Contextuality and probability in quantum mechanics and beyond
A theme issue compiled and edited by Samson Abramsky, Adán Cabello, Ehtibar N. Dzhafarov and Paweł Kurzyński

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About this issue

The word ‘contextuality’ has been on the lips of physicists since the 1970’s, related to a puzzling aspect of quantum theory: the outcomes of a quantum measurement cannot be understood in isolation from the entire experimental setup in which the measurement is made, including other quantum measurements performed together with the given one. Now, almost 50 years later, researchers are finally beginning to understand where this ‘contextuality’ comes from, and they are discovering how contextuality is connected to the power of quantum computers and future quantum technologies. They are also beginning to investigate the possibility of extending the notion of contextuality and the associated analytic tools beyond quantum physics, such as to computer databases and human decision making. This special issue is a collection of contributions reflecting key directions and approaches in this fascinating field of research.

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Cover image: Cover image adapted from Adán Cabello’s paper in this issue by Damir Dzhafarov; the original graphic was co-created by Sheila López Rosa.
The problem of quantum correlations and the totalitarian principle

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The totalitarian principle establishes that ‘anything not forbidden is compulsory’. The problem of quantum correlations is explaining what selects the set of quantum correlations for a Bell and Kochen–Specker (KS) contextuality scenario. Here, we show that two assumptions and a version of the totalitarian principle lead to the quantum correlations. The assumptions are that there is a non-empty set of correlations for any KS contextuality scenario and a statistically independent realization of any two KS experiments. The version of the totalitarian principle says that any correlation not forbidden by these assumptions can be produced. This paper contains a short version of the proof (presented elsewhere) and explores some implications of the result.

This article is part of the theme issue ‘Contextuality and probability in quantum mechanics and beyond’.

1. Introduction

John Wheeler conjectured that the universe is not ‘a machine governed by some magic equation’, but ‘a self-synthesizing system’ [1], in which ‘[e]verything is built on the unpredictable outcomes of billions upon billions of elementary … phenomena’ [2] that are, themselves, ‘lawless events’ [3]. It is difficult to picture a universe like that. Nevertheless, an interesting intellectual exercise is identifying signatures of such a universe and looking for them in our universe. A possible signature could be that Gell-Mann’s totalitarian principle [4] holds in it. The totalitarian principle states: ‘anything not forbidden is compulsory’. Of course, we have to clarify what is ‘anything’ and what makes anything ‘forbidden’.

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In this paper, we will assume that we are in a Wheelerian lawless universe and we ask ourselves what kind of non-locality and contextuality would be observed in such a universe. Our aim is to address a famous open problem in foundations of physics: identifying the principle that selects the quantum correlations for Bell [5,6] and Kochen–Specker (KS) contextuality [7–9] scenarios.

We assume that the reader has some previous knowledge of Bell non-locality and KS contextuality. However, we will start by reviewing all the concepts needed. In §2, we define Bell and KS contextuality scenarios, state the problem and recall the ‘solution’ quantum theory gives. In §3, we present our assumptions and the main result. In §4, we provide a short proof (an extended version can be found in [10]). In §5, we summarize the result. In §6, we discuss some implications and present some lines for future research.

2. The problem of quantum correlations

(a) Compatibility, non-disturbance and ideal measurements

We consider the set of theories that assign probabilities to the outcomes of measurements. We will denote by $P(x = a | \psi)$, the probability of obtaining outcome $a$ when measuring $x$ on state $\psi$. By ‘state’ we mean the object that encodes the expectations about the outcomes of future measurements. We do not assume any particular mathematical representation for the states, measurements, and outcomes.

**Definition 2.1.** A measurement $z$ with outcomes $c \in C$ is a coarse-graining of a measurement $x$ with outcomes $a \in A$ if, for all $c \in C$, there is $A_c \subseteq A$ such that, for all states $\psi$,

$$P(z = c | \psi) = \sum_{a \in A_c} P(x = a | \psi)$$

(2.1)

and $A_c \cap A_{c'} = \emptyset$ if $c \neq c'$.

**Definition 2.2.** Two measurements are compatible if they are coarse-grainings of the same measurement.

**Definition 2.3.** Two sets of measurements, $X = \{x_i\}$, with respective outcomes $a_i \in A_i$, and $Y = \{y_j\}$, with respective outcomes $b_j \in B_j$, such that every pair $(x_i, y_j)$ are compatible, are mutually non-disturbing if, for all $x_i \in X$, $a_i \in A_i$ and $y_j, y_k \in Y$,

$$\sum_{b_j \in B_j} P(x_i = a_i, y_j = b_j | \psi) = \sum_{b_k \in B_k} P(x_i = a_i, y_k = b_k | \psi),$$

(2.2)

and, for all $y_j \in Y$, $b_i \in B_i$ and $x_j, x_k \in X$,

$$\sum_{a_j \in A_j} P(x_j = a_j, y_i = b_i | \psi) = \sum_{a_k \in A_k} P(x_k = a_k, y_i = b_i | \psi).$$

(2.3)

Therefore, the marginal probabilities $P(x_i = a_i | \psi)$ are independent of the choice of $y_j \in Y_j$ and the marginal probabilities $P(y_i = b_i | \psi)$ are independent of the choice of $x_j \in X_j$.

**Definition 2.4.** A measurement is ideal (or sharp [11]) if

(i) it gives the same outcome when performed consecutive times on the same physical system,

(ii) it does not disturb compatible measurements, and

(iii) all its coarse-grainings satisfy (i) and (ii).
(b) Bell scenarios

A Bell experiment [5,6] involves two or more spatially separated agents (typically referred to as parties). Each party performs, on a different subsystem of a composite system, one measurement freely chosen from a fixed set. The choice of measurement of each party is space-like separated from the measurement outcomes observed by the other parties. Therefore, assuming that faster-than-light communication is impossible, measurements performed in the same round of a Bell experiment by different parties are mutually non-disturbing.

A Bell scenario is characterized by the number of parties, the number of measurements each party can perform, the number of outcomes of each measurement, and the relations of compatibility between the measurements. For example, the Clauser–Horne–Shimony–Holt (CHSH) or (2, 2, 2) Bell scenario [5,6] has two parties, each of them with two measurements, each of them with two outcomes, and every measurement of one party is compatible with every measurement of the other party.

The simplest quantum systems producing deviations from local realism in Bell scenarios are pairs of qubits. Quantum deviations from local realism require entangled states [12] and incompatible local measurements.

(c) Kochen–Specker contextuality scenarios

KS contextuality scenarios (hereafter KS scenarios for brevity) extend Bell scenarios to situations in which compatible measurements are not necessarily space-like separated in the sense of Bell experiments. A KS contextuality scenario is characterized by a set of ideal measurements, their outcomes and their relations of compatibility.

The restriction to ideal measurements in KS scenarios (restriction that does not exist in Bell scenarios) makes that, in KS scenarios, compatible measurements become mutually non-disturbing (as occurs in Bell scenarios). Any Bell scenario with ideal measurements is a KS scenario, but Bell scenarios with non-ideal measurements are not KS scenarios.

The assumptions of repeatability of the outcomes (i.e. condition (i) in the definition of ideal measurement) and mutual non-disturbance between measurements that are compatible (i.e. condition (ii)) justify the assumption of outcome non-contextuality for ideal measurements made for hidden variable theories in [7–9,13–17]. If conditions (i) and (ii) do not hold, then the assumption of outcome non-contextuality is not satisfied by classical systems [18].

Every KS set of quantum measurements (as defined in e.g. [9,19–21]) defines a KS scenario. There are also KS scenarios that do not require entire KS sets, as quantum deviations from the predictions of KS non-contextual hidden variable theories occur in scenarios with fewer measurements. Among the latter, there are deviations that occur for particular states [13] and deviations that occur for any state of a given dimension [16,17,22].

Quantum deviations of KS non-contextual hidden variable theories require quantum systems of dimension three (qutrits) or larger [8,9], and do not require entangled states. The simplest KS scenario in which qutrits produce KS contextuality is the Klyachko–Can–Binicioğlu–Shumovsky (KCBS) KS scenario [13], involving five measurements \( x_i \) with \( i = 1, \ldots, 5 \) (with two possible outcomes), such that \( x_i \) and \( x_{i+1} \) (with the sum taken modulo five) are compatible.

(d) Contexts and graphs of compatibility

**Definition 2.5.** A context in a Bell or KS scenario \( S \) is a subset of the measurements in \( S \) which only contains compatible (and mutually non-disturbing) measurements.

The relations of compatibility between the measurements in \( S \) can be pictured by a graph in which vertices represent measurements and edges relations of compatibility. A graph with this interpretation is called a graph of compatibility. For example, the graph of compatibility of the CHSH Bell scenario is a square and the graph of compatibility of the KCBS KS scenario is a pentagon.
In a graph of compatibility, contexts are represented by cliques. A clique is a set of vertices every pair of which are adjacent.

(e) Mutually exclusive events and graphs of exclusivity

The events of a Bell or KS scenario \( S \) and their relations of mutual exclusivity are determined by the measurements, outcomes and relations of compatibility between the measurements available in \( S \).

**Definition 2.6.** Two events of \( S \) are mutually exclusive when there is a measurement \( M \), defined using the measurements in \( S \), such that each event corresponds to a different outcome of \( M \).

For example, in the CHSH Bell scenario, the events are of the form \((x = a, y = b|\psi)\) with \( x, y, a, b \in \{0, 1\} \). Events \((x = a, y = b|\psi)\) and \((x' = a', y' = b'|\psi)\) are mutually exclusive if \( x = x' \) and \( a \neq a' \) or \( y = y' \) and \( b \neq b' \). For example, if \( x = x', a \neq a' \) and \( y \neq y' \), then \( M \) is the four-outcome measurement producing events \((x = a, y = 0|\psi), (x = a, y = 1|\psi), (x = a', y' = 0|\psi)\) and \((x = a', y' = 1|\psi)\).

The relations of mutual exclusivity between events can be pictured by a graph in which vertices represent events and edges relations of mutual exclusivity. A graph with this interpretation is called a graph of exclusivity [23,24].

There are two types of graphs of exclusivity. On the one hand, there are graphs in which the vertices and edges encode (using colours) the measurements and outcomes that define the numeration. For example, the graph of exclusivity in figure 2 is of this type.

On the other hand, there are graphs of exclusivity in which vertices and edges represent abstract events and relations of mutual exclusivity, respectively, without reference to any particular scenario. The vertices of these graphs have no labellings (except, possibly, a numeration). For example, the graph of exclusivity in figure 2 is of this type.

(f) Correlations

What we informally refer to as ‘correlations’ for a particular Bell or KS scenario \( S \) is a set \( p(S) \in \mathcal{P}(S) \) of probability distributions, one for each context. Following the terminology introduced in [25] (and used in, e.g. [26]), we will refer to every \( p(S) \) as a ‘behaviour’ for \( S \). In the literature \( p(S) \) is also called an ‘empirical model’ [27] or ‘probability model’ [28,29] for \( S \).

For a given Bell or KS scenario \( S \), every initial state and set of measurements produce a behaviour. For example, for the CHSH Bell scenario \( S_{\text{CHSH}} \), if, for simplicity, we denote probabilities \( P(x = a, y = b|\psi) \) as \( P(ab|xy) \), a behaviour can be represented by the matrix

\[
p(S_{\text{CHSH}}) = \begin{bmatrix}
P(00|00) & P(01|00) & P(10|00) & P(11|00) \\
P(00|01) & P(01|01) & P(10|01) & P(11|01) \\
P(00|10) & P(01|10) & P(10|10) & P(11|10) \\
P(00|11) & P(01|11) & P(10|11) & P(11|11) \end{bmatrix}.
\] (2.4)

Note that each row in the right-hand side of equation (2.4) contains the probabilities of the events of one context. Alternatively, \( p(S_{\text{CHSH}}) \) can be seen as an assignment of probabilities to the (suitably ordered) vertices of the graph of exclusivity \( G_{\text{CHSH}} \) in figure 1. In this case, we will represent \( p(S_{\text{CHSH}}) \) by a vector \( p(G_{\text{CHSH}}) \in [0, 1]^{V(G_{\text{CHSH}})} \), where \( V(G_{\text{CHSH}}) \) is the set of vertices of \( G_{\text{CHSH}} \).

For a given Bell (KS scenario) \( S \), the set of local realistic (KS non-contextual) behaviours is a closed convex polytope, i.e. a closed convex set whose boundaries are flat, called the local polytope (KS non-contextual polytope). The corresponding set in quantum theory is a convex set that, in general, is not a polytope. The local polytope for the CHSH Bell scenario is identical to...
Figure 1. Graph of exclusivity $G_{\text{CHSH}}$ of the 16 events of the CHSH Bell scenario. $(ab|xy)$ denotes the event $(x = a, y = b | \psi)$. Each colour corresponds to one of the measurements: red if $x$ is 0, yellow if $x$ is 1, cyan if $y$ is 0 and purple if $y$ is 1. Each event is characterized by the outcomes of two measurements. This is the reason why each vertex has two half circumferences. An empty (full) half circumference of a given colour denotes that the outcome of the measurement represented by that colour is 0 (respectively, 1).

the non-contextual polytope for the KS scenario involving four two-outcome ideal measurements and having a square as graph of compatibility. Similarly, the local polytope for any Bell scenario is identical to the non-contextual polytope for the KS scenario that has the same number of measurements, outcomes, and graph of compatibility.

(g) Constraints for behaviours for Bell and Kochen–Specker scenarios

For a fixed Bell or KS scenario $S$, every behaviour $p(S)$ must satisfy three constraints:

(A) Normalization: For every context $\{x, \ldots, z\}$ (with respective outcomes $a \in A, \ldots, c \in C$) in $S$,

$$
\sum_{a \in A, \ldots, c \in C} P(x = a, \ldots, z = c | \psi) = 1. \tag{2.5}
$$

Any subset of a context is also a context.

(B) Non-disturbance: Every pair $(X, Y)$ of mutually non-disturbing sets of measurements in $S$ must satisfy Conditions (2.2) and (2.3).

(C) The probability of each event of $S$ must only be a function of the state and measurement outcomes that define the event. For example, $P(x = a, y = b | \psi)$ must only be a function of $\psi$, $x = a$, and $y = b$. This constrains the behaviours since, for a fixed $S$, any behaviour must correspond to a fixed $\psi$ and a fixed set $(x = a, y = b)$. 

(h) Quantum behaviours for Bell and Kochen–Specker scenarios

Any behaviour \( p(S) \) for a Bell or KS scenario \( S \) allowed by quantum theory satisfies the following conditions:

(I) The initial state \( \psi \) of the system can be associated with a vector with unit norm \( |\psi\rangle \) in a
Hilbert space \( \mathcal{H} \).

(II) The state after performing any set \( \{x^{(i)}\} \) of compatible measurements in \( S \) and obtaining, respectively, outcomes \( \{a_i\} \) can be associated with a vector with unit norm
\[
|\psi'\rangle = N_i \prod_i E^{(i)}_{a_i} |\psi\rangle ,
\]
where \( N_i \) is a normalization constant and \( \{E^{(i)}_{a_i}\} \) are projection operators acting on \( \mathcal{H} \). The projection operator \( E^{(i)}_{a_i} \) corresponds to measurement \( x^{(i)} \) with outcome \( a_i \). The projection operators corresponding to different outcomes of the same measurement satisfy
\[
E^{(i)}_{a_j} E^{(i)}_{a_k} = \delta_{j,k} E^{(i)}_{a_i}
\]
and
\[
\sum_k E^{(i)}_{a_k} = I_i
\]
where \( I \) is the identity operator. If \( x^{(i)} \) and \( x^{(k)} \) are compatible measurements, then
\[
[E^{(i)}_{a_j}, E^{(k)}_{a_m}] = 0 \quad \forall j, m,
\]
where \([\ldots]\) denotes the commutator.

(III) The probability of obtaining \( \{a_i\} \) when measuring \( \{x^{(i)}\} \) on state \( \psi \) satisfies \( |\langle\psi' | \psi\rangle|^2 \),
where \( |\psi'\rangle \) is given by equation (2.6).

Remarkably, the characterization of the quantum behaviours is similar for Bell scenarios (in which we do not assume that measurements are ideal) and for KS scenarios (in which all measurements are ideal by definition). This reflects the fact that any quantum behaviour for a Bell scenario can be attained with ideal measurements. This follows from Neumark’s (also named Naimark’s) dilation theorem [30–34] that states that every generalized measurement in quantum theory (represented by a positive-operator valued measure (POVM)) can be implemented as an ideal quantum measurement (represented by a projection-valued measure (PVM)) on a larger Hilbert space. In a Bell scenario, any local POVM \( x \) admits a local dilation to a PVM that is common to every context in which \( x \) appears. Because of this, the set of quantum behaviours for the Bell CHSH scenario is identical to set of quantum behaviours for the KS scenario involving four two-outcome ideal measurements and having a square as graph of compatibility. And similarly for every Bell scenario.

(i) The problem of quantum correlations

The problem we address here is identifying the physical reason or principle that explains why the behaviours that are realizable for Bell and KS scenarios are those that satisfy conditions (I)–(III). The question we want to answer is where does the ‘irrational effectiveness’ [35] of the Hilbert space formalism supplemented with Born’s rule for singling out the physically realizable behaviours come from, why the quantum formalism is empirically successful.

None of the proposed principles (non-signalling [36], non-triviality of communication complexity [37], information causality [38], macroscopic locality [39], exclusivity [40] and local orthogonality [41]) has succeeded in selecting the quantum behaviours even in the simplest Bell scenario. In fact, for every non-trivial Bell scenario, there are non-quantum behaviours which seem to satisfy all these principles [42].
3. Result

(a) Assumptions

We make the following assumptions:

**Assumption 3.1.** There is a non-empty set of behaviours for any KS scenario.

**Assumption 3.2.** There is a statistically independent joint realization of any two KS experiments.

**Definition 3.3.** Two experiments \( A \) and \( B \) are statistically independent if the occurrence of any of the events of \( A \) (\( B \)) does not affect the probability of occurrence of any of the events of \( B \) (respectively, \( A \)).

Consequently, if \( A \) and \( B \) are statistically independent experiments and matrix \( p(S_A) \) is the behaviour for \( A \) (e.g. \( p(S_A) \) could be the one in equation (2.4)) and \( q(S_B) \) is the behaviour for \( B \), then an observer can define an experiment \( (A,B) \) with a behaviour given by \( p(S_A) \otimes q(S_B) \), where \( \otimes \) is the tensor product.

(b) Result

The aim of this paper is to prove the following:

**Theorem 3.4.** The set of behaviours \( \mathcal{P}(S) \) allowed by quantum theory for any Bell or KS scenario \( S \) is equal to the largest set allowed by assumptions 3.1 and 3.2.

(c) The totalitarian principle

The fact that the quantum set equals the largest set allowed by assumptions 3.1 and 3.2 implies that any behaviour allowed by these assumptions is compulsory in the sense that there exist a preparation and a set of measurements that produce it. This resembles Gell-Mann’s totalitarian principle [4]: ‘anything not forbidden is compulsory’.

The story of the totalitarian principle can be summarized as follows. In the context of the interactions between baryons, antibaryons and mesons, Gell-Mann made the observation that any process which is not forbidden by a conservation law is not only allowed but must be included in the sum over all paths which contribute to the outcome of the interaction. Gell-Mann named it the ‘principle of compulsory strong interactions’ [4] and commented that it ‘is related to the state of affairs that is said to prevail in a perfect totalitarian state. Anything that is not compulsory is forbidden’ [4]. After that, the principle started to be called ‘Gell-Mann’s totalitarian principle’ [43,44] and reformulated as ‘anything not forbidden is compulsory’. However, Trigg [45] and Weinberg [46] have pointed out that the author who deserves the credit for the totalitarian principle is T. H. White because, as Trigg remarks, ‘[i]n The Sword in the Stone, part 1 of The Once and Future King, Wart, the character who will later be King Arthur, is being educated by Merlin by being transformed into various animals. One of his experiences is as an ant, and he finds that the ant hill is run on the totalitarian principle’ [45]. Specifically, in ch. XIII of The sword in the stone [47], ‘EVERYTHING NOT FORBIDDEN IS COMPULSORY’ is the slogan carved over the entrance to each tunnel in the ant fortress.

In our version of the totalitarian principle, ‘anything’ refers to ‘any behaviour for a Bell or KS scenario’ and ‘forbidden’ means ‘forbidden by assumptions 3.1 and 3.2’.

4. Proof

A behaviour for scenario \( S \) satisfies the exclusivity principle (EP) [11,23,24,29,40,48–51] if the sum of the probabilities of the events of any set in which every two events are mutually exclusive in \( S \) is bounded by 1.
The proof of Theorem 3.4 begins with the following observations.

**Lemma 4.1.** The behaviours for any KS scenario must satisfy the EP.

*Proof.* In KS scenarios all measurements are ideal. It can be proven [10,11] that the EP holds for ideal measurements. Therefore, every behaviour for any KS scenario must satisfy the EP. ■

**Lemma 4.2.** The behaviours for any bipartite Bell scenario must satisfy the EP.

*Proof.* By definition of Bell scenario, behaviours must satisfy normalization and non-signalling (i.e. non-disturbance). It can be proven [10,23] that, for bipartite Bell scenarios, the set of behaviours satisfying the EP (applied to a single copy) is equal to the set of behaviours that satisfy normalization and the non-signalling principle. ■

Assumption 3.2 assures that there is a statistically independent joint realization of any two KS experiments A and B (including Bell experiments). This allows us to define experiments of the type (A, B) described before.

If A and B are KS experiments, then (A, B) can be seen as a single KS experiment. Therefore, lemma 4.1 assures that the behaviours for (A, B) must satisfy the EP.

If A and B are bipartite Bell experiments, then (A, B) can be seen as a bipartite Bell experiment. Therefore, lemma 4.2 assures that the behaviours for (A, B) must satisfy the EP.

If A is a KS experiment and B a bipartite Bell experiment, then (A, B) can be seen as a bipartite Bell experiment. Therefore, lemma 4.2 assures that the behaviours for (A, B) must satisfy the EP.

Similar arguments apply to n statistically independent experiments. In particular, the same behaviour \( p(S_A) \) for a Bell or KS experiment can be composed with itself as many times as we want. If \( p(S_A) \) occurs in n statistically independent experiments \( A_i \), then, by lemmas 4.1 and 4.2, the corresponding behaviour for the corresponding experiment \( (A_1, \ldots, A_n) \), that is, \( p(S_{A_1, \ldots, A_n}) = p(S_A)^\otimes n \), where \( p(S_A)^\otimes n \) denotes the tensor product of n copies of \( p(S_A) \), must satisfy the EP for any n.

Different sets of events may share the same graph of exclusivity G. This leads to the following definition:

**Definition 4.3.** The set \( \mathcal{P}(G) \) of assignments of probabilities to the vertices of graph G is the set of vectors \( p(G) \in [0, 1]^{V(G)} \) such that the components of \( p(G) \) are the probabilities of \( |V(G)| \) events with graph of exclusivity G in a behaviour for some Bell or KS scenario.

That is, \( \mathcal{P}(G) \) contains the vectors of probabilities with \( |V(G)| \) components corresponding to events that have G as graph of exclusivity produced in all Bell or KS scenarios.

**Lemma 4.4.** For any self-complementary graph of exclusivity G, the theta body of G, \( \text{TH}(G) \), is the largest set of assignments of probabilities \( \mathcal{P}(G) \) such that every \( p(G) \in \mathcal{P}(G) \) satisfies the EP applied to any number of independent copies of \( p(G) \) and such that \( p(G) \otimes q(G) \) satisfies the EP for every \( p(G), q(G) \in \mathcal{P}(G) \).

Given a graph G, \( \overline{G} \) denotes the complement of G, i.e. the graph with the same vertices as G and such that two distinct vertices of \( \overline{G} \) are adjacent if and only if they are not adjacent in G. A graph G is self-complementary if G and \( \overline{G} \) are isomorphic. The theta body of G, denoted \( \text{TH}(G) \), is a well-studied convex set in graph theory (e.g. [52,53]). It was introduced in [54] and, among the many ways to express it, the following one, using Dirac’s notation, is particularly useful for our purposes:

\[
\text{TH}(G) = \{ p(G) \in [0, 1]^{V(G)} : p_{ij} = |\langle x^{(i)}_{ai} | \psi \rangle |^2, |\langle x^{(i)}_{ai} | \psi \rangle | = 1, |\langle x^{(i)}_{ai} | x^{(j)}_{aj} | \psi \rangle | = 1, \langle x^{(i)}_{ai} | x^{(j)}_{aj} | \psi \rangle = 0, \forall (i, j) \in E(G) \},
\]

where \( E(G) \) is the set of edges of G.
Proof of Lemma 4.4. There are two necessary conditions that any candidate for \( \mathcal{P}(G) \) satisfying assumptions 3.1 and 3.2 must satisfy:

Condition 1: Any \( p(G) \in \mathcal{P}(G) \) must satisfy the EP applied to any number \( n \) of independent copies of \( p(G) \). Therefore, for any \( n \),

\[
\mathcal{P}(G) \subseteq \mathcal{E}^n(G),
\]

(4.2)

where

\[
\mathcal{E}^n(G) \equiv \{ p(G) \in [0, 1]^{V(G)} : p(G)^{\otimes n} \in \text{QSTAB}(G^{\otimes n}) \},
\]

(4.3)

where \( p(G)^{\otimes n} = p(G) \otimes \cdots \otimes p(G) \) \( (n \) times), \( G^{\otimes n} \) is the OR product of \( n \) copies of \( G \), and

\[
\text{QSTAB}(G) = \left\{ p(G) \in [0, 1]^{V(G)} : \sum_{c \subseteq C(G)} p_i \leq 1 \ \forall c \in C(G) \right\},
\]

(4.4)

where \( C(G) \) is the set of cliques of \( G \). The OR product (also called disjunctive or co-normal product) of \( G \) and \( G' \), denoted \( G \ast G' \), is the graph with \( V(G \ast G') = V(G) \times V(G') \) and \( ((i,i'),(j,j')) \in E(G \ast G') \) if and only if \( (i,j) \in E(G) \) or \( (i',j') \in E(G') \). QSTAB\((G)\) is a famous convex set in graph theory called the clique-constrained stable set polytope [52] (or fractional stable set polytope [52] or fractional vertex packing polytope [54]) of \( G \).

Condition 2: Any \( p(G), q(G) \in \mathcal{P}(G) \) must satisfy the EP applied to one copy of \( p(G) \) and one independent copy of \( q(G) \). This implies that

\[
\mathcal{P}(G) \subseteq \text{abl}[\mathcal{P}(G)],
\]

(4.5)

where \( \text{abl}[\mathcal{P}(G)] \) is the antiblocker of \( \mathcal{P}(G) \), defined as

\[
\text{abl}[\mathcal{P}(G)] = \{ q(G) \geq 0 : p(G) \cdot q(G) \leq 1 \ \forall p(G) \in \mathcal{P}(G) \},
\]

(4.6)

where \( \cdot \) is the dot product [52–54].

If \( G \) is self-complementary, then, for any \( n \),

\[
\text{abl}[\mathcal{E}^{n-1}(G)] \subseteq \text{abl}[\mathcal{E}^{n}(G)] \subseteq \mathcal{E}^{n}(G).
\]

(4.7)

Therefore, (4.2) implies that

\[
\mathcal{P}(G) \subseteq \lim_{n \to \infty} \mathcal{E}^{n}(G).
\]

(4.8)

and (4.5) implies that

\[
\mathcal{P}(G) \subseteq \lim_{n \to \infty} \text{abl}[\mathcal{E}^{n}(G)].
\]

(4.9)

If \( G \) is self-complementary, as \( n \) tends to infinity, \( \mathcal{E}^{n}(G) \) and \( \text{abl}[\mathcal{E}^{n}(G)] \) tend to \( \text{TH}(G) \) from above and below, respectively, and \( \text{TH}(G) \) is the largest set satisfying (4.8) and (4.9) (the other sets satisfying these conditions are subsets of \( \text{TH}(G) \)). Therefore, if \( G \) is self-complementary, the largest \( \mathcal{P}(G) \) is \( \text{TH}(G) \). In this case, \( \mathcal{P}(G) = \text{abl}[\mathcal{P}(G)] \) [52–54].

Lemma 4.4 states that for any self-complementary graph of exclusivity \( G \), the largest set of assignments of probabilities satisfying Conditions 1 and 2 is the one that contains all those assignments of probabilities that satisfy that

(I') The state of the system can be associated with a vector with unit norm \(|\psi\rangle\) in a vector space \( \mathcal{V} \) with an inner product.

(II') The state after performing, on state \( \psi \), a measurement \( x^{(i)} \) and obtaining outcome \( a_i \) can be associated with a vector with unit norm \(|x^{(i)}_{a_i}\psi\rangle\) in \( \mathcal{V} \). Post-measurement states corresponding to mutually exclusive events are associated with mutually orthogonal vectors.

(III') The probability of the event \( (x^{(i)}_{a_i}|\psi\rangle \) can be obtained as \(|\langle x^{(i)}_{a_i}\psi|\psi\rangle|^2\).

Interestingly, in quantum theory, for any \( G \), \( \mathcal{P}(G) = \text{TH}(G) \) [24]. Therefore, at least for self-complementary graphs of exclusivity, assumptions 3.1 and 3.2 select the quantum set.
Lemma 4.5. For any graph of exclusivity G, TH(G) is the largest set \( \mathcal{P}(G) \) of assignments of probabilities such that every \( p(G) \in \mathcal{P}(G) \) satisfies the EP applied to any number of independent copies of \( p(G) \) and such that \( p(G) \otimes q(G) \) satisfies the EP for every \( p(G), q(G) \in \mathcal{P}(G) \).

**Proof.** For any G, there is an operation that maps G into a self-complementary graph H(G) such that the largest \( \mathcal{P}[H(G)] \) allowed by assumptions 3.1 and 3.2 determines the largest \( \mathcal{P}(G) \) allowed by these assumptions. This map can be visualized as follows. Consider an experiment \( E \) producing \( n \) events \( \{e_{k}\}_{k=1}^{n} \) whose graph of exclusivity is G. Then, consider three additional mutually independent experiments: experiment \( X \), producing events \( \{x_{k}\}_{k=1}^{n} \) whose graph of exclusivity is \( G \), experiment \( Y \), producing events \( \{y_{k}\}_{k=1}^{n} \) whose graph of exclusivity is \( G \), and experiment \( Z \) producing events \( \{z_{k}\}_{k=1}^{n} \) whose graph of exclusivity is G. Now suppose an observer witnessing \( E, X, Y \) and \( Z \). Suppose that this observer has three independent coins \( A, B \) and \( C \), each of them producing two mutually exclusive events: \( A \) producing events \( a_{0} \) or \( a_{1} \), \( B \) producing \( b_{0} \) or \( b_{1} \), and \( C \) producing \( c_{0} \) or \( c_{1} \). Suppose that, using the four independent experiments and the three coins, the observer defines the following \( 4n \) events: \( \{(a_{0},e_{k}),(a_{1},b_{0},x_{k}),(b_{1},c_{0},y_{k}),(c_{1},z_{k})\}_{k=1}^{n} \), where, e.g., \( (a_{0},e_{1}) \) is the event in which coin \( A \) gives \( a_{0} \) and experiment \( E \) gives \( e_{1} \). H(G) is the graph of exclusivity of these \( 4n \) events. Figure 2 shows H(G) when G is an heptagon.

There are two properties of H(G) that are important for us. The first one is that any assignment of probabilities \( h[H(G)] \in \mathcal{P}[H(G)] \) can be implemented by suitably choosing assignments \( p(G) \in \mathcal{P}(G), x(G) \in \mathcal{P}(G), y(G) \in \mathcal{P}(G) \) and \( z(G) \in \mathcal{P}(G) \) for, respectively, \( \{e_{k}\}_{k=1}^{n}, \{x_{k}\}_{k=1}^{n}, \{y_{k}\}_{k=1}^{n} \) and \( \{z_{k}\}_{k=1}^{n} \), and assignments of probabilities \( a(K_{2}) \in \mathcal{P}(K_{2}), b(K_{2}) \in \mathcal{P}(K_{2}) \) and \( c(K_{2}) \in \mathcal{P}(K_{2}) \) for, respectively, \( \{a_{0},a_{1}\}, \{b_{0},b_{1}\} \) and \( \{c_{0},c_{1}\} \) (\( K_{2} \) is the complete graph on two vertices; the graph of exclusivity of the events of tossing a coin) [10]. Therefore, the largest \( \mathcal{P}(G) \) allowed by assumptions 3.1 and 3.2 can always be obtained from the largest \( \mathcal{P}[H(G)] \) allowed by these assumptions by suitably tracing out its elements.

The second property is that H(G) is self-complementary. Therefore, by lemma 4.4, the largest \( \mathcal{P}[H(G)] \) allowed by assumptions 3.1 and 3.2 is TH[H(G)]. Using these two properties, we conclude that the largest \( \mathcal{P}(G) \) allowed by assumptions 3.1 and 3.2 is TH(G).

A consequence of lemma 4.5 is that the set of behaviours for any given Bell or KS scenario S is a subset of TH(G), where \( G \) is the graph of exclusivity of all possible events of S. However,
TH(GS) may contain behaviours that are forbidden in S. To remove them, we need to take into account constraints (A), (B) and (C) for S (see §2).

The way constraints (A) and (B) for S remove elements of TH(GS) is easy to understand. The way constraint (C) for S excludes behaviours of TH(GS) is more subtle. To illustrate it, we will focus on the case that S is the CHSH Bell scenario. It is possible to produce any assignment of probabilities in TH(GS) if we have a suitable vector with unit norm $|\psi\rangle$ in a vector space $V$ (by Condition (I')) and 16 suitable vectors of unit norm (or rank-one projectors) and their orthogonal complements in $V$ (since measurements have only two outcomes) (by Condition (II')), so behaviours satisfy Condition (III'). However, in the CHSH Bell scenario we have only four two-outcome measurements. Therefore, we have only four pairs projector-orthogonal complement, each of them represented in figure 1 by one edge with a full half circumference in one extreme and an empty half circumference in the other extreme, all of the same colour. According to constraint (C), these four pieces must be combined exactly as shown in figure 1 to produce the events and explain their relations of mutual exclusivity.

It is not difficult to see that, for any given S, constraints (A), (B) and (C) applied after conditions (I'), (II') and (III') are equivalent to conditions (I), (II) and (III) (see §2h). See [10] for details. This finishes the proof of theorem 3.4.

5. Conclusion

We started by assuming that there is a non-empty set of behaviours for any KS scenario and a statistically joint realization of any two KS experiments. Then we showed that, for any specific Bell or KS scenario, the largest set of behaviours allowed by these assumptions is the set allowed by quantum theory.

This suggests a simple principle for quantum correlations: every behaviour that is not forbidden by these assumptions is feasible. That is, there is a preparation and a set of measurements that produces it. This result fits with Wheeler’s thesis that the universe lacks of laws for the outcomes of some experiments and with Born’s intuition that quantum theory is a consequence of the non-existence of ‘conditions for a causal evolution’ [55]. One can still assume that some laws and conditions for a causal evolution exist. However, then our result shows that they have no effect on the correlations allowed for Bell and KS scenarios.

6. Implications

In this final part, we explore some of the implications of theorem 3.4 (and of the lemmas used for its proof) and address some frequently asked questions.

(a) Specker’s triangle parable and Wright’s pentagon

In [7], within the framework of a parable involving an over-protective Assyrian prophet, Specker introduced the following behaviour for a scenario in which there are three measurements {1, 2, 3} whose graph of compatibility is a triangle (denoted as $C_3$) and whose possible outcomes are 0 and 1. If we denote as $P(a_ia_j|x_ix_j)$ the probability of obtaining outcomes $a_i$ and $a_j$ when measuring $x_i$ and $x_j$, respectively, a behaviour in this scenario can be represented by a matrix

$$p(S_{C_3}) = \begin{bmatrix} P(00|12) & P(01|12) & P(10|12) & P(11|12) \\ P(00|23) & P(01|23) & P(10|23) & P(11|23) \\ P(00|31) & P(01|31) & P(10|31) & P(11|31) \end{bmatrix}. \quad (6.1)$$

Specifically, Specker’s behaviour is

$$p_S(S_{C_3}) = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}. \quad (6.2)$$
It is easy to see that $p_S(S_3)$ violates the EP when we consider two independent copies of $p_S(S_3)$. Therefore, under assumptions 3.1 and 3.2, the proof of lemma 4.1 shows that $p_S(S_3)$ cannot be produced with ideal measurements. However, $p_S(S_3)$ can be trivially produced if we remove the assumption that the measurements are ideal [56,57].

The same argument and conclusion apply to a behaviour proposed by Wright in [58] for a scenario in which there are five measurements whose graph of compatibility is a pentagon (denoted as $C_5$). Using a similar notation to the one adopted in the previous example, a behaviour for this scenario can be represented by a matrix

$$p(S_3) = \begin{bmatrix}
P(00|12) & P(01|12) & P(10|12) & P(11|12) \\
P(00|23) & P(01|23) & P(10|23) & P(11|23) \\
P(00|34) & P(01|34) & P(10|34) & P(11|34) \\
P(00|45) & P(01|45) & P(10|45) & P(11|45) \\
P(00|51) & P(01|51) & P(10|51) & P(11|51)
\end{bmatrix}. \quad (6.3)$$

Specifically, Wright’s behaviour is

$$p_W(S_3) = \begin{bmatrix}
0 & 1 & 1 & 0 \\
0 & 1 & 1 & 0 \\
0 & 1 & 1 & 0 \\
0 & 1 & 1 & 0
\end{bmatrix}. \quad (6.4)$$

(b) Popescu–Rohrlich boxes

In [36], Popescu & Rohrlich (and previously other authors [59,60]) proposed a non-quantum behaviour for the CHSH Bell scenario that maximizes the violation of the CHSH Bell inequality without violating the condition of non-signalling. This behaviour, known as a pair of Popescu–Rohrlich boxes, can be expressed, using the convention introduced in equation (2.4), as follows:

$$p_{PR}(S_{CHSH}) = \begin{bmatrix}
\frac{1}{2} & 0 & 0 & \frac{1}{2} \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} \\
0 & \frac{1}{2} & \frac{1}{2} & 0
\end{bmatrix}. \quad (6.5)$$

$p_{PR}(S_{CHSH})$ violates the EP when we consider two independent copies of $p_{PR}$ [40,41]. Therefore, under assumptions 3.1 and 3.2, lemma 4.1 shows that a pair of statistically independent Popescu–Rohrlich boxes cannot be constructed with ideal measurements.

Moreover, a pair of statistically independent Popescu–Rohrlich boxes can be seen as a single bipartite Bell experiment. Therefore, according to lemma 4.2, the behaviour of this bipartite Bell experiment must satisfy the EP. But it does not.

(c) Almost quantum correlations

In [42], Navascués et al. presented, for every Bell scenario, a set of behaviours, called almost quantum behaviours, that satisfy all principles proposed to that date but contains non-quantum behaviours. For example, the following is a non-quantum almost quantum behaviour for the CHSH Bell scenario, using the convention introduced in equation (2.4):

$$p_{AQ}(S_{CHSH}) = \begin{bmatrix}
\frac{2993}{5500} & \frac{8}{1375} & \frac{137}{500} & \frac{22}{125} \\
107 & 139 & 139 & 37 \\
700 & 350 & 350 & 700 \\
\frac{7}{11} + \frac{\sqrt{2}}{9} & \frac{\sqrt{2}}{9} - \frac{\sqrt{2}}{9} & \frac{2}{11} - \frac{\sqrt{2}}{9} & \frac{\sqrt{2}}{9}
\end{bmatrix}. \quad (6.6)$$
For a given Bell scenario \( S \), the set of almost quantum correlations is a subset of \( \text{TH}(G_S) \) that satisfies the normalization and non-disturbance constraints for \( S \) (constraints (A) and (B) in §2) [42]. However, our result implies that every non-quantum behaviour in the set of almost quantum correlations for \( S \) fails to satisfy constraint (C) for \( S \). For the case of \( \mathbf{p}_{\text{AQ}}( \text{CHSH} ) \) in (6.6), this failure can be checked with a computer: \( \mathbf{p}_{\text{AQ}}( \text{CHSH} ) \) cannot be attained if we demand that 
\[
P(ab|xy) = |\langle \psi'|\psi \rangle|^2, \quad \text{with} \quad |\psi'\rangle = N_{ab|xy} E_a^{(x)} E_b^{(y)} |\psi\rangle,
\]
where \( N_{ab|xy} \) is a normalization constant, and \( E_a^{(x)} \) and \( E_b^{(y)} \) are projection operators corresponding to, respectively, measurement \( x \) with outcome \( a \) and measurement \( y \) with outcome \( b \), and such that for all \( x, E_a^{(x)} E_a^{(x')} = \delta_{a,a'} E_a^{(x)} \) and \( \sum_{a \in A} E_a^{(x)} = I \), for all \( y, E_b^{(y)} E_b^{(y')} = \delta_{b,b'} E_b^{(y)} \) and \( \sum_{b \in B} E_b^{(y)} = I \) and for all \( x, y, [E_a^{(x)}, E_b^{(y)}] = 0 \).

(d) Real versus complex quantum theory

Theorem 3.4 explains the origin of some of the most mysterious rules of quantum theory. However, it does not provide a full reconstruction of quantum theory. A natural question then is what else is needed to recover the whole formalism.

A first specific target follows from the observation that quantum correlations for Bell and KS scenarios admit representations both in real and complex vector spaces [61–64], while the full quantum theory is formulated in complex vector spaces. Why is it so?

In previous operational reconstructions of quantum theory, the complex-vector-space representation is enforced by imposing the axiom of ‘local tomography’ (the state of a composite system is determined by the joint probabilities it assigns to measurement outcomes on the component subsystems) [65–68]. Instead of this axiom, a purely physical reason enforcing the complex-vector-space representation could be the requirement that the laws of nature stay the same for all observers that are moving with respect to one another within an inertial frame. This suggests that the theory must be Lorentz-invariant at an ontological level. But this requires the theory to be free of instantaneous influences and holistic spaces inaccessible to the experimenters. In contrast to that, real-vector-space representations of quantum correlations seem to require [64] a holistic inaccessible ontological space. This observation suggests a way to attack the problem of why the complex-vector-space representation is worth further examination.

(e) Quantum logic and the exclusivity principle

As pointed out by Henson in [51], the EP is related to the notion of orthocoherence that appeared in quantum logic. ‘[A]n orthoalgebra is orthocoherent if and only if finite pairwise summable subsets are jointly summable’ [69]. The origin of orthocoherence can be traced back to Mackey’s axiom V in [70]. Interestingly, in the literature of quantum logic, since the end of the 1970s, orthocoherence is presented as ‘suspicious … as a fundamental principle’ [71]. Three related reasons are offered for that:

(a) ‘There has never been given any entirely compelling reason for regarding orthocoherence as an essential feature of all reasonable physical models’ [69].
(b) ‘[I]t is quite easy to manufacture simple and plausible toy examples that are not orthocoherent’ [71] (e.g. [7,58]).
(c) ‘[Orthocoherence] is not stable under formation of the tensor product’ [71] (see [72,73]).

By contrast, in this paper, we have seen that

(a’) A compelling reason why the EP is an essential feature of any reasonable physical theory is that the EP holds for events produced by ideal measurements. Ideal measurements must exist in any theory that contains classical physics as a particular case. There are also other reasons. For example, in [68], it is shown that two postulates are sufficient to guarantee the EP. The first postulate says that every state can be represented as
a probabilistic mixture of perfectly distinguishable pure states. The second postulate is that every set of perfectly distinguishable pure states of a given dimension can be reversibly transformed to any other such set of the same dimension. In [51], it is shown that irreducible third-order interference (a generalization of the idea that no probabilistic interference remains unaccounted for once we have taken into account interference between pairs of slits in an $n$-slit experiment) also implies the EP. Finally, in [74], it is shown that every Bayesian framework must include a set of ideal experiments that must satisfy the EP.

(b') As we have seen before, the toy examples in [7,58] (i.e. Specker’s triangle and Wright’s pentagon) are impossible or trivial, depending on whether or not we make the assumption that measurements are ideal.

(c') Observation (c) is not an obstacle but an opportunity. The fact that a behaviour $p(S)$ fails to satisfy the EP applied to $n$ copies indicates that $p(S)$ is forbidden under assumptions 3.1 and 3.2.

(f) Bohmian mechanics, many-worlds and QBism

It is interesting to compare the explanation of the origin of the Born rule suggested in this paper with other explanations given by some interpretations of quantum theory.

In the Bohmian interpretation [75–77], measurement outcomes are determined by a field (called the quantum potential) that permeates the universe. Each particle is at a certain position, and this position is governed by the quantum potential. However, the quantum potential is hidden to the experimenters, so experimenters are restricted to calculating the probability density to observe that the particle is at some position. The reason why outcomes happen with relative frequencies given by the Born rule is the initial state of the quantum potential and the initial positions of all particles [77].

In the Everettian interpretation of quantum theory [78], a measurement is a unitary transformation of a universal wave function that gives rise to a multiverse. Everettians and proponents of the decoherent (or consistent) histories interpretation of quantum theory [79] have made several attempts to justify the Born rule from simpler assumptions (e.g. [80–88]). However, each of these attempts in turn has attracted critical attention (e.g. [89–93]).

The problem is that any derivation of the Born rule that assumes that measurements can be represented by self-adjoint operators in a vector space $V$, outcomes correspond to their eigenvalues, and mutually exclusive results correspond to orthonormal basis is almost circular. Because then, for every $V$ of dimension $d$ greater than two, Gleason’s theorem [94] shows that the only possible states are vectors in $V$ and the only possible choice to assign a probability $P(v_i)$ to every vector $v_i$ in $V$ for any given vector $v$ in $V$ such that, for every orthonormal basis $\{v_i\}_{i=1}^d$ of $V$, the sum of the probabilities satisfies $\sum_{i=1}^d P(v_i) = 1$ and $P(v_i)$ only depends on $v_i$ (not on the orthonormal basis of $V$ considered) is $P(v_i) = |\langle v_i | v \rangle|^2$.

QBism [95] is a different type of interpretation. It does not assume any particular picture of the universe. For QBism, quantum theory is a personal tool for each agent. According to QBism, the Born rule is not a law of nature in the usual sense, but ‘an empirical addition to the laws of Bayesian probability’ [95] that a wise agent should follow in addition to the Bayesian coherence conditions. However, QBism does not clarify where does this empirical addition come from. In this respect, Theorem 3.4 could be an important contribution to QBism as it shows that the set of quantum behaviours does not require any empirical addition to the laws of Bayesian probability but follows from two natural assumptions that fit perfectly within a Bayesian framework.

(g) Emergence of classicality

Existing explanations of the emergence of classicality from quantum theory such as decoherence [96] and the restriction to coarse-grained measurements [97] assume the formalism of quantum theory. An interesting problem is understanding the emergence of classicality within the
framework proposed in this paper. An interesting observation in this sense is that, for any self-complementary graph of exclusivity $G$, the EP applied to a single copy selects a set, $E^1(G)$ (see §4) whose elements do not violate the EP with other elements if and only if these other elements belong to $\text{abl}(E^1(G))$, which is exactly the set of classical assignments of probability for $G$ [24]. This points out that the set of classical assignments of probability for $G$ is particularly robust under the EP and suggests that the problem of the emergence of classicality may be benefit from the approach to quantum theory proposed in this paper.

Data accessibility. This article has no additional data.

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