Journal of Physics A:
Mathematical and Theoretical

PAPER

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To cite this article: Rafael Wagner *et al* 2023 *J. Phys. A: Math. Theor.* **56** 505303

IOP Publishing — Journal of Physics A: Mathematical and Theoretical
J. Phys. A: Math. Theor. **56** (2023) 505303 (32pp) https://doi.org/10.1088/1751-8121/ad0bcc

Using a resource theoretic perspective to witness and engineer quantum generalized contextuality for prepare-and-measure scenarios

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Received 5 September 2023; revised 3 November 2023
Accepted for publication 10 November 2023
Published 27 November 2023

Abstract
We employ the resource theory of generalized contextuality as a tool for analyzing the structure of prepare-and-measure scenarios. We argue that this framework simplifies proofs of quantum contextuality in complex scenarios and strengthens existing arguments regarding robustness of experimental implementations. As a case study, we demonstrate quantum contextuality associated with any nontrivial noncontextuality inequality for a class of useful scenarios by noticing a connection between the resource theory and measurement simulability. Additionally, we expose a formal composition rule that allows engineering complex scenarios from simpler ones. This approach provides insights into the noncontextual polytope structure for complex scenarios and facilitates the identification of possible quantum violations of noncontextuality inequalities.

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Keywords: generalized contextuality, prepare-and-measure scenarios, quantum information, measurement simulability

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

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1. Introduction

Prepare-and-measure type experiments are essential setups corresponding to practical tasks, such as communication protocols, key distribution, computing, among many others. An important question in quantum information is finding quantum-over-classical advantages for these protocols. For this question to be rigorously approached, it is crucial to decide upon one of the various existing notions of *classicality*. Common choices include incoherent states [1, 2], Kochen–Specker (KS) noncontextuality [3], and Bell's notion of local causality [4, 5]. Throughout this work, we will consider the notion of classicality provided by generalized noncontextuality in [6]. This notion subsumes KS-noncontextuality [7–12], and has concrete relations with the others mentioned [13–16].

After it was proved that quantum theory is contextual in this generalized sense [6], several works have shown that contextuality underpins advantages in quantum protocols when compared to their classical counterparts. Some examples are parity oblivious tasks [13, 17], quantum state discrimination tasks [18], state-dependent quantum cloning [19], linear response processes [20] and quantum interrogation [21]. Nonetheless, finding novel techniques to detect quantum contextuality that are suitable to deal with complex scenarios is important for taking advantage of such a nonclassical feature in practical tasks.

The framework of resource theories provides a concrete and formal treatment for the quantification, manipulation and conversion of nonclassical resources [22, 23]. Despite the results outlined above, and the success of the resource theories of coherence [24–26], KS-contextuality [27–33], and nonlocality [34, 35], research on a resource theory for generalized contextuality is still in its infancy [36].

In this work, we provide novel tools in such direction. Following the linear characterization of generalized noncontextuality from [37] and the resource theory constructed from the underlying polytope structure presented in [36], we develop techniques to reduce complex scenarios to smaller ones, where the existence of contextuality serves as a witness for contextuality in the original scenario. These tools allow us to reinterpret the results of [38], as well as to witness the existence of quantum contextuality for a class of prepare-and-measure scenarios. Such a class encompasses the majority of already known proofs of contextual advantage and further generalizes it for a large class of experimental realizations. We also identify a class of scenarios with quantum violations for *all nontrivial nocontextuality inequalities*. Notably, we uncover that contextuality in the state-dependent cloning scenario of [19] is inherited from a product of simpler scenarios. Overall, these results highlight the potential usage of our techniques for witnessing and engineering nonclassical correlations in complex scenarios lifted from simpler ones.

In section 2, we briefly review the notion of generalized noncontextuality. Section 2.1 describes prepare-and-measure scenarios and how noncontextual ontological models attempt to explain the statistics arising from these experimental scenarios. Section 2.2 describes measurement simulability in operational theories, while section 2.3 discusses the elements of the resource theory we are considering, with a particular focus on the free operations. In section 3 we describe our results in general terms, using a link between simulability and the free operations of a resource theory (section 3.1), and a binary composition of scenarios (section 3.2). We then use these tools to witness and engineer quantum contextuality, in section 3.3. In section 4 we expose conclusions and perspectives.

2. Preliminaries

2.1. Generalized contextuality

Contextuality, as a notion of nonclassicality, is an inference between the operational description of an experimental setup and the ontological models one might prescribe to it. An operational theory is formally a process theory where processes are considered as lists of laboratory instructions with a probability rule [39]. To operationally describe a prepare-and-measure experiment, one must provide some set of laboratory procedures that prepare the studied system, together with a set of possible measurements that shall extract outcome information. The most general result from such procedures is described through conditional probabilities. We will consider the case of prepare-and-measure experiments with a finite set of preparation procedures, that we denote by $\mathbb{P} := \{P_j\}_{j\in J}$, and a finite set of measurement procedures, $\mathbb{M} := \{M_i\}_{i\in I}$, leading to some outcome results that we label $\mathbb{O}_{\mathbb{M}} \equiv K$. Capital letters K, J and I denote the set of labels with the same cardinality of the sets of primitives, $\mathbb{O}_{\mathbb{M}}, \mathbb{P}, \mathbb{M}$ respectively, while $|\cdot|$ represents the cardinality of the set (e.g. $|I|$ is the number of measurement procedures in the experimental scenario). The measurement *event* associated to obtaining outcome k for measurement M will be denoted $[k|M]$. Performing all the operations several times to acquire statistics will lead to a datatable of conditional probabilities, that we denote as B:

$$B := \{p(k|M_i, P_j)\}_{k\in K, i\in I, j\in J}. \tag{1}$$

We name B as the *behavior* of the system. Each physical realization will lead to some behavior B in the set of all possible behaviors. Operationally, there are more structures within an experimental description. For instance, it might be so that there are operationally equivalent ways to generate some statistics; as a standard example, consider the quantum preparations P_j[7] associated to preparations of the quantum states ρ^j,

$$\rho^1 = |0\rangle\langle 0|, \tag{2}$$

$$\rho^2 = |1\rangle\langle 1|, \tag{3}$$

$$\rho^3 = |+\rangle\langle +|, \tag{4}$$

$$\rho^4 = |-\rangle\langle -|. \tag{5}$$

For these preparation procedures, it is known that

$$\frac{1}{2}\rho^1 + \frac{1}{2}\rho^2 = \frac{1}{2}\rho^3 + \frac{1}{2}\rho^4, \tag{6}$$

meaning that the statistics for the measurement events $[k|M_i]$ will be the same for the above convex mixtures of $\{\rho^j\}_{j\in J}$. Such a description hints at what is understood as an *operational equivalence*.

Definition 1 (Operational equivalences). Let P, P' be two preparation procedures on an operational theory. Let $\mathcal{M}$ be a tomographically complete set of measurement procedures. Then, the procedures are operationally equivalent, and we write $P \simeq P'$, if and only if,

$$\forall [k|M], M \in \mathcal{M}, k \in \mathbb{O}_{\mathbb{M}}, \; p(k|M, P) = p(k|M, P'). \tag{7}$$

Equivalently, let $[k|M]$ and $[k'|M']$ be two measurement events, and $\mathcal{P}$ be a tomographically complete set of preparation procedures. Then, the events are operationally equivalent, and we write $[k|M] \simeq [k'|M']$, if and only if,

$$\forall P \in \mathcal{P}, \; p(k|M, P) = p(k'|M', P). \tag{8}$$

Let us imagine a situation in which an experimenter prepares single-photons and sends them through two different modes, that we denote 0 and 1. The experimenter then implements the procedure 'Send the single-photons through each mode with equal probability'. We call this procedure $P_{0/1}$. As another possibility, the experimenter can set-up a balanced beam-splitter between the two modes. In this case, they then implement the procedure 'Send, with equal probability, the single-photons through each mode, that later pass through a balanced beam-splitter.' We call this procedure $P_{+/-}$. Any conceivable measurement extracting mode information will not be able to distinguish between these two procedures, i.e. ideally $p(k|M, P_{0/1}) = p(k|M, P_{+/-})$, $\forall [k|M]$. Using the quantum formalism,

$$p(k|M, P_{0/1}) = \mathrm{Tr}\left(E_k\left(\frac{1}{2}\rho^1 + \frac{1}{2}\rho^2\right)\right) = \mathrm{Tr}\left(E_k\left(\frac{1}{2}\rho^3 + \frac{1}{2}\rho^4\right)\right) = p(k|M, P_{+/-}),$$

[7] More precisely, each state ρ_j defines an *equivalence class* $[P_j]$ of equivalent procedures implementing the same state.

for all possible POVMs $\{E_k\}_k$. The concept of operational equivalence will be fundamental in the definition of the generalized noncontextuality we will introduce.

Equivalences are part of the description of any operational theory, quantum or not; those denote the fact that some operational procedures (maybe defined as convex mixtures of others) cannot be distinguished using only the probabilities in the experiment. A set of non-trivial, fixed and finitely defined operational equivalences for the preparation procedures is denoted by $\mathbb{E}_{\mathbb{P}}$, when $a = 1, \ldots, |\mathbb{E}_{\mathbb{P}}|$,

$$\sum_j \alpha_j^a P_j \simeq \sum_j \beta_j^a P_j, \tag{9}$$

where $\sum_j \alpha_j^a = \sum_j \beta_j^a = 1$, and $0 \leqslant \alpha_j^a, \beta_j^a \leqslant 1$. At the level of the behaviors, we assume that convex mixtures of procedures will be respected, so that for all measurement events, we have

$$\sum_j \alpha_j^a p\left(k|M_i P_j\right) = \sum_j \beta_j^a p\left(k|M_i P_j\right). \tag{10}$$

Thus, each label a uniquely defines a vector $\boldsymbol{\gamma}_{\mathbb{P}}^a \equiv (\boldsymbol{\alpha}^a; \boldsymbol{\beta}^a)$ associated with the preparation procedures,

$$\boldsymbol{\gamma}_{\mathbb{P}}^a := \left(\alpha_1^a, \ldots, \alpha_{|J|}^a; \beta_1^a, \ldots, \beta_{|J|}^a\right). \tag{11}$$

Similarly for the measurement events, we define a set $\mathbb{E}_{\mathbb{M}}$, where the operational equivalences $b = 1, \ldots, |\mathbb{E}_{\mathbb{M}}|$,

$$\sum_{i,k} \alpha_{[k|M_i]}^b \left[k|M_i\right] \simeq \sum_{i,k} \beta_{[k|M_i]}^b \left[k|M_i\right] \tag{12}$$

uniquely define vectors $\boldsymbol{\gamma}_{\mathbb{M}}^b \equiv (\boldsymbol{\alpha}^b; \boldsymbol{\beta}^b)$,

$$\boldsymbol{\gamma}_{\mathbb{M}}^b := (\alpha_{[1|M_1]}^b, \ldots, \alpha_{[|K||M_1]}^b, \ldots, \alpha_{\left[|K||M_{|I|}\right]}^b; \tag{13}$$

$$\beta_{[1|M_1]}^b, \ldots, \beta_{[|K||M_1]}^b, \ldots, \beta_{\left[|K||M_{|I|}\right]}^b). \tag{14}$$

Hence, we define the sets $\mathbb{E}_{\mathbb{P}} := \{\boldsymbol{\gamma}_{\mathbb{P}}^a\}_{a=1}^{|\mathbb{E}_{\mathbb{P}}|}$ and $\mathbb{E}_{\mathbb{M}} := \left\{\boldsymbol{\gamma}_{\mathbb{M}}^b\right\}_{b=1}^{|\mathbb{E}_{\mathbb{M}}|}$, which completes the elements for the definition of a scenario. We say that an operational equivalence $\boldsymbol{\gamma}$ as defined above is trivial if $\boldsymbol{\alpha} = \boldsymbol{\beta}$.

Nontriviality is required to get rid of self-equivalences, since, for example, any preparation is always equivalent to itself in its own experimental setting. Hence, writing $\mathbb{E}_{\mathbb{M}} = \emptyset$ does not mean that there are no operational equivalences between measurement events, but that the experimentalist is not considering equivalences different from those of the form $M_1 \simeq M_1$ that represent no interesting constraints.

Definition 2 (Prepare-and-measure scenario). A prepare-and-measure scenario is constituted by the tuple $\mathbb{B}$ given by

$$\mathbb{B} = (\mathbb{P}, \mathbb{M}, \mathbb{O}_\mathbb{M}, \mathbb{E}_\mathbb{P}, \mathbb{E}_\mathbb{M})\,. \tag{15}$$

The first three elements in the tuple $\mathbb{B}$ are common to any prepare-and-measure experimental investigation, while the other two are required, as we will see later, for analyzing the existence of generalized contextuality. If a behavior B is obtained from prepare-and-measure implementations of the three first elements of $\mathbb{B}$, while satisfying the equivalences from the last two, we will often write $B \in \mathbb{B}$. Each element of any scenario $\mathbb{B}$ represents finitely chosen procedures available in a laboratory.

Whenever it is convenient, and since we are mostly interested in the labels for the procedures, we might follow the notation of [40], and write $\mathbb{B} = (|J|, |I|, |K|, \mathbb{E}_\mathbb{P}, \mathbb{E}_\mathbb{M})$. Notice that scenarios do not need to have tomographically complete sets of procedures, $\mathbb{P} \subset \mathcal{P}$, but the operational equivalences must hold for $\mathcal{P}$, the complete set of procedures.

As an example, which we shall consider when applying the techniques we develop in this work, is the simplest nontrivial scenario [13].

Definition 3 (Simplest scenario, $\mathbb{B}_{\mathbf{si}}$). The simplest nontrivial scenario, denoted $\mathbb{B}_{\text{si}}$, is composed by 2 dichotomic measurements M_1 and M_2 and 4 preparation procedures, $\mathbb{P} := \{P_i\}_{i=1}^4$. There are no equivalences for measurements, while preparations respect the equivalence relation

$$\frac{1}{2}P_1 + \frac{1}{2}P_2 \simeq \frac{1}{2}P_3 + \frac{1}{2}P_4. \tag{16}$$

In our notation, we have $\mathbb{B}_{\text{si}} := (4, 2, 2, \mathbb{E}_{\mathbb{P}.\text{si}}, \emptyset)$, where $\mathbb{E}_{\mathbb{P},\text{si}} = \{(1/2, 1/2, 0, 0; 0, 0, 1/2, 1/2)\}$.

Pusey [13] showed that this scenario is the one with the least experimental elements for which data can be contextual. Moreover, it was shown that there exists a mapping of this scenario into the Bell scenario investigated by Clauser *et al* [41]. The relationship between scenarios with such operational equivalences and Bell scenarios was also investigated in [15, 40].

The characterization of behaviors in [37] provides a fundamental aspect for contextuality theory when a finite set of operational procedures and equivalences are considered: the set of possible behaviors in $\mathbb{B}$ is in one-to-one correspondence with points in $\mathbb{R}^n$ forming a convex polytope. Inside this convex polytope of all behaviors obeying the operational equivalences, lies another polytope: the set of behaviors explained by *noncontextual ontological models*.

2.1.1. Ontological models.

In order to *explain* the conditional probabilities in a behavior $B \in \mathbb{B}$ we use the ontological models framework [10, 42, 43]. In such a framework, there exists some measurable set (Λ, Σ) of so-called *ontic states* $\lambda \in \Lambda$. These contain the full set of parameters representing the most accurate physical description of the system. From such a set of states, we construct probabilistic explanations for both preparation and measurement procedures in $\mathbb{B}$, such that:

$$\forall P \in \mathbb{P}, \exists \mu_P, \tag{17}$$

$$\forall M \in \mathbb{M}, \forall k \in \mathbb{O}_\mathbb{M}, \exists \xi_{[k|M]}, \tag{18}$$

where μ_P are probability measures over (Λ,Σ), for all $\lambda\in\Lambda$, $\xi_{[\cdot|M]}(\lambda)$ are probability distributions over the outcomes k, for any λ, and every $\xi_{[k|M]}$ is a measurable function for (Λ,Σ). Calling Π the set of all μ_P and Θ the set of all $\xi_{[k|M]}$ we have that an ontological model for B is a quadruple $(\Lambda,\Sigma,\Pi,\Theta)$ that recovers the conditional probabilities by means of

$$p(k|M_i,P_j)=\int_\Lambda \xi_{[k|M_i]}(\lambda)\,\mathrm{d}\mu_{P_j}(\lambda),\forall i,j,k. \tag{19}$$

The assumption of noncontextuality is defined as follows:

Definition 4 (Noncontextuality). A behavior in a prepare-and-measure scenario, $B\in\mathbb{B}$, is called *noncontextual* if there exists some ontological model $(\Sigma,\Lambda,\Pi,\Theta)$ for the behavior B such that the measures from Π respect operational equivalences of $\mathbb{E}_{\mathbb{P}}$, meaning

$$\sum_j \alpha_j^a P_j \simeq \sum_j \beta_j^a P_j \Rightarrow \sum_j \alpha_j^a \mu_{P_j}=\sum_j \beta_j^a \mu_{P_j}, \tag{20}$$

and the same for elements from Θ that are associated with equivalent procedures from $\mathbb{E}_{\mathbb{M}}$

$$\sum_{i,k}\alpha^b_{[k|M_i]}[k|M_i]\simeq\sum_{i,k}\beta^b_{[k|M_i]}[k|M_i]\Rightarrow\sum_{i,k}\alpha^b_{[k|M_i]}\xi_{[k|M_i]}=\sum_{i,k}\beta^b_{[k|M_i]}\xi_{[k|M_i]}. \tag{21}$$

In this way, noncontextual models provide an explanation for operational equivalences. Some processes are operationally indistinguishable because they have the same ontological counterparts. In even more direct terms, because they correspond to the same functions (or distributions) of the variables λ.

The set of behaviors that do have a noncontextual ontological explanation is fully characterized by a finite set of tight inequalities forming the so-called noncontextual polytope $NC(\mathbb{B})$ [37], see appendix A for an example. The behaviors that are incompatible with any noncontextual ontological explanation are said to be contextual. It is already established that operational descriptions of quantum theory, where POVMs represent measurements and density matrices represent preparations, can lead to contextual behaviors (see [38, 43, 44])– in particular, the simplest scenario in which such a violation can occur is given by $\mathbb{B}_{\text{si}}$.

Deciding if a behavior in a given scenario is noncontextual or not can be framed as a linear program, and is fully determined by the complete set of facet-defining noncontextuality inequalities characterizing the polytope $NC(\mathbb{B})$ [37]. Using hierarchies of semi-definite programs (SDPs), it is also possible to bound the set of quantum behaviors [40, 45]. However, in most situations, these numerical tools provide little intuition for generating novel analytical insights, and they become increasingly computationally demanding. This is especially evident when attempting to find all noncontextuality inequalities or applying SDP hierarchies to scenarios where $|I|,|J|,|K|\gg 2$.

The resource theoretic toolbox will be instrumental in providing simple yet important qualitative understanding of possibly large prepare-and-measure scenarios, while avoiding numerically demanding procedures. We will do so by leveraging the concept of measurement simulability, and by lifting inequalities present in smaller scenarios into more complex ones. Before delving into the key aspects of the resource theory of generalized contextuality, we will first explain measurement simulation within an operational-probabilistic theories perspective.

2.2. Measurement simulability

One notion that will be valuable to this work is that of measurement simulability. It was first stated for quantum measurements [46, 47] and recently studied in the context of generalized probabilistic theories [48]. The basic idea is to understand which measurement statistics can be obtained by using a given set of measurement apparatuses and classical (pre- or post-) processing. Here, we adapt the notion of measurement simulability to operational theories.

Definition 5 (Measurement simulability). Consider a set of $|I|$ measurement procedures $\mathbb{N} \equiv \{N_i\}_{i\in I}$, on a given operational theory, with outcome set K. Then, another measurement procedure set $\{M_{\tilde{i}}\}_{\tilde{i}\in\tilde{I}}$ on this operational theory, with outcome set $\tilde{K}$, is said to be $\mathbb{N}$-simulable if there exists classical pre-processings $q_M(i|\tilde{i})$ and post-processing $q_O^i(\tilde{k}|k)$ such that

$$\left[\tilde{k}|M_{\tilde{i}}\right] \simeq \sum_{i,k} q_O^i\left(\tilde{k}|k\right)[k|N_i]\, q_M\left(i|\tilde{i}\right) \tag{22}$$

for every $\tilde{k} \in \tilde{K}$ and $\tilde{i} \in \tilde{I}$. Above, $q_M(i|\tilde{i})$ is a conditional probability that, for each $\tilde{i}$, chooses N_i with probability $q_M(i|\tilde{i})$. Similarly, $q_O^i(\tilde{k}|k)$ define the probability of outcome $\tilde{k} \in \tilde{K}$ given $k \in K$ for each $i \in I$.

The aim of this definition is to take the concept of measurement simulability to the scope of operational theories. In such framework, as per definition 5, measurement simulability states *an equivalence of specific form* between the measurement procedure to be simulated and the set of measurements performing the simulation, in which the coefficients defining the equivalence are decomposed as $\beta_{[k_i|N_i]}^{\mathrm{sim}\tilde{M}_{\tilde{i}}} := q_M(i|\tilde{i})q_O^i(\tilde{k}|k)$.

As said before, measurement simulability has been defined in the framework of generalized probabilistic theories [48], broadening the previous and exclusively quantum definition [46, 47, 49]. In fact, these definitions follow from definition 5 by identifying the procedures that are operationally equivalent—similarly to ignoring/forgetting the particular ensemble that led to a quantum state ρ. This implication follows from the fact that one can obtain a generalized probabilistic description by starting with the operational theoretic one and then quotienting over the operational equivalences [39]. Therefore, one can understand definition 5 as taking measurement simulability to a more primitive description of experimental scenarios (operational theories), which carry more information than the description given by the GPT framework (or the previous quantum description [46]).

2.3. Resource theory

In general formulations of resource theories, the basic ingredients are *objects*, that may feature a specific resource, as well as operations among those objects [22, 36]. Objects without any resource, and operations incapable of creating them are called, respectively, free objects and free operations. Free operations define a pre-order: if an object o can be freely transformed into o', then o must have at least the same amount of resources as o'. This pre-order, in turn, must be respected by any monotone aiming to quantify the resource.

For the present work, we consider contextuality in any fixed prepare-and-measure scenario $\mathbb{B}$ as the resource, following [36]. Thus, we are interested in considering the objects as $B \in \mathbb{B}$, while the set of free objects is naturally defined by the polytope $NC(\mathbb{B})$. The set of free operations defining the resource theory we consider is the set of pre-processing preparations or measurements, together with post-processing of the measurement results [36].

Definition 6. Given a scenario $\mathbb{B} := (|J|, |I|, |K|, \mathbb{E}_{\mathbb{P}}, \mathbb{E}_{\mathbb{M}})$ we define the set of free operations $\mathcal{F}$ as the set of maps $T : \mathbb{B} \to T(\mathbb{B})$ such that

$$T : \{p(k|M_i, P_j)\}_{k\in K, i\in I, j\in J} \mapsto \left\{ \sum_{i,j,k} q_O^i\left(\tilde{k}|k\right) p(k|M_i, P_j)\, q_M\left(i|\tilde{i}\right) q_P\left(j|\tilde{j}\right) \right\}_{\tilde{k}\in\tilde{K}, \tilde{i}\in\tilde{I}, \tilde{j}\in\tilde{J}} \tag{23}$$

where $q_O^i : K \to \tilde{K}, q_M : \tilde{I} \to I, q_P : \tilde{J} \to J$ are stochastic maps between index sets, i.e. $q_P = (q_P(j|\tilde{j}))_{j,\tilde{j}}$ is a stochastic matrix, corresponding to operational primitives in the different scenarios defined for each $\mathbb{B}$ by $T(\mathbb{B}) := \left(|\tilde{J}|, |\tilde{I}|, |\tilde{K}|, \mathbb{E}_{T(\mathbb{P})}, \mathbb{E}_{T(\mathbb{M})}\right)$, for sets of operational equivalences defined for the procedures *after* the transformation T was performed. ◇

Experimentally, the procedures in $\mathbb{B}$ can be thought of as highly controlled experimental apparatuses, such as actions over superconducting qubits, programmable integrated interferometers, etc. However, the free operations must, intuitively, pertain to a class of processes available by classical machinery, such as introducing classical randomness, or relabeling procedures.

The free operations have an impact on the equivalence classes. For instance, the new coefficients for preparations, $\tilde{\boldsymbol{\alpha}}$ and $\tilde{\boldsymbol{\beta}}$ (for every s labeling the equivalences), are those obeying equations [36]

$$\alpha_j^s = \sum_{\tilde{j}\in\tilde{J}} \tilde{\alpha}_{\tilde{j}}^s q_P\left(j|\tilde{j}\right), \tag{24a}$$

$$\beta_j^s = \sum_{\tilde{j}\in\tilde{J}} \tilde{\beta}_{\tilde{j}}^s q_P\left(j|\tilde{j}\right), \tag{24b}$$

where $q_P(j|\tilde{j})$ are defined by the free operation (with similar relations for equivalences on measurements). The change in the operational equivalences is represented by the notation $\mathbb{E}_{\mathbb{P}} \xrightarrow{T} \mathbb{E}_{T(\mathbb{P})}$. Some particularly important features of the new equivalences are: first, the resulting equivalences in the new scenario may be trivial. This is so because we may have $\boldsymbol{\alpha} \neq \boldsymbol{\beta}$ *while* $q_P\boldsymbol{\alpha} = \tilde{\boldsymbol{\alpha}} = \tilde{\boldsymbol{\beta}} = q_P\boldsymbol{\beta}$, for q_P a (left) stochastic matrix. Second, no equivalences can be 'broken'; indeed, from (9),

$$\sum_{j\in J} \alpha_j^s P_j \simeq \beta_j^s P_j \implies \sum_{j,\tilde{j}} \tilde{\alpha}_{\tilde{j}}^s q_P\left(j|\tilde{j}\right) P_j \simeq \sum_{j,\tilde{j}} \tilde{\beta}_{\tilde{j}}^s q_P\left(j|\tilde{j}\right) P_j \implies \sum_{\tilde{j}\in\tilde{J}} \tilde{\alpha}_{\tilde{j}}^s \tilde{P}_{\tilde{j}} \simeq \sum_{\tilde{j}\in\tilde{J}} \tilde{\beta}_{\tilde{j}}^s \tilde{P}_{\tilde{j}}$$

where the new set of preparations $T(\mathbb{P}) \equiv \{P_{\tilde{j}}\}_{\tilde{j}\in\tilde{J}}$ are defined in the new scenario $T(\mathbb{B})$.

Finally, there are some different examples of monotones respecting the pre-order established by the free operations. The one we will use in this work is the l_1-distance from [36].

Definition 7. Let $\mathbb{B} := (|J|, |I|, |K|, \mathbb{E}_{\mathbb{P}}, \mathbb{E}_{\mathbb{M}})$ be any finitely defined prepare-and-measure scenario. The l_1-contextuality distance $\mathsf{d} : \mathbb{B} \to \mathbb{R}_+$ is defined by

$$\mathsf{d}(B) := \min_{B^*\in NC(\mathbb{B})} \max_{i\in I, j\in J} \sum_{k\in K} |p(k|M_i, P_j) - p^*(k|M_i, P_j)|. \tag{25}$$

Until now, we have been describing contextuality as a property: a data-set B either has it or not. The function above allows us to discuss contextuality as a quantity. With respect to d, we can now ask 'does B_1 have more contextuality than B_2?'.

The concept of quantifying abstract resources is one of the hallmarks of the formalization of general resource theories. The primary motivation for introducing quantifiers, such as the one above, is to correlate the success rates of tasks with the available resources (similar to determining how far a car can travel based on its fuel capacity).

This program has been surprisingly successful. To mention two examples related to quantum computation: Shor's algorithm [50] can be shown to depend on the amount of coherence [25] present in the computation, and success probabilities of computing Boolean non-linear functions, in a restricted measurement-based computational model, can be shown to depend on the amount of KS-contextuality [28]

Let us now mention one example which showcases that the use of resource theoretic quantifiers (in particular the contextuality l_1-quantifier of definition 7) can be broader than one might expect. In [51] this measure was used to bound nonclassicality in finite scenarios relevant to quantum Darwinism. This paradigm was proposed as an explanation for the emergence of objectivity from the quantum—and arguably non-objective—substrate [52]. Shortly speaking, quantum Darwinism poses that the information about a central system stored in small portions of its environment is redundant. This would imply that independent observers gathering information about the system through such portions of its environment (as we often do when assessing systems around us in our everyday life), will agree on the obtained information. This agreement between observers is the key to objectivity in the Darwinist program.

Brandão *et al* [53] showed that, under the circumstances that Darwinism is expected to hold (such as the presence of an environment with many parts), the quantum dynamics from the central system to some part j of the environment, Φ^j, is close to a measure-and-prepare map Φ^j_{obj}. This fact was shown by upper bounding the diamond norm $\|\Phi^j - \Phi^j_{\text{obj}}\|_\diamond$. Then, [51] showed that the l_1-distance lower bounds this quantity:

$$\mathsf{d}(B) \leqslant \frac{C}{\dim(\mathcal{H})} \|\Phi^j - \Phi^j_{\text{obj}}\|_\diamond, \tag{26}$$

where C is a constant, $\dim(\mathcal{H})$ is the system's of interest dimension and B is the statistics described by a finite scenario satisfying the operational properties of quantum Darwinism dynamics. This tells us that if a Darwinist process takes place, contextuality should be constrained. On the other side, Any value $\mathsf{d}(B) > 0$ in such a set-up signals, not only that a perfect process of quantum Darwinism has not taken place, but also by *how much*. Therefore, as we see, the understanding of a resource theory and its quantifiers can be helpful in a variety of fields, such as quantum computation or classical limits in open quantum systems dynamics.

3. Results

The results here reported are essentially obtained by exploring the defining feature of free operations; namely, that they cannot increase the resource (contextuality). The practical implication is that if T is a free operation and $T(B) \in T(\mathbb{B})$ is contextual, then B must be contextual on the original scenario, $\mathbb{B}$.

With this in mind, we first show how to reduce some complex scenarios to simpler ones by using measurement simulability. A practical implication of this is that we can attain/explore contextuality with easier implementations; with this perspective, we reinterpret the results of [38]. It is noteworthy that, in the resource-theoretic treatment of KS-contextuality, measurement simulation has also been investigated with the very same goal of understanding the simulation trade-off between scenarios [29], further investigated in [30, 31]. The results we will present regarding simulability and the conclusions drawn for the resource theory of generalized contextuality complement the existing knowledge in the KS-contextuality literature.

Secondly, we take the opposite path, showing how to build more complex scenarios from simpler ones—where important features of the simple scenarios are carried to the complex ones. This composition technique allows to engineer scenarios where all non-trivial facets exhibit quantum violations. Moreover, we conclude that the contextual advantage on the cloning task [19] is inherited from a simpler scenario. It is worth noting that the results obtained here will remain valid, or be easily generalized, if other resource theories encompassing broader families of free operations that include classical pre- and post-processing are constructed.

3.1. Simulability and free operations

We begin by showing that measurement simulation, as expressed in definition 5, physically implements a subset of the free operations.

Lemma 1 (Simulation is free). *Consider a $\{N_i\}_{i\in I}$-simulation of a set $\{M_{\tilde{i}}\}_{\tilde{i}\in\tilde{I}}$ and a set of preparations $\mathbb{P}$. Now consider the behaviors obtained by the simulating set $\{N_i\}_{i\in I}$, $B_N := \{p(k|N_i,P_j)\}_{k\in I, i\in I, j\in J}$, and those obtained by the simulated set $\{M_{\tilde{i}}\}_{\tilde{i}\in\tilde{I}}$, $B_M := \{p(\tilde{k}|M_{\tilde{i}},P_j)\}_{\tilde{k}\in\tilde{K},\tilde{i}\in\tilde{I},j\in J}$. The operation implemented by such a simulation, $T_{sim}: B_N \mapsto B_M$, is free.*

Proof. Measurement simulation acts as a map T_{sim} which takes the measurement events $[k|N_i]$, to the measurement events $\sum_{k,i} q^i_O(\tilde{k}|k)[k|N_i]q_M(i|\tilde{i})$. Due to linearity, the impact of simulation on behaviors is $T_{\text{sim}}(\{p(k|N_i,P_j)\}) = \{\sum_{k,i} q^i_O(\tilde{k}|k)p(k|N_i,P_j)q_M(i|\tilde{i})\}$. Now, the equivalence established by simulation, $[\tilde{k}|M_{\tilde{i}}] \simeq \sum_{k,i} q^i_O(\tilde{k}|k)[k|N_i]q_M(i|\tilde{i})$, implies

$$\sum_{k,i} q^i_O\left(\tilde{k}|k\right) p\left(k|N_i,P_j\right) q_M\left(i|\tilde{i}\right) = p\left(\tilde{k}|M_{\tilde{i}},P_j\right)\ \forall P_j \in \mathbb{P}. \tag{27}$$

By comparing the l.h.s. of equation (27) with the r.h.s. of equation (23), we see that T_{sim} is indeed a specific kind of free operation (obtained through simulation), which leaves preparations untouched. □

This lemma has a direct implication for quantum realizations (we will denote $\mathbb{M}^Q$ as the quantum realizations of the procedures $\mathbb{M}$):

Corollary 1. *Let $\mathbb{M}^Q_1, \mathbb{M}^Q_2$ be sets of quantum realizations of prepare-and-measure scenarios $\mathbb{B}_1, \mathbb{B}_2$, respectively. Then, if $\mathbb{M}^Q_1$ is $\mathbb{M}^Q_2$-simulable there exists a free operation $T: \mathbb{B}_2 \to T(\mathbb{B}_2) = \mathbb{B}_1$.*

One implication of the above results is that one can use simulations to derive simpler scenarios from complex ones. We discuss two simple instances of how this can be done: by manipulating measurement equivalences or by moving to a scenario having fewer measurements than the original one.

The first instance is a consequence of the impact of free operations on equivalence classes (as expressed in equation (24) for preparations). Indeed, by performing classical pre- and post-processing of events one might be able to engineer the equivalence classes of interest. This gives an alternative interpretation of the results of [38], that we proceed to briefly recall: In their work, the authors tackle the problem of practical impossibility to obey exactly the desired operational equivalences for the ideal quantum procedures, due to experimental errors. Assume that we want to test a noncontextuality inequality defined for a scenario $\mathbb{B}$. When operationally characterizing the procedures of $\mathbb{B}$ in a real experiment the noisy data effectively implements some other closely related scenario $\mathbb{B}^{\mathrm{p}}$. We call these the *primary procedures*. For concreteness, let us use preparations $\mathbb{P}^{\mathrm{p}}$ to express in precise terms the idea. The procedures $\mathbb{P}^{\mathrm{p}}$ correspond to those that can be characterized using the (robust) experimental implementations. In particular, the problem with these procedures is that they do not satisfy the ideal operational equivalences of the target scenario $\mathbb{B}$, with preparation procedures $\mathbb{P}$, in which case the noncontextuality inequality tested is not applicable.

By performing classical post-processing in the procedures, it is possible to obtain new *secondary* procedures that match the expected operational equivalences perfectly, *by construction*. The mapping can be framed as something of the form

$$P^{\mathrm{s}}_{\tilde{j}} = \sum_{j} q_P\left(\tilde{j}|j\right) P^{\mathrm{p}}_{j} \tag{28}$$

for all $j \in J$ labeling the elements of $\mathbb{P}^{\mathrm{p}}$. Properly choosing $p(\tilde{j}|j)$ allows the procedures $\mathbb{P}^{\mathrm{s}} := \{P^{\mathrm{s}}_{\tilde{j}}\}_{\tilde{j}}$ to satisfy the target operational equivalences of $\mathbb{B}$. With this, the behavior obtained from the secondary procedures can now be properly used to violate the inequality, that is now applicable.

To this approach one could provide the following criticism: Since we never obtain a noncontextual bound with respect to the primary (measured) procedures and their corresponding operational equivalences, what guarantees that we are not demonstrating contextuality of the secondary procedures only? The resource theory framework guarantees that:

Theorem 1. *Contextuality for behaviors obtained with the secondary procedures implies contextuality for behaviors obtained from the primary procedures.*

Proof. Recall that for the monotone d it is true that $\mathsf{d}(T(B)) \leqslant \mathsf{d}(B)$ for all $B \in \mathbb{B}$ and $T \in \mathcal{F}$ free operation. Transformations from primary to secondary procedures are of the form given by definition 6. Let us denote these operations as $T_{\mathrm{p}\to\mathrm{s}}$. This can be seen simply by noticing that $T_{\mathrm{p}\to\mathrm{s}}$ probabilistic mixes the secondary procedures given the primary ones, as is expressed by equation (28). Since $\forall T \in \mathcal{F}$, it is true that $\mathsf{d}(T(B)) > 0 \implies \mathsf{d}(B) > 0$, the fact that $B_{\mathrm{s}} = T_{\mathrm{p}\to\mathrm{s}}(B_{\mathrm{p}})$ implies $\mathsf{d}(B_{\mathrm{s}}) > 0 \implies \mathsf{d}(B_{\mathrm{p}}) > 0 \implies B_{\mathrm{re}}$ is contextual. □

With the resource-theoretic perspective here proposed, we can understand the methods of [38] as using a free operation to obtain new behaviors which obey the desired operational equivalences and still exhibit contextuality. Moreover, since the performed operation is free, we can add that their violations *also show contextuality for the original measurements, in the original scenario.* Notice that imposing assumptions on the possible experimental errors this argument can be extended to the ideal quantum realizations.

Let us now consider the use of measurement simulation to reduce a given scenario. We will consider the simplest case, where part of the measurements are erased. The following results are corollaries of lemma 1.

Corollary 2 (Trivial simulation). *Consider a scenario $\mathbb{B} = (|J|,|I|,|K|,\mathbb{E}_{\mathbb{P}},\mathbb{E}_{\mathbb{M}})$ and define another scenario $\mathbb{B}'$ obtained simply by discarding some of the measurements, i.e. $\mathbb{B}' = (|J|,|I'|,|K|,\mathbb{E}_{\mathbb{P}},\mathbb{E}'_{\mathbb{M}'})$ where $\mathbb{M}' \subset \mathbb{M}$ (thus, $|I'| \leqslant |I|$) and $\mathbb{E}'_{\mathbb{M}'} \subset \mathbb{E}_{\mathbb{M}}$. The transformation of erasing such procedures and equivalences among them, $T: \mathbb{B} \mapsto \mathbb{B}'$, is free.*

Proof. This transformation can be mathematically described as $T(B) = \{\sum_j p(k|N_i, P_j) q_M(i|i')\}$ where $q(i|i') = 1$ if $i = i'$ and 0 otherwise. □

This will be important to us, especially in the case where all remaining measurements are dichotomic and with no equivalences, $\mathbb{E}_{\mathbb{M}'} = \emptyset$. In other words, the case where one arises at simple generalizations of the simplest scenario definition 3 after discarding a subset of measurements. In this case, we know that there is a quantum realization of the measurements of the reduced scenario. That is,

Corollary 3. *Let $\mathbb{M} := \{M_i\}$ be any set of two-outcome operational measurements having a quantum realization $\mathbb{M}^Q$. Then, the quantum measurements $\mathbb{M}^Q_{si} := \{\frac{1}{\sqrt{2}}(\sigma_X + \sigma_Z), \frac{1}{\sqrt{2}}(\sigma_X - \sigma_Z)\}$ are $\mathbb{M}^Q$-simulable, for at least some quantum realization $\mathbb{M}^Q$ of $\mathbb{M}$.*

With the above results, we see that using simulations provided by a particular set of measurements may lead us to new, simpler, scenarios. If contextuality is witnessed in such scenarios, the resource theoretical perspective allows us to conclude that contextuality was present prior to the simplification process. Yet, the mere application of free operations $\mathbb{B}_{initial} \overset{T}{\mapsto} \mathbb{B}_{final}$ do not always help in *engineering* novel scenarios, or novel contextual behaviors, because we may not necessarily know from where the contextual behaviors $T(B) \in \mathbb{B}_{final}$ came from, among all the possible ones in the more complex scenarios $B \in \mathbb{B}_{initial}$, nor how to access them, since T needs not be injective. To that end, we introduce a formal composition rule $\boxplus$, presented in the next section 3.2. We will use such ideas in section 3.3 to engineer and witness quantum contextuality in more involved scenarios.

3.2. Composition of scenarios

In the previous section, we discussed how to use free operations (measurement simulability in particular) to obtain simpler scenarios. Here we take the opposite path, constructing complex scenarios from simpler ones. This particular construction allows one to obtain important information regarding the resource, which is inherited from the original, smaller, scenarios. This is based on the following definition,

Definition 8. Let $\mathbb{B}_1 = (|J_1|, |I_1|, |K_1|, \mathbb{E}_{\mathbb{P}_1}, \mathbb{E}_{\mathbb{M}_1})$, and $\mathbb{B}_2 = (|J_2|, |I_2|, |K_2|, \mathbb{E}_{\mathbb{P}_2}, \mathbb{E}_{\mathbb{M}_2})$ be two finitely defined prepare-and-measure scenarios, with behaviors $B_1 \in \mathbb{B}_1, B_2 \in \mathbb{B}_2$, seen as vectors $B_1 = (p(k_1|M_{i_1}, P_{j_1}))_{i_1,k_1,j_1}$, we then define:

(a) (Composition of scenarios) The target scenario $\mathbb{B} \equiv \mathbb{B}_1 \boxplus \mathbb{B}_2$ defined by the tuple,

$$(|J_1 \cup J_2|, |I_1 \cup I_2|, |K_1 \cup K_2|, \mathbb{E}_{\mathbb{P}_1 \cup \mathbb{P}_2}, \mathbb{E}_{\mathbb{M}_1 \cup \mathbb{M}_2})$$

has the operational equivalences of both scenarios defined as, for $\{a\}_{a=1}^{|\mathbb{E}_{\mathbb{P}_1 \cup \mathbb{P}_2}|} := \{a_1\}_{a_1=1}^{|\mathbb{E}_{\mathbb{P}_1}|} \cup \{a_2\}_{a_2=1}^{|\mathbb{E}_{\mathbb{P}_2}|}$, that we denote $\gamma^a_{\mathbb{P}_1 \cup \mathbb{P}_2} \in \mathbb{E}_{\mathbb{P}_1 \cup \mathbb{P}_2}$,

$$\gamma^a_{\mathbb{P}_1 \cup \mathbb{P}_2} := \begin{cases} (\boldsymbol{\alpha}^{a_1}, \mathbf{0}; \boldsymbol{\beta}^{a_1}, \mathbf{0}), & a = a_1 \\ (\mathbf{0}, \boldsymbol{\alpha}^{a_2}, \mathbf{0}; \boldsymbol{\beta}^{a_2}), & a = a_2 \end{cases}. \tag{29}$$

The analogous definition holds for the operational equivalences for measurement events by a change $P \to M$ and $a \to b$.

(b) (Composition of behaviors) The binary operation $\boxplus$ is defined as the vertical stacking of vectors from the scenarios $\mathbb{B}_1, \mathbb{B}_2$ towards $\mathbb{B}$, i.e.

$$B_1 \boxplus B_2 := \begin{pmatrix} p\left(k_1|M_{i_1}, P_{j_1}\right) \\ p\left(k_2|M_{i_2}, P_{j_2}\right) \end{pmatrix}. \tag{30}$$

With $i_1 \in I_1$, $|I_1| = |\mathbb{M}_1|$ and similarly for all other labels.

As an operational constraint, the target scenario *does not* consider the probabilities obtained with hybrid procedures, i.e. those of the form

$$p\left(k_1|M_{i_1}, P_{j_2}\right), p\left(k_2|M_{i_1}, P_{j_1}\right) \notin B_1 \boxplus B_2. \tag{31}$$

Note that compositions of multiple scenarios are constructed in sequence and are associative.

This binary operation essentially appends two given scenarios. The geometrical consequences of such composition will be important, as it will allow us to build an intuition of the resulting noncontextual polytope. This is described by the following lemma:

Lemma 2 (Geometrical consequences, from [54–56]). *Let $P \subset \mathbb{R}^n$, $Q \subset \mathbb{R}^m$ be two convex polytopes. Then, the product defined by*

$$P \times Q := \left\{ \begin{pmatrix} p \\ q \end{pmatrix} : p \in P, q \in Q \right\} \subset \mathbb{R}^{n+m}, \tag{32}$$

is again a convex polytope. Let $|V(P)|$ and $|V(Q)|$ represent the number of vertices of each of the convex polytopes P and Q, then, we also have that $|V(P\times Q)| = |V(P)| \cdot |V(Q)|$. Let $|F(P)|$ define the number of facets of the convex polytope P, and similarly for the convex polytope Q. Then, we have that $|F(P\times Q)| = |F(P)| + |F(Q)|$.

One important feature of the binary operation is the following result.

Theorem 2. *The binary operation $\boxplus$ preserves the resource:*

$$B_1 \in NC(\mathbb{B}_1), B_2 \in NC(\mathbb{B}_2) \Leftrightarrow B_1 \boxplus B_2 \in NC(\mathbb{B}_1 \boxplus \mathbb{B}_2).$$

We prove this theorem in appendix B, but we provide some intuition here. ($\Rightarrow$) If there exists a noncontextual ontological model for each part B_1 and B_2, respecting the operational equivalences of both scenarios, then in the new scenario $\mathbb{B} := \mathbb{B}_1 \boxplus \mathbb{B}_2$ the operational equivalences are inherited according to (29), so that we can choose the set of ontic states $\Lambda_1 \sqcup \Lambda_2$, and construct a noncontextual model for any B using the model of the parts, over this larger ontic space. ($\Leftarrow$) Now, on the other way around, if there exists a noncontextual ontological model for any behavior $B_1 \boxplus B_2$ there must exist one for its parts, by simply restricting the probability distributions to the correct labels since the operational equivalences are of the form of equation (29). An implication of $\boxplus$ preserving the resource is that it does not increase the l_1-distance quantifier:

Lemma 3. *Let $\mathbb{B} := (|J|, |I|, |K|, \mathbb{E}_{\mathbb{P}}, \mathbb{E}_{\mathbb{M}})$ be any finitely defined prepare-and-measure scenario. The l_1-contextuality distance $\mathsf{d} : \mathbb{B} \to \mathbb{R}_+$ (see definition 7) is subbadditive under the binary operation $\boxplus$. This means that for $B_1 \in \mathbb{B}_1$ and $B_2 \in \mathbb{B}_2$ we get:*

$$\mathsf{d}(B_1 \boxplus B_2) \leqslant \mathsf{d}(B_1) + \mathsf{d}(B_2). \tag{33}$$

In other words, theorem 2 (and its manifestation through the l_1-distance) tells us that this composition preserves the structure of the noncontextual behaviors; therefore, if $B_1 \boxplus B_2 \in \mathbb{B}_1 \boxplus \mathbb{B}_2$ is contextual, then it must be true that either B_1 or B_2 is contextual (or both). We remark that similar results have been shown for KS-contextuality using the *contextual fraction* monotone [28]. Abramsky *et al* [29] presented the monotonicity rules for the fraction with respect to different composition rules between empirical models. Moreover, they have also shown that if a given model simulates another, the latter must have less contextual fraction than the former.

Lemma 2 is also proved in appendix B. Both lemma 2 and theorem 2 give interesting tools to understand a complex scenario. Indeed, if we are able to decompose a given scenario as $\mathbb{B} = \mathbb{B}_1 \boxplus \mathbb{B}_2 \boxplus \ldots \boxplus \mathbb{B}_n$, we can obtain resourceful behaviors on $\mathbb{B}$ by building on resourceful behaviors on its components, $\mathbb{B}_l (l \in \{1, \ldots, n\})$. In this sense, $\mathbb{B}$ can be engineered from the control an experimenter has of its parts. The resulting scenario, together with its behaviors, will also be known, and with a known lower bound in the contextuality with respect to the l_1-distance monotone. Behaviors in the parts $\mathbb{B}_1, \ldots, \mathbb{B}_n$ will dictate what are the behaviors given by the whole $\mathbb{B}$, and how to access them.

3.3. Witnessing quantum contextuality

In sections 3.1 and 3.2, we exposed general results that show how a resource-theoretic approach provides interesting tools to analyze complex contextuality scenarios. Namely, by reducing a scenario via erasing procedures, designing equivalences or looking for a nice decomposition in terms of the product (30); we can also use such a product to build up complex scenarios that preserve the resource. Here we take advantage of those results to engineer and witness *quantum* contextuality. In particular, we show that scenarios of a particular form always feature quantum contextuality and that the contextual advantage present in the cloning scenario [19] is actually inherited from a simpler scenario (that we name $\mathbb{B}_6$).

3.3.1. Using free operations. Here we present examples in which one can prove the existence of quantum contextuality in certain scenarios by taking advantage of free operations in the resource-theoretic approach. In particular, we use free operations (such as the trivial simulation discussed in corollary 2), to take these scenarios to the simplest one ($\mathbb{B}_{\text{si}}$, see definition 3), and still find contextual quantum realizations. The idea is represented in figure 1.

In what follows, we discuss scenarios of a specific structure in which we can apply such a technique.

Example 1. Consider scenarios of the kind $\mathbb{B} := (4, |I|, 2, \mathbb{E}_{\mathbb{P},si}, \emptyset), |I| \geqslant 2$. There is always a quantum behavior $B \in \mathbb{B}$ and a free operation towards the simplest scenario, i.e. $T \in \mathcal{F}$ where $T(\mathbb{B}) = \mathbb{B}_{\text{si}}$, such that $T(B) \in \mathbb{B}_{\text{si}}$ is a quantum contextual behavior.

In other words, every prepare-and-measure scenario that can be written as above will have at least some quantum realization that is contextual. Such contextual behavior *may be* understood as a quantum advantage in such a scenario, as suggested by the resource-theoretic approach.

Proof. Since there are no equivalences among measurements, we can choose any set $\mathbb{M}^Q$ with $|I|$ procedures to be a realization of the measurement procedures $\mathbb{M}$. Finally, we can use the strategy of trivial simulation described in corollary 2 to take $\mathbb{B}$ to $\mathbb{B}_{\text{si}}$, simply by erasing all but two measurements. Finally, we can use the quantum realizations providing contextual advantage in this scenario, which proves our example.

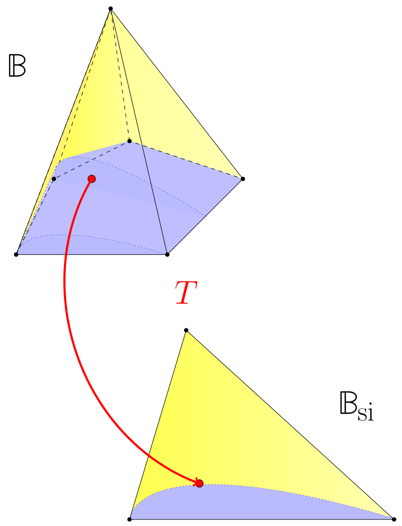


Figure 1. Free operations as a tool for witnessing quantum contextuality in complex scenarios. By finding the existence of a free transformation T towards quantum contextual behaviors in already known scenarios, such as the simplest scenario $\mathbb{B}_{\rm si}$ from [13], one can attest contextuality in the original case.

Even though the above completes our proof, we might profit from an explicit description of such a procedure. Let a quantum realization of the measurement procedures $\mathbb{M} = \{M_i\}_{i\in I}$ from the scenario $\mathbb{B}$ be such that each measurement is a projective measurement, with $\mathbb{M}^Q = \mathbb{M}^Q_{\rm si} \cup \{M_3^{\rm proj},\dots,M_I^{\rm proj}\}$, for $M_i^{\rm proj}$ a projective measurement for all $i = 3,\dots,|I|$. Now, define maps q^i_O, q_M as

$$q^i_O\left(\tilde{k}|k\right) = \delta_{k,\tilde{k}} \tag{34}$$

$$q_M\left(i|\tilde{i}\right) = \begin{cases} 1 \text{if } \; i \in \{0,1,2\} \\ 0, \text{otherwise.}\end{cases} \tag{35}$$

For any measurement event represented by the quantum operators $E^{\tilde{i}}_{\tilde{k}}$ from the POVMs $M_{\tilde{i}} \in \mathbb{M}^Q_{\rm si}$, we have

$$E^{\tilde{i}}_{\tilde{k}} = \sum_{i,k} q^i_O\left(\tilde{k}|k\right) E^i_k q_M\left(i|\tilde{i}\right). \tag{36}$$

Let the quantum realization of the preparation procedures in $\mathbb{B}$ be that given in equations (2)–(5). These can also be a quantum realization for $\mathbb{B}_{\rm si}$, since the preparation structure of both scenarios is the same. Then, if we define the free operation T using the maps in equations (36) and (34), we can notice that the following holds,

$$
\begin{aligned}
p\left(k|M_i,P_j\right) &= \mathrm{Tr}\left(E^i_k\rho^j\right) \xrightarrow{T} \\
&\to \sum_{i,k} q^i_O\left(\tilde{k}|k\right)\mathrm{Tr}\left(E^i_k\rho^j\right)q_M\left(i|\tilde{i}\right) \\
&= \mathrm{Tr}\left(\sum_{i,k} q^i_O\left(\tilde{k}|k\right)E^i_k q_M\left(i|\tilde{i}\right)\rho^j\right) \\
&= \mathrm{Tr}\left(E^{\tilde{i}}_{\tilde{k}}\rho^j\right) = p\left(\tilde{k}|M_{\tilde{i}},P_j\right),
\end{aligned}
$$

where $E^{\tilde{i}}_{\tilde{k}}$ are the POVM elements of the measurement procedures in $\mathbb{M}^Q_{\mathrm{si}}$, discussed in the appendix C. Therefore we might access the quantum contextual behavior from $\mathbb{B}_{\mathrm{si}}$ that is maximally quantum contextual [6, 57]. Since T is a free operation, the specific quantum realization we used in the domain $\mathbb{B}$ cannot be noncontextual. □

Applying the same reasoning to preparation procedures, a generalization follows:

Example 2. Consider scenarios of the kind $\mathbb{B} := (|J|,|I|,2,\mathbb{E}_{\mathbb{P}},\emptyset)$, with $|J|$ even, $|J| \geqslant 4$ and $|I| \geqslant 2$, and $\mathbb{E}_{\mathbb{P}} = \mathbb{E}_{\mathbb{P},\mathrm{si}} \cup \mathbb{E}'$, where $\mathbb{E}'$ does not involve the first four preparations. There is always a quantum behavior $B \in \mathbb{B}$ and a free operation $T \in \mathcal{F}$, with image $T(\mathbb{B}) = \mathbb{B}_{\mathrm{si}}$ the simplest scenario such that $T(B) \in \mathbb{B}_{\mathrm{si}}$ is a quantum contextual behavior.

It is clear that there exists a quantum contextual behavior for such a scenario since we can consider the same quantum contextual behavior from example 1, and complete the procedures with anything such that the equivalences $\mathbb{E}'$ do not involve the first four procedures. Then, there will certainly exist some pre-processings from these towards the preparations (3)–(5), with the same description as the one given by corollary 2.

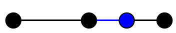
3.3.2. Using the composition. In this section, we take advantage of the consequences of theorem 2 to witness quantum contextuality. Namely,

Corollary 4. *Consider a behavior $B_1 \boxplus B_2$, with $B_1 \in \mathbb{B}_1$ and $B_2 \in \mathbb{B}_2$, that has some quantum realizations and is contextual. Then, B_1 or B_2 must be contextual. Mathematically,*

$$B_1 \boxplus B_2 \in QC\left(\mathbb{B}_1 \boxplus \mathbb{B}_2\right) \tag{37}$$

$$\iff B_1 \in QC\left(\mathbb{B}_1\right) \text{ or } B_2 \in QC\left(\mathbb{B}_2\right) \tag{38}$$

where $QC(\mathbb{B})$ is the set of contextual points in the scenario that have some quantum realization.

Hence, using the composition $\boxplus$, we are constructing higher-dimensional polytopes that will inherit quantum contextuality from its lower-dimensional components. Thus, whenever very complex scenarios can be understood as the product of lower-dimensional ones, we can find the arising noncontextual polytope structure from the product elements and build up quantum violations from those in the components. We shall see examples of how this can be done. First, let us give an intuitive geometric view of why complex scenarios acquire quantum contextuality from simple ones. Let  be the pictorial representation of a prepare-and-measure experimental scenario, meaning that this is some convex polytope $\mathbb{B}$ with the quantum set (first three nodes) containing the left black line and the one in blue (color

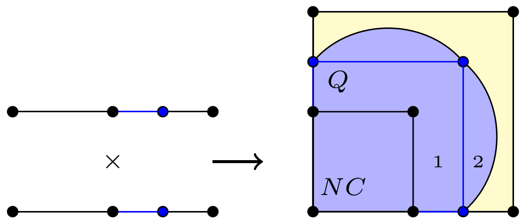


Figure 2. Representation of the polytope structure arising from the product scenario. We stress that it is not clear how the new form of the *quantum* set $Q(\mathbb{B})$ should be, even though it is clear the polytope structure for both NC and the larger polytope of statistics. In this picture we have used the fact that $NC(\mathbb{B}) \subseteq Q(\mathbb{B})$. From the convex nature of $Q(\mathbb{B})$, the product scenario must have a quantum contextual set that is at least of the form given by region 1, but it could also be given by region 2 and the study of maximal violations for noncontextuality inequalities shall answer such questions, see [58, 59] (color online).

online; three lines between four nodes, first one represents the noncontextual set of behaviors, the second represents the quantum and the third the post-quantum). Then, the product $\mathbb{B} \boxplus \mathbb{B}$ between two of these 1-dimensional convex polytopes will be such as represented in figure 2.

From figure 2, we see that if one constructs very complex scenarios, when they are associated with decompositions of $\mathbb{B}^{\boxplus n}$ for n as large as we could imagine, the resource is always present.

The arguably simplest construction one might consider is to take sequential products of the simplest scenario, $\mathbb{B} := \mathbb{B}_{\text{si}}^{\boxplus n}$. Interestingly, using some symmetry arguments and the tight noncontextuality inequalities of the simplest scenario, we can obtain the following result for such construction:

Lemma 4. *For any scenario of the form $\mathbb{B} := \mathbb{B}_{si}^{\boxplus n}$, $n \geqslant 1$, every tight and nontrivial noncontextuality inequality will be violated by some quantum contextual behavior.*

We provide a proof in appendix D. Therefore, for these scenarios, there exist quantum contextual behaviors *with respect to all (nontrivial) noncontextuality inequalities that define the polytope $NC(\mathbb{B})$*. A resource theoretic consequence arises as a corollary from such lemma.

Corollary 5 (Quantum advantages for $\mathbb{B} = \mathbb{B}_{\text{si}}^{\boxplus n}$). *Consider a quantum information task that has a success rate defined by a function $g : \mathbb{B} \to \mathbb{R}_+$, for $\mathbb{B}$ of the form of $\mathbb{B}_{si}^{\boxplus n}$, such that the noncontextual bound for the success, $g^{NC}(B) \leqslant \delta$, for some $\delta \in \mathbb{R}$, can be expressed as a linear combination of the noncontextuality inequalities of $NC(\mathbb{B})$. Then, there exists a quantum behavior B^Q such that $g(B^Q) > \delta$.*

Thus, lemma 4 represents a general proof of quantum *advantage* in tasks related to scenarios of the form $\mathbb{B}_{\text{si}}^{\boxplus n}$, for $n \geqslant 2$ (whenever the success rate of the operational task is defined by a function g that is a convex-linear function of the noncontextuality inequalities $NC(\mathbb{B}_{\text{si}})$).

As another notable example, we discuss the quantum cloning scenario from [19] which we name as $\mathbb{B}_{\text{qc}}$. This is an operational scenario that reproduces the statistics for an important quantum task known as state-dependent quantum cloning, in which contextuality underpins quantum advantage [19].

In this scenario, we have a set

$$\mathbb{P}_{\text{qc}} := \{P_s, P_{s^\perp} \mid s \in \{a, b, \alpha, \beta, aa, bb\}\}$$

with preparation operational equivalences

$$\frac{1}{2}P_a + \frac{1}{2}P_{a^\perp} \simeq \frac{1}{2}P_b + \frac{1}{2}P_{b^\perp}, \tag{39}$$

$$\frac{1}{2}P_\alpha + \frac{1}{2}P_{\alpha^\perp} \simeq \frac{1}{2}P_{aa} + \frac{1}{2}P_{aa^\perp}, \tag{40}$$

$$\frac{1}{2}P_\beta + \frac{1}{2}P_{\beta^\perp} \simeq \frac{1}{2}P_{bb} + \frac{1}{2}P_{bb^\perp}. \tag{41}$$

For the measurement procedures, we have the six binary-outcome ones $M_s, s \in \{a, b, \alpha, \beta, aa, bb\}$, with no operational equivalences. The example below captures the polytope structure of this scenario as from smaller ones.

Example 3 (Quantum cloning inherits contextuality from $\mathbb{B}_6$). The scenario $\mathbb{B}_{\text{qc}}$ related to the state-dependent quantum cloning task, can be written as

$$\mathbb{B}_{\text{qc}} = \mathbb{B}_6 \boxplus \mathbb{B}_6 \boxplus \mathbb{B}_6, \tag{42}$$

where $\mathbb{B}_6 := (4, 6, 2, \mathbb{E}_{\mathbb{P},\text{si}}, \emptyset)$. The *inner* polytope structure of $\mathbb{B}_{\text{qc}}$ is then given by $\mathbb{B}_6$.

We needed to add some symmetries associated with the fact that the scenario $\mathbb{B}_6^{\boxplus 3}$ would have 18 measurement procedures, therefore making notice of the symmetry $I_1 = I_2 = I_3 \implies I := I_1 \cup I_2 \cup I_3 = I_1 = \{a, b, \alpha, \beta, aa, bb\}$. And also that $K_1 = K_2 = K_3$. Under these circumstances equation (42) holds.

Recall that the operational equivalences within any scenario provide the fundamental constraints of the generated data over noncontextual models. As such, the example above shows that the equivalences from $\mathbb{B}_{\text{qc}}$ can be framed as compositions of those from $\mathbb{B}_{\text{si}}$. Hence, the operational structure underpinning the cloning scenario is simply that of a composition of those pertaining to the simplest scenario.

This example is also helpful to discuss some aspects of the map $\boxplus$, in particular,

$$NC(\mathbb{B}_{\text{qc}}) = NC(\mathbb{B}_6) \times NC(\mathbb{B}_6) \times NC(\mathbb{B}_6). \tag{43}$$

This example allows us to conclude the following: equation (42) is a proof of quantum contextuality in the quantum cloning scenario, since $\mathbb{B}_6$ has quantum contextual behaviors. The first point is in agreement with [19, 60] providing a new understanding of the advantage in the cloning scenario, i.e. in terms of quantum contextuality present in the smaller $\mathbb{B}_6$.

4. Discussion

In this work, we use the resource theory of contextuality introduced in [36]. We examine, with a resource theoretic perspective, the preservation of contextuality due to measurement simulability; known techniques used in experimental tests of contextuality; and the polytope structure of novel composed scenarios. These composed scenarios can be interpreted as a strategy for extending inequalities from smaller scenarios to larger ones.

To elaborate, we establish a connection between the simulation of measurements in operational theories with free operations and the creation of simpler scenarios achieved by omitting certain measurements. Furthermore, by recognizing that mixing is formally a free operation, we offer a new interpretation of the engineering of operational equivalences used in the tests detailed in [38]. We conclude that the free operations provide a simple and rigorous argument in favor of the experimental conclusions drawn from [38] regarding the use of secondary procedures as a tool for witnessing contextuality from imperfect equivalences.

Moreover, we introduce a composition of scenarios allowing the construction of complex scenarios while conserving the resource. This brings light to the importance of the resource theory developed in [36], especially in situations limited by the intrinsic complexity of numerically studying correlation polytopes.

We then apply the techniques to analyze *quantum* contextuality, leading to both foundational and practical implications. We have demonstrated that there always exists quantum contextual behaviors for a class of prepare-and-measure scenarios—and such a class encompasses the scenarios from [13, 17–19]. We also show that quantum contextuality is present for every nontrivial facet of the noncontextual polytope for scenarios of the form $\mathbb{B}_{\text{si}}^{\boxplus n}$. Moreover, we show that the scenario related to the task of state-dependent cloning, $\mathbb{B}_{\text{qc}}$, can be decomposed in terms of the simpler scenario $\mathbb{B}_6$. Thus, we can conclude that the quantum resource present in $\mathbb{B}_{\text{qc}}$ is inherited from quantum contextuality in $\mathbb{B}_6$. This also allows one to understand $NC(\mathbb{B}_{\text{qc}})$ via the inequalities of $NC(\mathbb{B}_6)$, which is a much simpler computational task.

4.1. Relation with previous work

Resource theoretic investigations of prepare-and-measure (generalized) contextuality scenarios remain largely unexplored. In this work, we have presented various qualitative and quantitative results that analyze the specific structure of these scenarios. We believe these findings can be important in practical applications, enabling the development of novel demonstrations of quantum contextuality, or the lack thereof, akin to the successful application of the monotone d, as seen in [51], for constraining the emergence of noncontextuality under quantum Darwinism.

On the contrary, for a different yet related notion of contextuality, namely KS contextuality, not only there is a vast literature devoted to formalizing a resource theory of it [27–29, 32, 61–63], but also its application to relevant tasks [31, 64, 65]. In this case, very similar constructions, such as the operation $\boxplus$ we have considered here, have been introduced for empirical models in the resource theory of KS-contextuality in [29], as we have pointed out before. Our description differs from theirs since it uses a fairly *different* notion of nonclassicality, namely, generalized contextuality. Those differences are not only present at a conceptual level, but result in a completely different scenario description, with fairly different tools. For example, the various quantum states used are present operationally in the description of a generalized contextuality scenario, while those are left out from the definition of scenarios used for studying KS-contextuality. Consequently, there is no compelling argument for why results from generalized contextuality scenarios should apply to the measurement scenarios in the KS formalism, and vice-versa. Yet, the existing literature on KS-contextuality is certainly suggestive of the future directions to be considered.

4.2. Further directions

The examples here discussed are far from exhausting the possibilities of the tools developed. Therefore, finding other physically appealing scenarios, or introducing novel composition rules beyond $\boxplus$ is an interesting perspective. Further investigations could also use small perturbations over the quantum measurements [66], and with the help of contextuality monotones, try to understand how much can one perturb the quantum behaviors and still witness contextuality, which is important for experimental implementation of generalized noncontextuality.

One potential venue of exploration involves studying the interplay between the composition rule $\boxplus$ and scenarios relevant for quantum computation. For instance, it remains unclear the relevance of generalized contextuality in some measurement-based schemes of quantum computation [67, 68]. Possibly, each measurement step leads to some defined scenario $\mathbb{B}$, and the sequence of measurements leading to some sequence $\mathbb{B}_1 \boxplus \cdots \boxplus \mathbb{B}_n$. Furthermore, it is likely that the resource theory of generalized contextuality will play a leading role in explaining hardness of classically simulating quantum computations for the so-called Λ-polytope method [69–71], that provides an ontological model that is measurement noncontextual, but preparation contextual, and for which it is unknown what nonclassical resources drive the simulation overhead.

To conclude, our work motivates the utilization of resource-theoretic analysis of generalized contextuality, as we provide new qualitative insights into the underlying polytope structure within prepare-and-measure scenarios. We have demonstrated the applicability of the composition rule $\boxplus$, which can be interpreted as an instance of a lifting of noncontextuality inequalities. Formally, lifting has been successfully employed in analyzing other pertinent quantum information polytopes, such as Bell inequalities that define facets in local polytopes [72]. Nevertheless, the formal lifting strategies for noncontextuality inequalities in prepare-and-measure scenarios remain an uncharted territory, lacking a formal complete description. We hope our work paves the way for future investigations, encouraging exploration in this direction.

Data availability statement

No new data were created or analysed in this study.

Acknowledgments

The authors would like to thank Ana Belén Sainz and Marcelo Terra Cunha for their helpful comments on an early version of this work.

R W, A T and B A would like to thank National Council for the Improvement of Higher Education (CAPES) and National Council for Scientific and Technological Development (CNPq) for their support during this research. RDB thanks São Paulo Research Foundation (Fapesp), which supported this work via Project Numbers 2016/24 162-8 and 2019/02 221-0, and acknowledges support by the Digital Horizon Europe project FoQaCiA, Foundations of quantum computational advantage, GA No. 101070558, funded by the European Union. B A was supported financially by São Paulo Research Foundation, Auxílio à Pesquisa—Jovem Pesquisador, Grant Number $2020/06454-7$. B A and R D B acknowledge funding from Instituto Serrapilheira, Chamada 2020.

Appendix A. Noncontextual polytope for the simplest scenario

With the methods developed by [37] it is possible to fully characterize the noncontextual polytope for the scenario $\mathbb{B}_{\text{si}}$. For a given behavior $B \in \mathbb{B}_{\text{si}}$ using the shorthand for $p(1|M_i,P_j) = p_{ij}$ we have that the facets of the noncontextual polytope are tightly characterized by the following set of inequalities:

$$0 \leqslant p_{ij} \leqslant 1,\ \forall M_i, P_j \tag{A1}$$

$$p_{12} + p_{22} - p_{14} - p_{23} \leqslant 1 \tag{A2}$$

$$p_{12} + p_{22} - p_{13} - p_{24} \leqslant 1 \tag{A3}$$

$$p_{22}+p_{13}-p_{12}-p_{24}\leqslant 1 \tag{A4}$$
$$p_{12}+p_{23}-p_{22}-p_{14}\leqslant 1 \tag{A5}$$
$$p_{22}+p_{14}-p_{12}-p_{23}\leqslant 1 \tag{A6}$$
$$p_{23}+p_{14}-p_{12}-p_{22}\leqslant 1 \tag{A7}$$
$$p_{12}+p_{24}-p_{22}-p_{13}\leqslant 1 \tag{A8}$$
$$p_{13}+p_{24}-p_{22}-p_{12}\leqslant 1. \tag{A9}$$

Taken from [37, 56].

Appendix B. Proof of theorem 2

Proof. Let $B_1\in NC(\mathbb{B}_1), B_2\in NC(\mathbb{B}_2)$. Hence, there are $(\Sigma^{(i)},\Lambda^{(i)},\Pi^{(i)},\Theta^{(i)})$ where $\Pi^{(i)}$ and $\Theta^{(i)}$, $i=1,2$, respect the operational equivalences at the ontological model level respectively for each scenario. For sets of labels we define $K_i, I_i, J_i, \{a_i\}, \{b_i\}$ as before (see definition 8), for their respective operational primitives from $\mathbb{B}_i$. The scenarios are finite and the operational equivalences are fixed and finite as well, so each set ranges over a finite set of labels.

$$K := K_1\cup K_2$$
$$I := I_1\cup I_2$$
$$J := J_1\cup J_2$$
$$\{a\}_{a=1}^{|\mathbb{E}_{\mathbb{P}_1\cup\mathbb{P}_2}|} := \{a_1\}_{a_1=1}^{|\mathbb{E}_{\mathbb{P}_1}|}\cup\{a_2\}_{a_2=1}^{|\mathbb{E}_{\mathbb{P}_2}|},$$
$$\{b\}_{b=1}^{|\mathbb{E}_{\mathbb{M}_1\cup\mathbb{M}_2}|} := \{b_1\}_{b_1=1}^{|\mathbb{E}_{\mathbb{M}_1}|}\cup\{b_2\}_{b_2=1}^{|\mathbb{E}_{\mathbb{M}_2}|}.$$

From the definition of noncontextuality at the ontological model level, we have the equations below. Here and throughout this appendix we simplify the notation to $p(k|M_i,P_j)\equiv p(k|i,j)$.

$$p(k_1|i_1,j_1)=\sum_{\lambda_1\in\Lambda_1}\xi_{[k_1|i_1]}(\lambda_1)\,\mu_{j_1}(\lambda_1), \tag{B1}$$
$$p(k_2|i_2,j_2)=\sum_{\lambda_2\in\Lambda_2}\xi_{[k_2|i_2]}(\lambda_2)\,\mu_{j_2}(\lambda_2), \tag{B2}$$
$$\sum_{j_1}\left(\alpha_{j_1}^{a_1}-\beta_{j_1}^{a_1}\right)\mu_{j_1}(\Omega_1)=0,\ \forall a_1,\forall\Omega_1\in\Sigma_1 \tag{B3}$$
$$\sum_{j_2}\left(\alpha_{j_2}^{a_2}-\beta_{j_2}^{a_2}\right)\mu_{j_1}(\Omega_2)=0,\ \forall a_2,\forall\Omega_2\in\Sigma_2 \tag{B4}$$
$$\sum_{k_1,i_1}\left(\alpha_{[k_1|i_1]}^{b_1}-\beta_{[k_1|i_1]}^{b_1}\right)\xi_{[k_1|i_1]}(\lambda_1)=0,\ \forall\lambda_1,b_1, \tag{B5}$$
$$\sum_{k_2,i_2}\left(\alpha_{[k_2|i_2]}^{b_2}-\beta_{[k_2|i_2]}^{b_2}\right)\xi_{[k_2|i_2]}(\lambda_2)=0,\ \forall\lambda_2,b_2. \tag{B6}$$

In (B3)–(B6), $\xi_{[\cdot|i_1]}\in\Theta^{(1)}, \mu_{j_1}\in\Pi^{(1)}$, and similarly for the remaining distributions. If we consider the product between the behaviors, $B_1\boxplus B_2$, we can construct a novel ontological model using as the ontic space $\Lambda := \Lambda^{(1)}\sqcup\Lambda^{(2)}$ the disjoint union between the two sets. We then define $\tilde{\xi}_{[k|i]}:\Lambda\to[0,1]$ as,

$$\tilde{\xi}_{[k|i]}(\lambda) := \begin{cases} \xi_{[k_1|i_1]}(\lambda_1), & \lambda = (\lambda_1, 1) \\ \xi_{[k_2|i_2]}(\lambda_2), & \lambda = (\lambda_2, 2) \end{cases}$$

$$\forall \lambda \in \Lambda, \sum_{k \in K} \tilde{\xi}_{[k|i]}(\lambda) = \begin{cases} \sum_{k \in K} \tilde{\xi}_{[k|i_1]}(\lambda), \text{if } i \in I_1 \\ \sum_{k \in K} \tilde{\xi}_{[k|i_2]}(\lambda), \text{if } i \in I_2 \end{cases} = \begin{cases} \sum_{k_1 \in K_1} \tilde{\xi}_{[k_1|i_1]}(\lambda), \text{if } i \in I_1 \\ \sum_{k_1 \in K_1} \tilde{\xi}_{[k_1|i_2]}(\lambda), \text{if } i \in I_2 \end{cases} = \begin{cases} 1, \\ 1 \end{cases} = 1.$$

So that the extended functions are normalized in the ontic space Λ. We have considered that, whenever $i \in I_1 \cap I_2$ any function $\xi_{[k_1|i_1]}$ or $\xi_{[k_2|i_2]}$ will serve, we then just need to pick one and use it for our noncontextual ontological model. This means that if we have two scenarios with the same procedures, $\{M_1, M_2\}, \{M_1, M_2\} \to \{M_{1_1}, M_{2_1}, M_{1_2}, M_{2_2}\} \equiv \{M_1, M_2\}$. Therefore we can recognize if two procedures are simply the same. In this sense, we can have that the number of procedures in $\mathbb{B}_{\text{si}}$ and $\mathbb{B}_{\text{si}}^{\boxplus n}$ are the same so that we simplify the scenario's description.

For $\tilde{\mu}_j$, the ontic spaces are finite and we write $\tilde{\mu}_j(\{\lambda\}) \equiv \tilde{\mu}_j(\lambda)$. Let $j \in J$, we define that, if $j \in J_1$,

$$\tilde{\mu}_j(\lambda) := \begin{cases} \mu_{j_1}(\lambda), & \text{if } \lambda = (\lambda_1, 1) \\ 0, & \text{if } \lambda = (\lambda_2, 2) \end{cases}$$

and similarly if $j \in J_2$. Again, when $j \in J_1 \cap J_2$ we choose one of the ontological descriptions as our fixed definition for the preparation procedure associated with it. With this definition, we have that, for any $j \in J$,

$$\sum_{\lambda \in \Lambda} \tilde{\mu}_j(\lambda) = \sum_{\lambda = (\lambda_1, 1) \in \Lambda} \tilde{\mu}_j(\lambda) + \sum_{\lambda = (\lambda_2, 2) \in \Lambda} \tilde{\mu}_j(\lambda)$$

and, whenever $j \in J_1$ or $j \in J_2$ we recover the normalization condition from the already defined distributions in the parts. We then obtain that any $p(k|i,j)$ in $B_1 \boxplus B_2$ will have an ontological description,

$$\begin{aligned} \sum_{\lambda \in \Lambda_1 \sqcup \Lambda_2} \tilde{\xi}_{[k|i]}(\lambda) \tilde{\mu}_j(\lambda) &= \begin{cases} \sum_{\lambda \in \Lambda} \tilde{\xi}_{[k_1|i_1]}(\lambda) \tilde{\mu}_{j_1}(\lambda), & \text{if } k,i,j \in K_1, I_1, J_1 \\ \sum_{\lambda \in \Lambda} \tilde{\xi}_{[k_2|i_2]}(\lambda) \tilde{\mu}_{j_2}(\lambda), & \text{if } k,i,j \in K_2, I_2, J_2 \end{cases} \\ &= \begin{cases} \sum_{\lambda_1 \in \Lambda_1} \xi_{[k_1|i_1]}(\lambda_1) \mu_{j_1}(\lambda_1), & \text{if } k,i,j \in K_1, I_1, J_1 \\ \sum_{\lambda_2 \in \Lambda_2} \xi_{[k_2|i_2]}(\lambda_2) \mu_{j_2}(\lambda_2), & \text{if } k,i,j \in K_2, I_2, J_2 \end{cases} \\ &= \begin{cases} p(k_1|i_1, j_1), & \text{if } k,i,j \in K_1, I_1, J_1 \\ p(k_2|i_2, j_2), & \text{if } k,i,j \in K_2, I_2, J_2 \end{cases} = B_1 \boxplus B_2. \end{aligned}$$

Notice that in the new scenario $\mathbb{B}_1 \boxplus \mathbb{B}_2$ it is at play our operational constraint that the preparations of the parts do not interact with the measurements of one another. The operational equivalences defined in the scenario $\mathbb{B}_1 \boxplus \mathbb{B}_2$ are the ones from (29), so we need to study the following objects:

$$\sum_j \left(\alpha_j^a - \beta_j^a\right) \tilde{\mu}_j(\lambda), \ \forall \lambda \in \Lambda_1 \sqcup \Lambda_2, \forall \gamma^a \in \mathbb{E}_{\mathbb{P}_1 \cup \mathbb{P}_2}. \tag{B7}$$

It will be true, for all $\lambda \in \Lambda_1 \sqcup \Lambda_2$, the following holds,

$$\sum_j \left(\alpha_j^a - \beta_j^a\right) \tilde{\mu}_j(\lambda) = \underbrace{\sum_{j_1} \left(\alpha_{j_1}^a - \beta_{j_1}^a\right) \tilde{\mu}_{j_1}(\lambda)}_{\stackrel{(B3)}{=}0} + \underbrace{\sum_{j_2} \left(\alpha_{j_2}^a - \beta_{j_2}^a\right) \tilde{\mu}_{j_2}(\lambda)}_{\stackrel{(29)}{=}0} = 0, \forall \boldsymbol{\gamma}_{\mathbb{P}_1 \cup \mathbb{P}_2}^a = \boldsymbol{\gamma}_{\mathbb{P}_1 \cup \mathbb{P}_2}^{a_1}$$

$$\sum_j \left(\alpha_j^a - \beta_j^a\right) \tilde{\mu}_j(\lambda) = \underbrace{\sum_{j_1} \left(\alpha_{j_1}^a - \beta_{j_1}^a\right) \tilde{\mu}_{j_1}(\lambda)}_{\stackrel{(29)}{=}0} + \underbrace{\sum_{j_2} \left(\alpha_{j_2}^a - \beta_{j_2}^a\right) \tilde{\mu}_{j_2}(\lambda)}_{\stackrel{(B4)}{=}0} = 0, \forall \boldsymbol{\gamma}_{\mathbb{P}_1 \cup \mathbb{P}_2}^a = \boldsymbol{\gamma}_{\mathbb{P}_1 \cup \mathbb{P}_2}^{a_2}.$$

And for all $\lambda \in \Lambda_1 \sqcup \Lambda_2$ we also have, $\forall \boldsymbol{\gamma}_{\mathbb{M}_1 \cup \mathbb{M}_2}^b = \boldsymbol{\gamma}_{\mathbb{M}_1 \cup \mathbb{M}_2}^{b_1}$,

$$\begin{aligned}\sum_{k,i} \left(\alpha_{[k|i]}^b - \beta_{[k|i]}^b\right) \tilde{\xi}_{[k|i]}(\lambda) = & \underbrace{\sum_{k_1,i_1} \left(\alpha_{[k_1|i_1]}^{b_1} - \beta_{[k_1|i_1]}^{b_1}\right) \tilde{\xi}_{[k_1|i_1]}(\lambda_1)}_{\stackrel{(B5)}{=}0} \\ & + \underbrace{\sum_{k_2,i_2} \left(\alpha_{[k_2|i_2]}^{b_1} - \beta_{[k_2|i_2]}^{b_1}\right) \tilde{\xi}_{[k_2|i_2]}(\lambda_2)}_{\stackrel{(29)}{=}0} = 0,\end{aligned}$$

and $\forall \boldsymbol{\gamma}_{\mathbb{M}_1 \cup \mathbb{M}_2}^b = \boldsymbol{\gamma}_{\mathbb{M}_1 \cup \mathbb{M}_2}^{b_2}$,

$$\begin{aligned}\sum_{k,i} \left(\alpha_{[k|i]}^b - \beta_{[k|i]}^b\right) \tilde{\xi}_{[k|i]}(\lambda) = & \underbrace{\sum_{k_1,i_1} \left(\alpha_{[k_1|i_1]}^{b_2} - \beta_{[k_1|i_1]}^{b_2}\right) \tilde{\xi}_{[k_1|i_1]}(\lambda_1)}_{\stackrel{(29)}{=}0} \\ & + \underbrace{\sum_{k_2,i_2} \left(\alpha_{[k_2|i_2]}^{b_1} - \beta_{[k_2|i_2]}^{b_1}\right) \tilde{\xi}_{[k_2|i_2]}(\lambda_2)}_{\stackrel{(B6)}{=}0} = 0.\end{aligned}$$

This proves that the ontological model constructed is noncontextual for the behavior $B_1 \boxplus B_2$ whenever B_1, B_2 are also noncontextual behaviors.

For the $(\Leftarrow)$ part of the proof, suppose that the behavior $B_1 \boxplus B_2$ has a noncontextual ontological model $(\Sigma, \Lambda, \Pi, \Theta)$. We know that this $\mathbb{B}_1 \boxplus \mathbb{B}_2$ scenario has the same operational equivalences as both the scenarios $\mathbb{B}_1$ and $\mathbb{B}_2$ divided, by means of the weight vectors, e.g. $(\alpha_1^{a_1}, \alpha_2^{a_1}, \ldots, \alpha_{j_1}^{a_1}, 0, \ldots, 0)$. Hence, there exists an ontological model for B_1 inherited from $B_1 \boxplus B_2$ using the operational equivalences:

$$\sum_j \left(\alpha_j^a - \beta_j^a\right) \mu_j(\lambda) = 0, \forall \lambda \implies \sum_{j_1} \left(\alpha_{j_1}^a - \beta_{j_1}^a\right) \mu_{j_1}(\lambda) = 0, \forall \lambda, \forall \boldsymbol{\gamma}_{\mathbb{P}_1 \cup \mathbb{P}_2}^a \in \mathbb{E}_{\mathbb{P}_1 \cup \mathbb{P}_2},$$

where we can restrict $\{a\}$ to some set of labels $\{a_1\}$ and reduced vectors $\gamma_{\mathbb{P}}^{a_1}$ by cutting the zeros. We get the same for the behavior B_2. The ontological description of the probabilities we get immediately:

$$p(k_1|i_1,j_1) := \sum_{\lambda\in\Lambda} \xi_{[k=k_1|i=i_1]}(\lambda)\,\mu_{j=j_1}(\lambda), \tag{B8}$$

for any $k_1,i_1,j_1 \in K_1,I_1,J_1$, and similarly,

$$p(k_2|i_2,j_2) := \sum_{\lambda\in\Lambda} \xi_{[k=k_2|i=i_2]}(\lambda)\,\mu_{j=j_2}(\lambda). \tag{B9}$$

□

B.1. l_1-distance

We prove lemma 3 as follows: Recall that the l_1-distance monotone is defined as,

$$\mathsf{d}(B) := \min_{B^*\in NC(\mathbb{B})} \max_{i,j} \sum_k |p(k|i,j) - p^*(k|i,j)|. \tag{B10}$$

Let B_1^* and B_2^* be the noncontextual behaviors achieving the minimum in equation (B10). Denoting $(p^*(k|i,j))_{k\in K, i\in I, j\in J} \equiv B_1^* \boxplus B_2^*$,

$$\begin{aligned}
&\mathsf{d}(B_1 \boxplus B_2)\\
&\quad\leqslant \max_{i,j}\sum_k |p(k|i,j) - p^*(k|i,j)|\\
&\quad= \max_{i,j}\left\{\left\{\sum_k |p_1(k_1|i_1,j_1) - p_1^*(k_1|i_1,j_1)|\right\} \cup \left\{\sum_k |p_2(k_2|i_2,j_2) - p_2^*(k_2|i_2,j_2)|\right\}\right\}\\
&\quad= \max\left\{\max_{i_1,j_1}\sum_k |p_1(k_1|i_1,j_1) - p_1^*(k_1|i_1,j_1)|, \max_{i_2,j_2}\sum_k |p_2(k_2|i_2,j_2) - p_2^*(k_2|i_2,j_2)|\right\}\\
&\quad= \max\{\mathsf{d}(B_1), \mathsf{d}(B_2)\} \leqslant \mathsf{d}(B_1) + \mathsf{d}(B_2).
\end{aligned}$$

Appendix C. Quantum realization in the simplest scenario

Consider the so-called simplest scenarios $\mathbb{B}_{\text{si}}$ from definition 3. In this scenario there are no operational equivalences between the measurement procedures $\mathbb{M} := \{M_1, M_2\}$. A possible quantum contextual realization within the simplest scenario was presented in [13, 17], where we simply consider that M_1, M_2 are given by the POVMs, $M_1 = \frac{1}{\sqrt{2}}(\sigma_X + \sigma_Z), M_2 = \frac{1}{\sqrt{2}}(\sigma_X - \sigma_Z)$. For the preparations we can simply take, as is usual, the preparations (2)–(5), such that this realization gives rise immediately to the correct operational equivalences for preparation procedures from $\mathbb{B}_{\text{si}}$. For a sufficiently large number of repeated procedures, we get the following probabilistic data table (we omit probabilities corresponding to $1-p$ events).

Since we have a full characterization of the noncontextual polytope for such scenario [37] we notice that table 1 is *contextual* because it violates Ineq. (A8)

$$p_{12} + p_{24} - p_{22} - p_{13} = 0.8535 + 0.8525 - 0.1464 - 0.1464 = 1.4132 > 1.$$

Table 1. Data-table for the final statistics obtained by quantum predictions.

	ρ^1	ρ^2	ρ^3	ρ^4
E_1^1	0.1464	0.8535	0.1464	0.8535
E_1^2	0.8535	0.1464	0.1464	0.8535

Appendix D. Permutations of contextual vertices

In this appendix, we prove lemma 4. There are three partial results we need:

1. The set of vertices of the polytope of all behaviors $\mathbb{B}_{\text{si}}$, is the set of deterministic assignments that respect the operational equivalences associated with the preparation procedures. Therefore there is always a permutation $T_{v\to w}$ between any two vertices from $\mathbb{B}_{\text{si}}$. Since any permutation is also a free operation, we need to show that $T_{v\to w}$ is a special kind of free operation, one that satisfies,

$$B \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \Leftrightarrow T_{v\to w}(B) \in C(\mathbb{B}) \setminus NC(\mathbb{B}).$$

   This will be true whenever $T_{v\to w}$ is a permutation of elements in the behavior $B \in \mathbb{B}_{\text{si}}$.
2. To do so, we will use the contextual measure $\mathsf{d} : \mathbb{B} \to \mathbb{R}_+$. We need to show that

$$B \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \implies \mathsf{d}(B) > 0. \tag{D1}$$

3. We need to show that for any quantum contextual behavior $B \in \mathbb{B}_{\text{si}}^{\boxplus n}$, $n \geqslant 1$, there always exists some transformation $T_{v\to w}$ between contextual vertices of $\mathbb{B}_{\text{si}}^{\boxplus n}$ that maintains this behavior inside the set $\mathbb{B}_{\text{si}}^{\boxplus n}$. This will be true for $\mathbb{B}_{\text{si}}^{\boxplus n}$ because for any $n \geqslant 1$, some of the features regarding the polytope structure of the simplest scenario will remain.

We then proceed with the demonstration of these lemmas.

Lemma 5. *Let* $\mathbb{B} := (|J|, |I|, |K|, \mathbb{E}_{\mathbb{M}}, \mathbb{E}_{\mathbb{P}})$ *be any finitely defined prepare-and-measure scenario. Let* $\mathsf{d} : \mathbb{B} \to \mathbb{R}_+$ *be the* l_1*-contextuality monotone defined in lemma 3. Then, the following holds:*

$$B \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \implies \mathsf{d}(B) > 0. \tag{D2}$$

Proof. Let $B \in C(\mathbb{B}) \setminus NC(\mathbb{B})$. Then, $\mathsf{d}(B) = 0$ implies that,

$$\begin{aligned}
&\min_{B^* \in NC(\mathbb{B})} \max_{i,j} \sum_k |p(k|i,j) - p^*(k|i,j)| = 0 \implies \\
&\exists B^* \in NC(\mathbb{B}), \max_{i,j} \sum_k |p(k|i,j) - p^*(k|i,j)| = 0, \implies \\
&\forall i \in I, \forall j \in J, \sum_k |p(k|i,j) - p^*(k|i,j)| = 0 \implies \\
&\forall i \in I, \forall j \in J, \forall k \in K, |p(k|i,j) - p^*(k|i,j)| = 0
\end{aligned}$$

which implies that $B = B^*$, contradiction. Therefore, we must have that $\mathsf{d}(B) > 0$. □

Lemma 6. *Let $\mathbb{B} := (|J|, |I|, |K|, \mathbb{E}_{\mathbb{M}}, \mathbb{E}_{\mathbb{P}})$ be any finitely defined prepare-and-measure scenario. Let $P \in \mathcal{F}$ defined such that, for all $i \in I$, $q_O^i : K \to \tilde{K} = K$, $q_M : \tilde{I} = I \to I$, $q_P : \tilde{J} = J \to J$ are permutation matrices. Then,*

$$B \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \Leftrightarrow P(B) \in C(\mathbb{B}) \setminus NC(\mathbb{B}). \tag{D3}$$

Whenever $P \in \mathcal{F}$ is defined by permutation matrices we call P a free permutation. If a free operation satisfies equation (D3) we will refer to this operation as a completely free operation.

Proof. We want to show that free permutations are completely free transformations. Let $B \in \mathbb{B}$, and let $P \in \mathcal{F}$ be a free permutation. Since $P \in \mathcal{F}$ we immediately have that

$$B \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \Leftarrow P(B) \in C(\mathbb{B}) \setminus NC(\mathbb{B}).$$

Therefore, we need to show that the arrow $\Rightarrow$ holds. Note that the action of P is simply to rearrange the labels. We denote this by using the tilde notation,

$$B := (p(k|i,j))_{k\in K, i\in I, j\in J} \mapsto P(B) = \left(p\left(\tilde{k}|\tilde{i},\tilde{j}\right)\right)_{\tilde{k}\in K, \tilde{i}\in I, \tilde{j}\in J}.$$

This implies that, using the l_1-monotone,

$$\begin{aligned}\mathsf{d}(B) &= \min_{B^*\in NC(\mathbb{B})} \max_{i\in I, j\in J} \sum_{k\in K} |p(k|i,j) - p^*(k|i,j)| \\ &= \min_{B^*\in NC(\mathbb{B})} \max_{\tilde{i}\in I, \tilde{j}\in J} \sum_{\tilde{k}\in K} |p\left(\tilde{k}|\tilde{i},\tilde{j}\right) - p^*\left(\tilde{k}|\tilde{i},\tilde{j}\right)| = \mathsf{d}(P(B)).\end{aligned}$$

We can then conclude that,

$$B \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \overset{\text{Lemma 5}}{\Longrightarrow} \mathsf{d}(B) > 0 \implies \mathsf{d}(P(B)) > 0 \implies P(B) \in C(\mathbb{B}) \setminus NC(\mathbb{B}) \tag{D4}$$

whenever P is a free operation constructed from permutation matrices. □

Lemma 7. *Let $\mathbb{B}_{si}$ be the simplest scenario, as defined in definition 3. The noncontextual polytope $NC(\mathbb{B}_{si})$ has eight facet-defining noncontextuality inequalities, that we associate with affine-linear functionals $\{h_i\}_{i=1}^8$, with $h_i : \mathbb{R}^8 \to \mathbb{R}$. Then, for each affine-functional h_i there is one, and only one vertex $B_v \in V(\mathbb{B}_{si})$, for $V(\mathbb{B}_{si})$ the set of vertices of the convex polytope $\mathbb{B}_{si}$, that violates the noncontextuality inequality associated with $h_i(B) \leqslant 0$.*

Proof. Writing the functionals $h_i(B) \leqslant 0$ is equivalent to writing the noncontextuality inequalities given by equations (A1)–(A9). The polytope $NC(\mathbb{B}_{\rm si})$ has many other noncontextuality inequalities but these constitute the non-trivial tight noncontextuality inequalities. The lemma is proven then by construction: table 2 has all elements of $V(\mathbb{B}_{\rm si})$, where we choose $B \equiv \begin{pmatrix} p_{11}, p_{12}, p_{13}, p_{14} \\ p_{21}, p_{22}, p_{23}, p_{24}\end{pmatrix}$.

Table 2. Table of deterministic vertices from $C(\mathbb{B}_{\mathrm{si}})$. Vertices violating one of the tight noncontextuality inequalities defined by (A1)–(A9) correspond to contextual deterministic behaviors (see inequalities below). Note that for this scenario noncontextual vertices of $NC(\mathbb{B}_{\mathrm{si}})$ need not be deterministic.

	$(1,1,1,1)$	$(1,0,0,1)$	$(1,0,1,0)$	$(0,1,0,1)$	$(0,1,1,0)$	$(0,0,0,0)$
$(1,1,1,1)$	$\begin{pmatrix}1,1,1,1\\1,1,1,1\end{pmatrix}$	$\begin{pmatrix}1,0,0,1\\1,1,1,1\end{pmatrix}$	$\begin{pmatrix}1,0,1,0\\1,1,1,1\end{pmatrix}$	$\begin{pmatrix}0,1,0,1\\1,1,1,1\end{pmatrix}$	$\begin{pmatrix}0,1,1,0\\1,1,1,1\end{pmatrix}$	$\begin{pmatrix}0,0,0,0\\1,1,1,1\end{pmatrix}$
$(1,0,0,1)$	$\begin{pmatrix}1,1,1,1\\1,0,0,1\end{pmatrix}$	$\begin{pmatrix}1,0,0,1\\1,0,0,1\end{pmatrix}$	$\begin{pmatrix}1,0,1,0\\1,0,0,1\end{pmatrix}$	$\begin{pmatrix}0,1,0,1\\1,0,0,1\end{pmatrix}$	$\begin{pmatrix}0,1,1,0\\1,0,0,1\end{pmatrix}$	$\begin{pmatrix}0,0,0,0\\1,0,0,1\end{pmatrix}$
$(1,0,1,0)$	$\begin{pmatrix}1,1,1,1\\1,0,1,0\end{pmatrix}$	$\begin{pmatrix}1,0,0,1\\1,0,1,0\end{pmatrix}$	$\begin{pmatrix}1,0,1,0\\1,0,1,0\end{pmatrix}$	$\begin{pmatrix}0,1,0,1\\1,0,1,0\end{pmatrix}$	$\begin{pmatrix}0,1,1,0\\1,0,1,0\end{pmatrix}$	$\begin{pmatrix}0,0,0,0\\1,0,1,0\end{pmatrix}$
$(0,1,0,1)$	$\begin{pmatrix}1,1,1,1\\0,1,0,1\end{pmatrix}$	$\begin{pmatrix}1,0,0,1\\0,1,0,1\end{pmatrix}$	$\begin{pmatrix}1,0,1,0\\0,1,0,1\end{pmatrix}$	$\begin{pmatrix}0,1,0,1\\0,1,0,1\end{pmatrix}$	$\begin{pmatrix}0,1,1,0\\0,1,0,1\end{pmatrix}$	$\begin{pmatrix}0,0,0,0\\0,1,0,1\end{pmatrix}$
$(0,1,1,0)$	$\begin{pmatrix}1,1,1,1\\0,1,1,0\end{pmatrix}$	$\begin{pmatrix}1,0,0,1\\0,1,1,0\end{pmatrix}$	$\begin{pmatrix}1,0,1,0\\0,1,1,0\end{pmatrix}$	$\begin{pmatrix}0,1,0,1\\0,1,1,0\end{pmatrix}$	$\begin{pmatrix}0,1,1,0\\0,1,1,0\end{pmatrix}$	$\begin{pmatrix}0,0,0,0\\0,1,1,0\end{pmatrix}$
$(0,0,0,0)$	$\begin{pmatrix}1,1,1,1\\0,0,0,0\end{pmatrix}$	$\begin{pmatrix}1,0,0,1\\0,0,0,0\end{pmatrix}$	$\begin{pmatrix}1,0,1,0\\0,0,0,0\end{pmatrix}$	$\begin{pmatrix}0,1,0,1\\0,0,0,0\end{pmatrix}$	$\begin{pmatrix}0,1,1,0\\0,0,0,0\end{pmatrix}$	$\begin{pmatrix}0,0,0,0\\0,0,0,0\end{pmatrix}$

Each vertex defining a deterministic contextual behavior violates one, and only one, noncontextuality inequality

$$h_1(B) = p_{12} + p_{22} - p_{14} - p_{23} - 1 \leqslant 0 \to h_1\left(\begin{pmatrix}0,1,1,0\\0,1,0,1\end{pmatrix}\right) > 0$$
$$h_2(B) = p_{12} + p_{22} - p_{13} - p_{24} - 1 \leqslant 0 \to h_2\left(\begin{pmatrix}0,1,0,1\\0,1,1,0\end{pmatrix}\right) > 0$$
$$h_3(B) = p_{22} + p_{13} - p_{12} - p_{24} - 1 \leqslant 0 \to h_3\left(\begin{pmatrix}1,0,1,0\\0,1,1,0\end{pmatrix}\right) > 0$$
$$h_4(B) = p_{12} + p_{23} - p_{22} - p_{14} - 1 \leqslant 0 \to h_4\left(\begin{pmatrix}0,1,1,0\\1,0,1,0\end{pmatrix}\right) > 0$$
$$h_5(B) = p_{22} + p_{14} - p_{12} - p_{23} - 1 \leqslant 0 \to h_5\left(\begin{pmatrix}1,0,0,1\\0,1,0,1\end{pmatrix}\right) > 0$$
$$h_6(B) = p_{23} + p_{14} - p_{12} - p_{22} - 1 \leqslant 0 \to h_6\left(\begin{pmatrix}1,0,0,1\\1,0,1,0\end{pmatrix}\right) > 0$$
$$h_7(B) = p_{12} + p_{24} - p_{22} - p_{13} - 1 \leqslant 0 \to h_7\left(\begin{pmatrix}0,1,0,1\\1,0,0,1\end{pmatrix}\right) > 0$$
$$h_8(B) = p_{13} + p_{24} - p_{22} - p_{12} - 1 \leqslant 0 \to h_8\left(\begin{pmatrix}1,0,1,0\\1,0,0,1\end{pmatrix}\right) > 0.$$

In terms of the polytope structure, each contextual behavior $B \in \mathbb{B}_{\mathrm{si}}$ violates at least one inequality, and therefore for some $h \in \{h_i\}_{i=1}^{8}$ and some $B_v \in V(\mathbb{B})$, we have that both $h(B) > 0$ and $h(B_v) > 0$. □

Lemma 8. *Whenever $B_v, B_w \in V(\mathbb{B}_{si})$ are contextual vertices, there exists a free permutation $T_{v\to w}$ satisfying the following:*

$$\forall B \in \mathbb{B}_{\mathrm{si}} \implies T_{v\to w}(B) \in \mathbb{B}_{\mathrm{si}}. \tag{D5}$$

Table 3. Free permutations acting over $\mathbb{B}_{\text{si}}$. Each one of these operations is such that they leave the polytope $\mathbb{B}_{\text{si}}$ invariant. They also leave $c(\mathbb{B})_{si}$ invariant, meaning that each vertex is sent to another vertex in the polytope.

Element	Result	q_O	q_M	q_P
α	$\begin{pmatrix} p_{12},p_{11},p_{13},p_{14} \\ p_{22},p_{21},p_{23},p_{24} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
β	$\begin{pmatrix} p_{11},p_{12},p_{14},p_{13} \\ p_{21},p_{22},p_{24},p_{23} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
γ	$\begin{pmatrix} p_{21},p_{22},p_{23},p_{24} \\ p_{11},p_{12},p_{13},p_{14} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
δ	$\begin{pmatrix} p_{13},p_{14},p_{11},p_{12} \\ p_{23},p_{24},p_{21},p_{22} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$

Since free permutations are completely free operations, we have that there exists a quantum contextual behavior violating all noncontextuality inequalities of $\mathbb{B}_{si}$.

Proof. Let $\Gamma(\mathbb{B}_{\text{si}})$ be the symmetry group of the polytope $\mathbb{B}_{\text{si}} \subset \mathbb{R}^8 \subset \mathbb{R}^{16}$. For any convex polytope $\mathbb{B}_{\text{si}}$, the symmetry group $\Gamma(\mathbb{B}_{\text{si}})$ is finite. To each symmetry $\alpha \in \Gamma(\mathbb{B}_{\text{si}})$ we associate a (faithful) representation $T : \Gamma(\mathbb{B}_{\text{si}}) \to \text{Aut}(\mathbb{R}^8)$. Define $c(\mathbb{B}_{\text{si}}) := \text{ConvHull}\left(V(\mathbb{B}_{\text{si}}) \setminus V(NC(\mathbb{B}_{\text{si}}))\right)$. Then, we have that the polytope $c(\mathbb{B}_{\text{si}})$ is vertex-transitive, i.e. there exists an element of $\Gamma(\mathbb{B}_{\text{si}})$ that sends any vertex of $c(\mathbb{B}_{\text{si}})$ to any other vertex. To see this we consider the group elements $\alpha, \beta, \gamma, \delta$ defined by their representation matrices as, for any point $\begin{pmatrix} p_{11},p_{12},p_{13},p_{14} \\ p_{21},p_{22},p_{23},p_{24} \end{pmatrix} \in \mathbb{B}_{\text{si}}$:

The free operations that we associate with the group elements $\alpha, \beta, \gamma, \delta \in \Gamma(\mathbb{B}_{\text{si}})$, present in table 3 they constitute free permutations. Each one of these operations is such that they constitute a proof that $c(\mathbb{B}_{\text{si}})$ is a vertex-transitive convex polytope. To prove so we simply notice that we can make a graph, such that each contextual point is a vertex of the graph, and each edge is a free permutation between the vertices. Figure 3 we construct this graph; since this graph is completely connected, there is always a symmetry (free permutation) between any two vertices[8] and we conclude that $c(\mathbb{B}_{\text{si}})$ is a vertex-transitive convex polytope.

Since there exists a bijection between nontrivial violations given by equations (A1)–(A9), and contextual vertices in the scenario $\mathbb{B}_{\text{si}}$ we have that if $B \in \mathbb{B}_{\text{si}}$ violates an inequality associated with B_v a contextual vertex, since $c(\mathbb{B}_{\text{si}})$ is vertex-transitive there exists a symmetry $T_{v \to w}$, that is a free permutation that can be read from figure 3, such that $T_{v \to w}(B)$ violates any other noncontextuality inequality associated with any other contextual vertex $B_w \in V(c(\mathbb{B}_{\text{si}}))$. Therefore, let $B^Q \in \mathbb{B}_{\text{si}}$ be the quantum contextual behavior given by table 1. There exists a

[8] The set $\mathcal{F}$ of free operation is closed under composition.

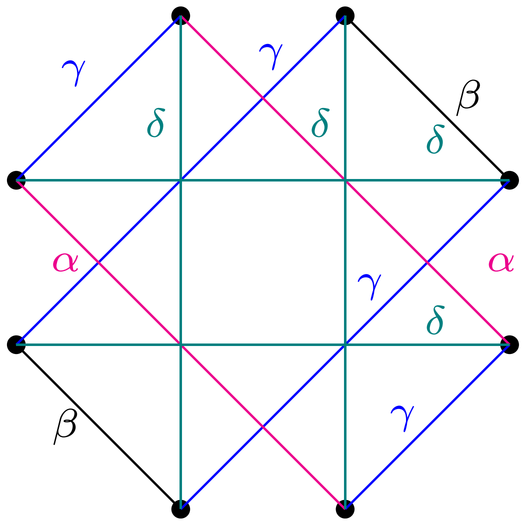


Figure 3. Graph of transformations between contextual vertices.

free permutation that sends B^Q to a region of the polytope $\mathbb{B}_{\mathrm{si}}$ that violates any other noncontextuality inequality. □

Now that we know that this is a true feature of $\mathbb{B}_{\mathrm{si}}$, we can prove the result from the text (lemma 4), that we rewrite here.

Lemma 9. *For any scenario of the form* $\mathbb{B} := \mathbb{B}_{si}^{\boxplus n}$, $n \geqslant 1$, *every tight noncontextuality inequality will have a quantum contextual behavior.*

Proof. Since we know that this is true for $n = 1$ we can try to prove this by induction. Let the set of non-trivial noncontextuality inequalities for $\mathbb{B}_{\mathrm{si}}$ be defined by $H_1 := \{h_i : h_i(B) \leqslant 0, i \in \{1,\ldots,8\}\}$. For $\mathbb{B}$ and $\mathbb{B}_{\mathrm{si}}^{\boxplus(n-1)}$ we use similar definitions, denoting H the set of functionals corresponding to inequalities of $NC(\mathbb{B})$, and H_{n-1} for $NC(\mathbb{B}_{\mathrm{si}}^{\boxplus(n-1)})$. Since we know that $NC(\mathbb{B}) = NC(\mathbb{B}_{\mathrm{si}}) \times NC(\mathbb{B}_{\mathrm{si}}^{\boxplus(n-1)})$ we have that H is the set of linear functionals such that, for all $\mathbb{B} \ni B = B_1 \boxplus B_2$,

$$\begin{aligned} H := &\{h : h(B) = h_1(B_1) \leqslant 0, \text{for some } h_1 \in H_1\} \\ &\cup \{h : h(B) = h_2(B_2) \leqslant 0, \text{for some } h_2 \in H_{n-1}\}. \end{aligned} \tag{D6}$$

Therefore, as our hypothesis, we suppose that there exists a quantum contextual behavior B^Q such that, for all $h \in H_{n-1}$ we have that $h(B^Q) > 0$. Since, for H_1 we know that this is also true and that H is given by equation (D6), we have that for every $h \in H$ there exists some $B^Q \in \mathbb{B}$ such that $h(B^Q) > 0$. We conclude that this must be true for all $n \geqslant 1$. □

Notice that equation (D6) is another way of stating that the number of facets in a convex polytope that is the product of two convex polytopes gets summed. This is clear by noticing that we can associate the sets H to matrices that define the convex polytope via an H-representation, and by proving lemma 2, from where it is clear how the set of inequalities (convex-linear functions in the terminology of the sets H) is upgrated for the product polytope.

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