicate the average over a number of trials. In each trial, the quantity $(v_{\text{max}} - v_{\text{mid}})(v_{\text{mid}} - v_{\text{min}})$ is 1 only if the outcomes are distinct (i.e. 0, 1, 2), and zero otherwise (e.g. 0, 1, 1, 1). The other summands in equation (66) are calculated in this way. For any noncontextual value assignment of $A, B, C, D$, it may be checked that the LHS is bounded above by 2. On the other hand, for XOS theory, the LHS of (66) attains the algebraic maximum of 4.

The above consideration about other possible structures prompts us to reflect on why compatibility in QM does not seem to be unextendable. Here we propose that this is ‘the most natural’ for a nonclassical theory. The reason is that otherwise, nonseparability would intervene mysteriously at some higher despite compatibility at lower orders. This would mean that nonseparability does not occur as a consequence of failure of extendability of congruence. Thus, the ‘nice’ connection to intransitivity of congruence would be lost, making the theory more complicated. From this perspective, QM is a natural nonclassical theory, which provides a possible explanation for the absence of OS type correlations in QM.

9. Ontology for contextual theories

From the perspective of $\Sigma$-ontology, basic nonclassicality of a regular theory arises essentially because of the compressive action of $\varphi_\Sigma$ on the underlying simplex $\Sigma_{\nu}$ (the map $\varphi_\star$ adds attractive features like pure state preparability). The simplex $\Sigma_{\nu}$ itself has a direct product structure and is quite classical. In particular, the underlying versions of the measurements are separable, meaning that any state $\psi$ has a JD over the values of the measurements. This idea forms the basis of the underlying simplex $\Sigma_{\nu}$. Higher nonclassicality will be seen to correspond to the addition of a further fundamental type of nonclassicality, which occurs when the underlying simplex itself deviates from the direct product structure form, leading to quantum contextuality.

When a contextuality inequality is violated and hence no JD exists, the underlying simplex $\Sigma_{\nu}$ of the type described earlier, which assumes separable measurements, does not exist. One can still envisage an underlying simplex, provided we enlarge the convex direct product suitably. We shall find that the convex contextual product, denoted by the symbol $\boxtimes$, fulfills this requirement. Essentially, the operation $\boxtimes$ is a recursive application of $\otimes$ to combinations of measurements. This will be used to define an underlying simplex, $\Sigma_{\nu}^{\otimes}$, suitable for contextual-ity. Here $\theta$ is the ‘valency’ of an measurement, meaning the number of other measurements it must combine with, to determine the full measurement context. We shall sometimes indicate the valency by a subscript to the $\otimes$ operator.

Suppose $\theta = 1$, so that the context is specified by a single fiducial measurement. Given fiducial measurements $X, Y, Z, \ldots$, we define

$$\Sigma_X \boxtimes_1 \Sigma_Y \boxtimes_1 \Sigma_Z \boxtimes_1 \cdots \equiv \Sigma_{XY} \otimes \Sigma_{YZ} \otimes \Sigma_{XZ} \otimes \cdots,$$

(68)

where $\Sigma_{XY} = \Sigma_X \otimes \Sigma_Y$, and so on. For $\theta = 2$, the RHS will contain operands such as $\Sigma_{XYZ}$, meaning that the context is specified by two measurements, an example of which is studied later. Here it suffices to note that, as with the convex direct product, if the convex sets being combined are simplexes, then the convex contextual product is a simplex. In general, the marginal probabilities $P_X, P_Y, P_Z, \cdots$ are not well defined, which may be averted by imposing additional backward consistency conditions. In the absence of backward consistency, the full combined space will be of the form $\Sigma_{XYZ} \otimes \Sigma_{XYZ}^{(1)} \otimes \Sigma_{XYZ}^{(2)} \cdots$, i.e. probabilities are explicitly specified for different valencies.
In particular, the vertices of convex set $\Sigma_{\theta}^{\bullet}$ are in general classical (deterministic) contextual configurations, meaning, they correspond to a classical mechanism to reproduce contextual behavior. The underlying simplex $\Sigma_{\theta}$ introduced in section 7 corresponds to $\theta = 0$.

An example for a classical contextual configuration suitable to simulate the OS theory would be as follows: the properties $X, Y, Z$ have definite values 0, 0, 1, except that if $X$ is measured along with $Y$, then a hidden mechanism causes a ‘signal’ to be transmitted from $Y$ to $X$ instructing $X$ to flip its bit value. This may be represented as follows:

$$
\begin{array}{c|c}
\text{input} & \text{output} \\
XY & 10 \\
YZ & 01 \\
ZX & 10 \\
\end{array}
$$

For the OS theory, there are $4^3 = 64$ classical contextual configurations such as (69), which constitute the vertices of a 63-simplex, denoted $\Sigma_{\theta}^{\bullet}$, or simply $\Sigma_{\theta}^{\bullet}$, given by:

$$
\Sigma_{\theta}^{\bullet} = \Sigma_X \uplus \Sigma_Y \uplus \Sigma_Z.
$$

Our strategy will be to use this object as the underlying simplex and impose backward consistency on the gdit space derived by application of the compression operation $\varphi_{\theta}$.

In g-type ontology, the action of $\varphi_{\theta}$ on $\Sigma_{\theta}^{\bullet}$ is a transformation analogous to that of going from the form of equation (1) to that of equation (7). Under this mapping, the classical contextual configuration equation (69) yields

$$
\begin{array}{c|c}
\text{input} & \text{output} \\
XY & 10 \\
YZ & 01 \\
ZX & 10 \\
\end{array}
$$

which can be represented more conventionally as:

$$
\begin{array}{c|c}
\text{input} & \text{output} \\
XY & 10 \\
YZ & 01 \\
ZX & 10 \\
\end{array}
$$

the contextual gdit, since it is the gdit version of these classical deterministic configurations.

Since compression $\varphi_{\theta}$ preserves the extreme points, there are 64 contextual gdits, whose convex hull is the corresponding gdit theory space $\Sigma_{\theta}^{\bullet}$, the underlying contextual gdit space, with dimension $3 \times (4 - 1) = 9$ (a 7-fold reduction in dimensionality).

This contextual gdit violates the ‘no-signaling’ conditions for single systems, more precisely, non-contextuality of probabilities in the sense of Gleason’s theorem [55, 56]:

$$
\begin{align*}
P(a|AB) &= P(a|AC), \\
P(b|BA) &= P(b|BC), \\
P(c|CA) &= P(c|CB),
\end{align*}
$$

where $P(a|AB)$ denotes the probability to obtain outcome $a$ when $A$ is measured alongside $B$.

It is convenient to compose the crumpling map in terms of two sub-mappings:

$$
\varphi_* = \varphi_{\theta} \circ \varphi_{\theta}^+.
$$

The mapping $\varphi_{\theta}^+ : \Sigma_{\theta}^{\bullet} \rightarrow \Sigma^+$ imposes the ‘contextual no-signaling’ conditions (73), where $\Sigma^+$ refers to the contextual no-signaling polytope, i.e. the largest convex set embedded in $\Sigma_{\theta}^{\bullet}$, consistent with contextual no-signaling. Obviously, $\Sigma \subseteq \Sigma^+$, and mapping $\varphi_{\theta}^- : \Sigma^+ \rightarrow \Sigma$. 

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For a theory of 3-input-\(n\)-outcome systems, equation (73) would impose \(\mathcal{N}_G \equiv 3(n - 1)\) conditions, whilst the dimension of the contextual gdit theory \(\Sigma_{\mathcal{G}}\) underlying the OS theory would be \(\mathcal{D}_{\mathcal{G}} \equiv 3(n^2 - 1)\). Therefore, with imposition of conditions (73), the dimension of the contextual no-signaling polytope \(\Sigma^+\), embedded within the gdit polytope \(\Sigma_{\mathcal{G}}\) is, \(\mathcal{D}_{\mathcal{G}} - \mathcal{N}_G = 3n(n - 1)\). By tomographic separability, the nonsimplex \(\Sigma\) for a 3-input-\(n\)-output regular theory has dimension \(3(n - 1)\). Therefore the map \(\varphi^+ : \Sigma^+ \to \Sigma\) involves a further \(n\)-fold reduction of dimensionality (for a discussion on dimensionality mismatch in a different context, see [57]).

Example. The following six contextual OS gdits

| Input | \(Q_A^1\) | \(Q_A^2\) | \(Q_B^1\) | \(Q_B^2\) | \(Q_C^1\) | \(Q_C^2\) |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| \(AB\) | 01        | 10        | 01        | 10        | 01        | 10        |
| \(BC\) | 10        | 01        | 01        | 10        | 10        | 01        |
| \(CA\) | 01        | 10        | 10        | 10        | 01        | 10        |

each of which violates the OS inequality, by reaching the algebraic minimum of \(-3\). In equation (74), the first column is the pair of joint inputs, and each other column is the output corresponding to a given deterministic contextual box \(Q^j\). Here the box \(Q_A^1\) is just the gdit represented in equation (72). The superscript corresponds to the measurement for which a Kochen-Specker contradiction would arise in a realistic assignment of values.

The vertices of the contextual no-signaling polytope \(\Sigma^+\) derived from the above contextual gdit polytope has vertices formed by equally mixing a gdit like \(Q_A^1\) and its ‘partner’ gdit \(Q_A^2\), where the latter is obtained from the former by flipping the outcome bits, and \(j \in \{A, B, C\}\). For the contextual gdits in (74), we obtain the three nonsignaling contextual boxes \(Q^j \equiv \frac{1}{2} \left( Q_A^j + Q_B^j \right)\), which violate equation (66) by reaching its algebraic minimum, but respect the Gleason no-signaling conditions (73).

Any state in the polytope generated by these contextual no-signaling boxes \(Q^j\) has uncertainty \(U = \frac{1}{2}\) as per (25), where the uncertainty arises from the underlying mixing. We observe that the no-signaling feature is essentially equivalent to backward consistency. Therefore, any such state in \(\Sigma^+\) is backward consistent, in contrast to states in \(\Sigma_{\mathcal{G}} - \Sigma^+\), in particular, the contextual gdits \(Q^j\). The \(Q^j\)'s are the contextuality analogues of the PR boxes [58, 59], which violate the CHSH inequality for quantum nonlocality to its algebraic maximum.

The complementarity between signaling and randomness in the context of nonlocality [60], based on techniques developed in [61], and first conjectured in [62, 63], can be formulated analogously for contextuality, reported elsewhere. Similarly, one may consider the single-system analog of device-independent quantum cryptography [64–67], based on contextuality inequalities [68].

As in the case of OS theory, the underlying contextual simplex \(\Sigma_{\mathcal{G}}^\circ\) for the XOS theory can be constructed with vertices given by classical signaling configurations. Under the map \(\varphi^\circ\), these configurations transform to XOS contextual gdits, which are the vertices of the underlying contextual gdit polytope, \(\Sigma_{\mathcal{G}}^\circ\). Three such contextual gdits, which are the XOS equivalents of (74), are:
each of which violates the XOS contextuality inequality (66) to its algebraic maximum of 4. As in the OS case, each contextual XOS gdit $R_j$ violates contextual no-signaling.

Under the crumpling map $\varphi^*: \Sigma^* \rightarrow \Sigma^+$ we obtain the contextual no-signaling polytope $\Sigma^+$ appropriate to the XOS toy theory, whose vertices include contextual boxes, one of which is obtained by taking a uniform average $\frac{1}{3} (R_1 + R_2 + R_3)$.

Finally, it is worth contrasting our combinatoric approach to contextuality from that of [30, 50, 51], where graph theoretic representations of contextuality and nonlocality are explored, which we mentioned in section 7. One key difference is that in our approach, the adjacent vertices of the graph representing a contextuality situation are compatible measurements, whereas in [30] they are exclusive events associated with a pair of measurements and in [50] with orthogonal vectors in $\mathbb{R}^d$. The difference in these approaches may be attributed to the different motivations. For example, in [30], the authors aim to uncover a fundamental axiom to explain the level of quantum violation of contextuality inequalities, whereas our motivation here has been to interpret contextuality as a higher-level manifestation of nonclassicality, that is fundamentally associated with the nonsimplicial character.

### 10. Conclusions

For a class of general probability theories of single systems, we point out that a number of nonclassical features like multiple pure-state decomposability, measurement disturbance, lack of certain universal operations, measurement uncertainty and no-cloning, can be accounted for by the assumption that the state space is not a simplex. These nonclassical features can be explained in terms of an epistemic interpretation for which an underlying simplex serving as a noncontextual ontological model. A base-level nonclassical theory would be nonclassical in the sense of possessing a no-cloning theorem etc, but would lack KS contextuality. An example of such a theory is Spekkens toy theory [25]. For contextuality, the further assumption about the intransitivity of congruence is necessary.

In Spekkens’ toy theory, a single system has three measurements (‘questions’). All equal mixtures of maximal knowledge states of the three measurements are operationally indistinguishable, meaning that the state space is non-simplicial, though in that work it was not described geometrically, but instead as a manifestation of the ‘knowledge-balance’ principle. On the other hand, all of three measurements are pairwise incongruent, so that the possibility of intransitivity of pairwise congruence does not arise. Our result thus explains why the theory reproduces many nonclassical features, but not KS contextuality. Therefore, in response to Spekkens’ open question [25, section IX], as to what other principle, besides the knowledge-balance principle, is required to capture the remaining quantum phenomena, our approach suggests: namely, the intransitivity or unextendability of pairwise congruence.

Here we only consider single systems, without reference to correlated systems, in contrast to various current foundational studies. Thus, in the absence of other assumptions, all nonclassical features derived in our study are logically independent of whether or not the theory in question is nonlocal or nonsignaling.
By identifying nonclassical features that are logically related and those that are logically independent in any regular theory, our approach could provide a new perspective for axiomatic reconstructions of QM [2, 7, 41, 69–72].

In QM, various nonclassical features are tied closely together by the single theme of noncommutative algebra, making it difficult to discern basic interdependence from independence. Our approach helps disentangle the relationship between different nonclassical features. For instance, it shows that any nonclassical theory $T$ with a no-cloning theorem is also expected to possess measurement uncertainty and measurement disturbance. Thus, these latter features do not require any ‘further explanation’.

Finally, we believe that the explanatory value of an axiomatic approach is enhanced by the choice of axioms that appear ‘natural’ and that are naturally connected with each other. Thus, once one isolates the most elementary surprise about a theory and identifies it as the basic axiom, this should lead us smoothly to the other axiom(s). In our work, it may be hoped that pairwise measurement incongruence serves as such a basic axiom for QM, which then naturally leads to the question of (in)congruence among multiple properties, leading to contextuality.

The requirement of naturalness of axioms is not entirely aesthetic, but based on our perception that fulfilling it would position us in the state of ‘the right ignorance’ that would guide us to the right questions answering which would enable us to understand why QM has this particular mathematical structure.

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