




Inequalities witnessing coherence, nonlocality, and contextualityRafael Wagner ^{1,2,*} Rui Soares Barbosa ^{1,†} and Ernesto F. Galvão ^{1,3,‡}¹*INL – International Iberian Nanotechnology Laboratory, 4715-330 Braga, Portugal*²*Centro de Física, Universidade do Minho, 4710-057 Braga, Portugal*³*Instituto de Física, Universidade Federal Fluminense, Niterói – Rio de Janeiro, 24210-340, Brazil*

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Quantum coherence, nonlocality, and contextuality are key resources for quantum advantage in metrology, communication, and computation. We introduce a graph-based approach to derive classicality inequalities that bound local, noncontextual, and coherence-free models, offering a unified description of these seemingly disparate quantum resources. Our approach generalizes recently proposed basis-independent coherence witnesses, and it recovers all noncontextuality inequalities of the exclusivity graph approach. Moreover, violations of certain classicality inequalities witness preparation contextuality. We describe an algorithm to find all such classicality inequalities, and we use it to analyze some of the simplest scenarios.

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Nonclassical resources provided by quantum theory are key to quantum advantage for information processing [1–8]; see [9–11] for comprehensive reviews of applications. Many different nonclassical features of quantum mechanics have been identified, studied, witnessed, and quantified [4,12–27]. It is natural to wonder to what extent different quantum resources can be characterized in a unified way. Here we address this question by proposing a single formalism that yields inequalities bounding three different notions of classicality: noncontextual, local, and coherence-free models.

A number of modern approaches to contextuality have successfully incorporated nonlocality as a special case [28–31]. The relationship between this unified notion of nonclassical correlations and coherence, however, has been harder to establish. One roadblock is that most approaches to characterize coherence presuppose the choice of a fixed reference basis [11]. Recently, different approaches have been proposed to study a basis-independent notion of coherence [26,32], dubbed *set coherence* in Ref. [26]. A recent approach, upon which the present work builds, derives witnesses of basis-independent coherence using only relational information between states in the form of two-state overlaps [32]. Still, so far there has been no clear identification between nonlocality and contextuality on the one hand, and coherence on the other. There are examples of models that mimic quantum coherence *without* displaying contextuality or nonlocality, such as the toy models from Refs. [33,34], while on the other hand incoherent states—even maximally mixed states—can of course be used to witness state-independent quantum contextuality [35,36]. Theory-independent approaches have been used to compare relevant types of nonclassical resources [23,27,37], but an understanding of the special case of coherence and

contextuality is still lacking. A better understanding of the relationship between these two fundamental manifestations of nonclassicality has both important foundational impact and potential technological applications.

Building on the study of coherence using two-state overlaps [32], we propose a framework that associates with any (simple) graph G a probability polytope C_G of edge weightings. Vertices of the graph G represent probabilistic processes, while edges of G correspond to correlations between neighboring processes. We show that the faces of the polytope C_G describe bounds on noncontextual, local, and coherence-free models, depending on the interpretation of vertices of the graph G as preparations and measurements. The description of three notions of classicality under a single framework represents a significant conceptual advance towards clarifying the source of quantum computational advantage.

II. FRAMEWORK**A. The classical polytope C_G**

Let $G = (V(G), E(G))$ be an undirected graph, which we call the *event graph*. We consider edge weightings $r : E(G) \rightarrow [0, 1]$, which assign a weight $r_e = r_{ij}$ to each edge $e = \{i, j\}$ of G . We regard these weightings as points forming a polytope, the unit hypercube, $r \in [0, 1]^{E(G)}$.

To define the *classical polytope* $C_G \subseteq [0, 1]^{E(G)}$, take each vertex $i \in V(G)$ to represent a random variable A_i with values belonging to an alphabet Λ , and suppose these are jointly distributed. This determines an edge weighting r where each weight r_{ij} is the probability that the processes corresponding to vertices i and j output equal values, i.e.,

$$r_{ij} = P(A_i = A_j).$$

An edge weighting r is in the classical polytope C_G if it arises in this fashion from jointly distributed random variables $(A_i)_{i \in V(G)}$. Each weight r_{ij} is then a measure of the correlation between the output values of A_i and of A_j . In the case of dichotomic values $\Lambda = \{+1, -1\}$, this quantity is related to

*rafael.wagner@inl.int

†rui.soaresbarbosa@inl.int

‡ernesto.galvao@inl.int

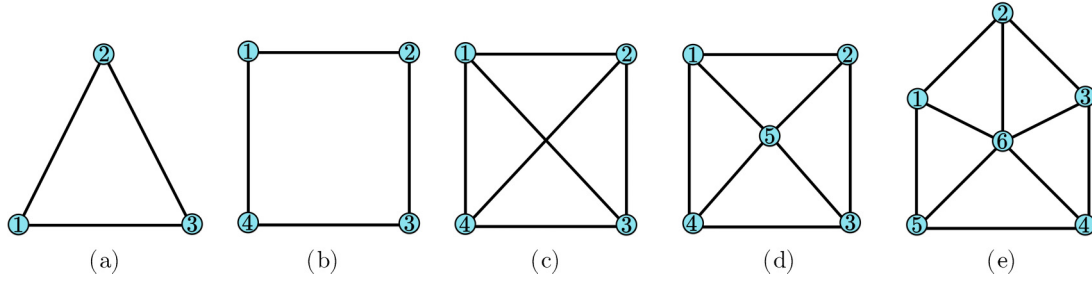


FIG. 1. Event graphs corresponding to bounds on classical models. Each of these graphs can be used to obtain the following nonclassicality inequalities: (a) constrained CHSH inequality; (b),(d) CHSH Bell locality inequality; (c) new K_4 classically inequality from Eq. (2), and (e) Klyachko, Can, Binicioğlu, and Schumovsky (KCBS) noncontextuality inequality.

the expected value of the product by $\langle A_i A_j \rangle = 2r_{ij} - 1$ [38]. An (alternative) formal description of C_G is given in detail in Appendix A.

B. Inequalities defining C_G

The inequalities defining the polytope C_G impose logical conditions determining the set of classical edge weightings. The existence of nontrivial facets of C_G can be illustrated with the example of Fig. 1(a), the three-vertex complete graph K_3 , with edge weights r_{12}, r_{23}, r_{13} . We cannot have, e.g.,

$$r_{12} = 1, \quad r_{23} = 1, \quad r_{13} = 0,$$

as this would contradict transitivity of equality on the deterministic values corresponding to each of the three vertices: $A_1 = A_2 = A_3 \neq A_1$. In Ref. [32] it was shown that the only nontrivial inequalities for the n -cycle event graph C_n are

$$-r_e + \sum_{e' \neq e} r_{e'} \leq n - 2, \quad \text{for each } e \in E(C_n). \quad (1)$$

Incidentally, these inequalities have been known at least since the work of Boole [39–41].

We now give a high-level description of an algorithm to completely characterize C_G for general event graphs G . We start by enumerating the vertices of C_G . These are all the “deterministic” labelings of the edges of G with values in $\{0, 1\}$ that are logically consistent with transitivity of equality. The facets of C_G can then be found using standard convex geometry tools [42].

Whether a given deterministic edge labeling is consistent—and therefore a vertex of C_G —can be checked in linear time on the size of G by a graph traversal. However, it is unnecessary to generate all $2^{|E(G)|}$ -many labelings and discard the inconsistent ones. Instead, one can directly generate only the consistent ones by searching through underlying value assignments to the vertices of G . Despite being much more efficient for most graphs, this also quickly becomes unavoidably intractable due to the exponentially increasing number of vertices of the polytope C_G . We deepen this discussion in Appendix A.

Using the method just outlined, we find all facets of C_G for some small graphs, including all graphs shown in Fig. 1. Interestingly, already for K_4 , shown in Fig. 1(c), a new type of facet appears that is different from the cycle inequalities in Eq. (1). These new facets of K_4 are described by the inequalities of the form

$$(r_{12} + r_{13} + r_{14}) - (r_{23} + r_{34} + r_{24}) \leq 1 \quad (2)$$

up to label permutations.

In Appendix B, we prove that certain constructions of graphs by combining smaller graphs do not give rise to new facet inequalities, trimming the class of graphs worth analyzing. In Appendix C, we list all facet inequalities of the classical polytopes for the complete graphs K_4, K_5 , and K_6 . We also give numerically found examples of quantum violations—witnessing basis-independent coherence in the sense described in the next section—of all nontrivial facets of K_4 and K_5 . All the new inequalities and quantum violations found, together with the code used to obtain them, which is applicable to analyze C_G for an arbitrary graph G , are made available in an associated Git repository [43]. In Appendix D, we generalize the inequalities of Eq. (2) to complete graphs of $n \geq 4$ vertices, and we prove that these define facets of the classical polytopes C_{K_n} for all such n . This yields an infinite family h_n of new classicality inequalities not previously described in the literature. The first three new inequalities from this family (h_4, h_5, h_6) have recently been experimentally violated, serving to benchmark quantum photonic devices [44].

We now proceed to describe how the inequalities obtained for the abstract scenarios considered above establish bounds both on coherence-free models and on noncontextual/local models. Each type of operational scenario suggests an interpretation for edge weights, and naturally imposes further constraints on them, resulting in cross-sections of the polytope C_G . These cross-sections recover known noncontextuality/locality polytopes, as well as basis-independent coherence witnesses.

III. C_G BOUNDS COHERENCE-FREE MODELS

Most commonly, coherence is defined for a quantum state with respect to a fixed basis, as the presence of nonzero off-diagonal elements in its density matrix (in that basis) [45,46]. Recently, Refs. [26,32] proposed a *basis-independent* notion of coherence as a property of a *set of states*: this is said to be *coherent* when the states in the set are not simultaneously diagonalizable, i.e., when there is no basis in which all their density matrices are diagonal, or equivalently, if the states in the set do not pairwise commute. Otherwise, the set is said to be *coherence-free*, or *incoherent*.

In Ref. [32], basis-independent coherence witnesses were described using only pairwise overlaps $r_{ij} = \text{Tr}(\rho_i \rho_j)$ among a set of quantum states, focusing on witnesses provided by violations of the cycle inequalities in Eq. (1). We explain the interpretation of the facet inequalities of C_G as basis-

independent coherence witnesses, generalizing the results of Ref. [32] to *any* event graph G .

Let G be any graph with n vertices. Consider a general separable state of n quantum systems of the same type (e.g. qudits), each associated with a vertex of the graph. Each edge of G is given a weight equal to the overlap between the two states of its incident vertices. These overlaps can be estimated using the well-known SWAP test [47]. In Ref. [32] it was shown that the facet-inequalities of C_G describe necessary conditions on the set of overlaps, i.e., on edge weightings of G , for the set of single-system states to be coherence-free, that is, all of them diagonal in a common single-system basis. This is so because for such a coherence-free set of states, the overlap r_{ij} equals the probability of obtaining equal outcomes in independent measurements of the states associated with vertices i and j using the observable that projects onto the reference basis.

IV. C_G BOUNDS LOCAL AND NONCONTEXTUAL MODELS

The faces of C_G can also be understood as bounds on non-contextual models [48,49]. A simple first approach consists in having vertices of G represent measurements, while edges identify two-measurement contexts, i.e., pairs of observables that can be measured simultaneously. The weight of an edge corresponds to the probability, with respect to a given global state, that the two incident measurements yield equal outcomes. A necessary and sufficient condition for the existence of a noncontextual model whose behavior is consistent with a given edge weighting is the existence of a global probability distribution (on outcome assignments to all measurements) whose marginals recover the correct outcome probabilities. This is the content of the Fine-Abramsky-Brandenburger theorem [29,50,51].

Such a global distribution, when it exists, can also be interpreted as a classical coherence-free model. This dual role of global probability distributions is the link connecting coherence-free models and noncontextual models, and allowing violations of facet inequalities of C_G to witness either property, depending on the interpretation of the scenario at hand.

In general, this simple approach, interpreting vertices as measurements and edges as equality of outcome in two-measurement contexts, is not sufficient to capture contextuality in full generality (see [31], Section 2.5.3). Even restricting to contextuality scenarios whose maximal contexts have size two, the facets of C_G are not necessarily facet, or even tight, noncontextuality inequalities, except in the case of dichotomic measurements (see [52], Theorem 38), where equality of outcomes fully determines the measurement statistics. An important example is the Clauser-Horne-Shimony-Holt (CHSH) inequality.

Encoding some contextuality scenarios requires the imposition of further constraints, which geometrically determine cross-sections on the classical polytope C_G . These constraints may, for example, represent operational symmetries of the measurement scenario, e.g., making two vertices equal, or they may encode given conditions on the compatibility of observables. One example is the exclusivity constraint present in the Cabello-Severini-Winter (CSW) graph approach [28].

We now show how both CHSH and the original three-setting Bell inequality can be obtained from cycle inequalities, before describing a more systematic approach that recovers all noncontextuality inequalities obtainable from the exclusivity graph approach [28,31].

We remark that we treat Bell nonlocality as an instance of contextuality, in which measurement compatibility is ensured by spacelike separation between various parties who locally measure a shared multipartite system. This view of nonlocality as a special case of contextuality is well established, e.g., in Refs. [29,30], although there are important subtle differences when considering free transformations in a resource-theoretic setup [53].

A. Example: CHSH inequality from the four-cycle graph C_4

It is easy to check from Eq. (1) that the four-cycle graph C_4 , shown in Fig. 1(b), has four nontrivial facets given by the inequality

$$r_{12} + r_{23} + r_{34} - r_{14} \leq 2, \quad (3)$$

and label permutations thereof. We translate this into the CHSH [54] Bell scenario, with Alice locally measuring one of two rank-1 projectors A_1 or A_2 , and Bob locally measuring either B_1 or B_2 , on the singlet state $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. As a contextuality scenario, the CHSH graph C_4 is a graph with no clique with more than two vertices, and the only nontrivial noncontextuality inequality is given in terms of correlations. From the event graph perspective, each vertex can be understood as a two-outcome measurement at either Alice or Bob. It is easy to check that the overlap between two single-qubit projectors A, B is the probability of obtaining different outcomes [55] when measuring those projectors on each part of the singlet state: $r_{AB} = p_{\neq}^{AB} = 1 - p_{=}^{AB}$. Using this interpretation, the facet of C_4 given by Eq. (3) can be rewritten as

$$p_{\neq}^{A_1 B_1} + p_{\neq}^{A_2 B_1} + p_{\neq}^{A_2 B_2} - p_{\neq}^{A_1 B_2} \leq 2, \quad (4)$$

which is a well-known way to write the CHSH inequality [56]. This same procedure can be used to obtain chained Bell inequalities [57,58] from cycle inequalities.

B. Example: Original Bell inequality from the three-cycle graph C_3

If on the C_4 graph we have just analyzed we impose the constraint that one of the edge weights equal 1, then we recover the nontrivial facets for the three-cycle C_3 , namely $r_{12} + r_{23} - r_{13} \leq 1$ and label permutations. The embedded tetrahedron with these three facets delimits the local correlations in the original two-party Bell inequality [49], featuring three settings at each party, and assuming perfect anticorrelation for pairs of aligned settings. For a geometrical description of the ellipse of quantum correlations, see Ref. [59].

C. Example: CHSH inequality from the five-vertex wheel graph W_5

An alternative way of interpreting an event graph as a contextuality scenario involves having a single vertex, the handle, represent a quantum state, and all the others represent measurement operators. Take the five-vertex wheel graph W_5

of Fig. 1(d) as an instructive example. A simple calculation shows that if we impose $r_{12} = r_{34}$ and $r_{23} = r_{14}$, then adding together four three-cycle inequalities for this graph recovers the CHSH inequality in the form of Eq. (4). The quantum realization of this graph scenario has the central vertex 5 representing a singlet state, with the other vertices representing the four projectors measured jointly by Alice and Bob. The imposed constraints reflect the fact that opposing edges represent the same quantity, the overlap between the two projectors locally measured by one of the parties.

V. RECOVERING ALL NONCONTEXTUALITY INEQUALITIES OF THE EXCLUSIVITY GRAPH FORMALISM

The second approach to obtaining the CHSH inequality does not rely on particular properties of the singlet state. The use of a handle vertex to represent a state can be generalized to other scenarios, as we now describe.

In the *exclusivity graph approach* to contextuality, one considers a graph H whose vertices represent measurement events [60] (in a quantum realization, projection operators), and edges connect mutually exclusive events (in the quantum setting, orthogonal projectors). In this formalism, the noncontextual behaviors are described by a well-known construction, the stable polytope of the graph H , denoted $\text{STAB}(H)$ [31]. This is reviewed in detail in Appendix E. In brief, the vertices or extreme points of the polytope $\text{STAB}(H)$ are (the characteristic functions of) subsets of $V(H)$ that do not contain any pair of adjacent vertices. More intuitively, perhaps, they correspond to truth-value assignments to the measurement events, i.e., functions $V(H) \rightarrow \{0, 1\}$, such that no two exclusive events are deemed true, i.e., no two adjacent vertices are assigned the value 1.

We can understand this setup in terms of our formalism as follows. We define an event graph H_\star obtained from the exclusivity graph H by adding a new vertex connected to all other vertices. This new vertex is used to represent a handle state ψ . Formally, H_\star is given by $V(H_\star) := V(H) \sqcup \{\psi\}$ and $E(H_\star) := E(H) \cup \{\{v, \psi\} \mid v \in V(H)\}$. The structure of the exclusivity graph H is then used to force a constraint on edge weightings of H_\star , namely that all edges already present in H be assigned zero weight. The resulting cross-section $C_{H_\star}^0 := \{r \in C_{H_\star} \mid \forall e \in E(H), r_e = 0\}$ of the polytope C_{H_\star} , which moreover is a subpolytope, then carries information about the noncontextual behaviors in $\text{STAB}(H)$. Formally, in Appendix E, we exhibit an isomorphism between the polytopes $\text{STAB}(H)$ and $C_{H_\star}^0$ for any exclusivity graph H . As a consequence, we show that the *facet-defining noncontextuality inequalities bounding noncontextual behaviors for H are precisely the facet-defining inequalities of $C_{H_\star}^0$* . Moreover, these inequalities can be obtained from the inequalities defining facets of the whole classical polytope C_{H_\star} by removing (i.e., setting to zero) the variables r_e with $e \in E(H)$.

A. Example: KCBS noncontextuality inequality

We illustrate this mapping between formalisms with the noncontextuality inequality obtained by Klyachko, Can, Binicioğlu, and Schumovsky (KCBS) [61], and expressed in the CSW formalism in Ref. [28].

Starting with the five-cycle graph $H = C_5$ interpreted as an exclusivity graph, then H_\star is the six-vertex wheel graph W_6 of Fig. 1(e). The central vertex represents a quantum state, while neighboring vertices in the outer five-cycle represent mutually exclusive measurement events (quantum mechanically: orthogonal projectors) so as to impose $r_{vw} = 0$ for neighboring v and w in this outer subgraph. The KCBS noncontextuality inequality is a bound on weightings of the edges connected to the central vertex:

$$\sum_{v=1}^5 r_{v6} \leq 2. \quad (5)$$

Note that each edge weight r_{v6} in Eq. (5) is the probability of successful projection of the central vertex state onto the projector associated with vertex v .

In our framework, this inequality is obtained from a facet-defining inequality of C_{W_6} ,

$$\begin{aligned} & -r_{12} - r_{23} - r_{34} - r_{45} - r_{15} \\ & + r_{16} + r_{26} + r_{36} + r_{46} + r_{56} \leq 2, \end{aligned}$$

by imposing the exclusivity (or orthogonality) condition of null edge weights on the five-cycle outer subgraph.

VI. CYCLE INEQUALITIES WITNESS PREPARATION CONTEXTUALITY

In addition to considering different approaches to Kochen-Specker noncontextuality, one can also consider different *notions* of noncontextuality. One such proposal, put forth by Spekkens in Ref. [62], is that of preparation (generalized) noncontextuality [7,63–66]. We consider once more a quantum realization of the event graph representing vertices as states and edges as two-state overlaps. In Appendix F we prove that *violations of the inequalities for the classical polytope of the cycle event graph C_n are witnesses of preparation contextuality*. This result is shown for a class of prepare-and-measure operational scenarios [63,64], which includes quantum theory viewed as an operational theory. In contrast to quantum theory, the well-known noncontextual toy theory of Ref. [33] does not violate these event graph inequalities if vertices of the event graph are taken to represent toy theory states.

VII. DISCUSSION AND FUTURE DIRECTIONS

We proposed a new graph-theoretic approach that unifies the study of three different quantum resources, namely contextuality, nonlocality, and coherence. Nonclassicality inequalities are obtained as facets of a polytope C_G of edge weightings associated with an *event graph* G , with suitable constraints that depend on the chosen interpretation of vertices as quantum states or measurements, as required by each scenario.

Connections with the theory of contextuality were presented with respect to different approaches and definitions. In particular, we recovered all inequalities of the CSW exclusivity graph approach [28], and we explicitly derived CHSH and KCBS inequalities as examples. We also showed that for cycle graphs the classical polytope bounds Spekkens preparation noncontextuality.

It would be interesting to understand whether these results can be made more robust. In particular, we observed that the noncontextuality inequalities for an exclusivity graph H are obtained from the inequalities of a classical polytope C_H , by assigning weight zero to some edges. But many of these inequalities of C_H , allow for deviations from such null weights without leaving the classical polytope C_H . This suggests that perhaps those inequalities could still be interpreted as a robust form of noncontextuality inequalities, where exclusivity is relaxed.

Future research directions include characterizing this framework in the landscape of general probabilistic theories (GPTs) and understanding how this approach bounds relational unitary invariants involving three or more states, such as Bargmann invariants [67]. It would also be interesting to relate violation of our inequalities with advantage in quantum protocols, as recently done by some of us in [68] for the task of quantum interrogation.

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APPENDIX A: CHARACTERIZING THE CLASSICAL POLYTOPE

In Ref. [32], Galvão and Brod derived the facet-defining inequalities of the classical polytope C_{C_n} of the n -cycle event graph C_n , as discussed in the main text. The construction uses an argument based on Boole's inequalities for logically consistent processes [39]. In the main text we discuss that, in fact, *any* event graph, and not only cycle graphs, can be used to bound classicality of different forms.

In this Appendix, we consider the computational problem of characterizing the classical polytope C_G for any event graph G . We propose a simple algorithm for computing all its vertices and facets. This proceeds by first calculating the list of vertices of C_G , i.e., its V-representation, and then finding its facet-defining inequalities, i.e., its H-representation, using standard convex geometry tools. As discussed in the main text, this last step is computationally efficient on the size of the polytope. However, the overall efficiency of the procedure is intrinsically limited by the fact that the number of vertices and facets of C_G grows exponentially on the size of G . The brunt of this Appendix is dedicated to computing the set of vertices of C_G .

After setting out the formal definitions, we characterize the edge $\{0, 1\}$ -labelings $E(G) \rightarrow \{0, 1\}$ that respect logical consistency conditions and thus correspond to the vertices of C_G . This characterization yields an efficient procedure for checking whether such an edge labeling is a vertex of C_G , whose complexity we analyze.

However, when the goal is to generate all vertices of C_G , it is needlessly wasteful to generate all the $2^{|E(G)|}$ -many edge $\{0, 1\}$ -labelings and then filter them one by one. Instead, we present a procedure that generates the edge labelings that are vertices of C_G by generating vertex labelings underlying them, thus limiting the search through the space $\{0, 1\}^{E(G)}$ of edge labelings. Even though it might output the same vertex more than once, the method works well, especially for dense graphs. It is optimal for the complete graphs K_n , which, as we will see in Appendix C, are our main examples of interest. We observe that the number of vertices of the polytope C_{K_n} is given by a well-known combinatorial sequence, known as the Bell numbers [69], which count the number of partitions of a set, precisely the space that is searched by this procedure. Finally, we discuss an alternative method that might be more efficient for sparse graphs.

1. Basic definitions

We start with the relevant definitions.

Definition 1. A graph $G = (V(G), E(G))$ consists of a finite set $V(G)$ of vertices and a set $E(G)$ of edges, which are two-element subsets of $V(G)$, i.e., sets of the form $\{v, w\}$, where $v, w \in V(G)$ are distinct vertices.

Note that the graphs we consider in this text are so-called *simple* graphs: they are undirected (since $\{v, w\} = \{w, v\}$), have at most one edge between any two vertices v and w , and have no loops (i.e., they have no edges from a vertex to itself). In one well-delimited passage, however, we will need to consider *possibly loopy graphs*, which may have loops. This corresponds to dropping the requirement that v and w be distinct in the definition above. A possibly loopy graph is said to be *loop-free* if it has no loops, i.e., if it is a bona fide (simple) graph.

Definition 2 (Labelings and coloring). A *vertex labeling* by a set Λ , or a *vertex Λ -labeling* for short, is a function $\lambda : V(G) \rightarrow \Lambda$ assigning to each vertex a label from Λ . It is called a *coloring* if $\{v, w\} \in E(G)$ implies $\lambda(v) \neq \lambda(w)$. The graph G is said to be k -colorable for $k \in \mathbb{N}$ when it admits a coloring by a set of size k .

Similarly, an *edge labeling* by a set Λ , or an *edge Λ -labeling* for short, is a function $\alpha : E(G) \rightarrow \Lambda$ assigning a label from Λ to each edge. When $\Lambda = [0, 1]$, we call this an *edge weighting*.

Definition 3 (Chromatic number). The *chromatic number* of a graph G , written $\chi(G)$, is the smallest $k \in \mathbb{N}$ such that G is k -colorable.

In the classical, deterministic situation modeled by our framework, we consider a vertex labeling of a graph G by an arbitrary labeling set Λ . However, operationally, we do not have access to the vertex labels, but only to the information of whether the labels of neighboring edges are equal or different.

Definition 4. Given any vertex labeling $\lambda : V(G) \rightarrow \Lambda$, its *equality labeling* ϵ_λ is the edge $\{0, 1\}$ -labeling given by

$$\epsilon_\lambda : E(G) \rightarrow \{0, 1\},$$

$$\epsilon_\lambda \{v, w\} := \delta_{\lambda(v), \lambda(w)} = \begin{cases} 1 & \text{if } \lambda(v) = \lambda(w), \\ 0 & \text{if } \lambda(v) \neq \lambda(w). \end{cases}$$

We are interested in characterizing the edge $\{0, 1\}$ -labelings that arise as equality labelings of vertex labelings.

Definition 5. An edge $\{0, 1\}$ -labeling $\alpha : E(G) \rightarrow \{0, 1\}$ is said to be Λ -realizable if it is the equality labeling of some vertex Λ -labeling, i.e., if $\alpha = \epsilon_\lambda$ for some $\lambda : V(G) \rightarrow \Lambda$. If Λ has size $k \in \mathbb{N}$, we say that α is k -realizable.

We write $\text{Eq}(G)$ for the set of realizable edge labelings of G (with any Λ), and $\text{Eq}_k(G)$ for the set of k -realizable ones. We have that $\text{Eq}_k(G) \subseteq \text{Eq}_{k'}(G)$ whenever $k \leq k'$, and $\text{Eq}(G) = \bigcup_{k \in \mathbb{N}} \text{Eq}_k(G)$. Moreover, $\text{Eq}(G) = \text{Eq}_{|V(G)|}(G)$ because a vertex labeling uses at most one distinct label per vertex of the graph.

We often refer to these realizable edge $\{0, 1\}$ -labelings as the *classical* edge labelings. By the inclusion $\{0, 1\} \subseteq [0, 1]$, we can think of any edge $\{0, 1\}$ -labeling as a (deterministic) edge weighting. This gives an alternative description of the classical polytope C_G in the main text.

Definition 6. Given a graph G , its *classical polytope* $C_G \subseteq [0, 1]^{E(G)}$ is the convex hull of the set $\text{Eq}(G)$ seen as a set of points in $[0, 1]^{E(G)}$.

2. Characterizing the vertices of C_G

We now consider the question of determining whether a given edge $\{0, 1\}$ -labeling is realizable (as the equality labeling of some vertex labeling).

Given $\alpha : E(G) \rightarrow \{0, 1\}$, define a relation \sim_α on the set of vertices of G whereby $v \sim_\alpha w$ if and only if there is a path from v to w through edges labeled by 1, i.e., there is a sequence $e_1, \dots, e_n \in E(G)$ such that $v \in e_1$, $w \in e_n$, $e_i \cap e_{i+1} \neq \emptyset$, and $\alpha(e_i) = 1$. This is easily seen to be an equivalence relation.

It yields the following characterization of the classical edge labelings:

Proposition 1. An edge labeling $\alpha : E(G) \rightarrow \{0, 1\}$ is realizable (i.e., classical) if and only if for all edges $\{v, w\} \in E(G)$, $v \sim_\alpha w$ implies $\alpha(\{v, w\}) = 1$.

In other words, an edge labeling $\alpha : E(G) \rightarrow \{0, 1\}$ fails to be realizable precisely when there is an edge $\{v, w\} \in E(G)$ such that $v \sim_\alpha w$ and $\alpha(\{v, w\}) = 0$. In terms of the underlying vertex labelings, such a situation would violate the transitivity of equality.

A slightly different perspective is given by using α to construct a new graph that ‘‘collapses’’ G through paths labeled by 1. Note that this construction yields a possibly loopy graph.

An edge $\{0, 1\}$ -labeling α partitions the edges of G into two sets. This determines two graphs $G_{\alpha=0}$ and $G_{\alpha=1}$, both with the same vertex set as G , but each retaining only the edges of G with the corresponding label, i.e., for each $b \in \{0, 1\}$,

$$V(G_{\alpha=b}) := V(G),$$

$$E(G_{\alpha=b}) := \{e \in E(G) \mid \alpha(e) = b\}.$$

A possibly loopy graph G/α is then defined as follows:

(i) Its vertices are the connected components of $G_{\alpha=1}$, or equivalently, the equivalence classes of \sim_α .

(ii) There is an edge between two connected components A and B of $G_{\alpha=1}$ whenever there exist vertices $v \in A$, $w \in B$, such that $\{v, w\} \in E(G_{\alpha=0})$.

Lemma 1. Let $\alpha : E(G) \rightarrow \{0, 1\}$ and Λ be any set. There is a one-to-one correspondence between Λ -realizations of α and Λ -colorings of G/α .

Proof. Let $\lambda : V(G) \rightarrow \Lambda$ such that $\alpha = \epsilon_\lambda$. If $v \sim_\alpha w$, then $\lambda(v) = \lambda(w)$ by propagating equality along the path labeled by 1. Hence, the map $\kappa : V(G/\alpha) \rightarrow \Lambda$ given by $\kappa([v]) := \lambda(v)$ is well defined. Now, an edge $e \in E_{G/\alpha}$ is of the form $e = \{\{v\}, \{w\}\}$ for some $v, w \in V(G)$ such that $\alpha(\{v, w\}) = 0$. Since $\alpha = \epsilon_\lambda$, this means that $\lambda(v) \neq \lambda(w)$, hence $\kappa([v]) \neq \kappa([w])$. Thus, κ is a coloring.

Conversely, given a coloring $\kappa : V_{G/\alpha} \rightarrow \Lambda$, set $\lambda(v) := \kappa([v])$. Let $e = \{v, w\} \in E(G)$. If $\alpha(e) = 1$, then $[v] = [w]$, hence $\lambda(v) = \lambda(w)$ because κ is a coloring. If $\alpha(e) = 0$, then $\{[v], [w]\} \in E_{G/\alpha}$, hence $\lambda(v) \neq \lambda(w)$. In either case, $\alpha(e) = \epsilon_\lambda(e)$.

The two processes just described are inverses of one another. \blacksquare

Corollary 1. An edge $\{0, 1\}$ -labeling is Λ -realizable if and only if the possibly loopy graph G/α is Λ -colorable. In particular, it is realizable (i.e., classical) if and only if G/α is loop-free.

Proposition 2. Checking whether an edge $\{0, 1\}$ -labeling for a graph G is realizable can be done in time $O(n + m)$, where $n = |V(G)|$ and $m = |E(G)|$. Checking k -realizability in a given $k \geq 3$ is NP-complete.

Proof. For the first part, transverse the graph $G_{\alpha=1}$ using a depth-first search (DFS). When visiting each vertex, run through all the departing edges of $G_{\alpha=0}$ to see if any is linked to an already visited vertex in the connected component of $G_{\alpha=1}$ currently being traversed. If any is found, reject α .

For the second part, use Corollary 1 to reduce to graph coloring: a graph G is k -colorable if and only if the constant 0 edge labeling is realizable. \blacksquare

The procedure outlined in the proof above is described below in more detail using pseudocode.

Input: graph G with $V(G) = \{1, \dots, N\}$,
edge-labeling $\alpha : E(G) \rightarrow \{0, 1\}$

Output: whether α is realizable, hence a vertex of the polytope C_G .

global variable d_i **for each** $i \in V(G)$

global variable c_i **for each** $i \in V(G)$

procedure MAIN ()

$d_i \leftarrow$ false **for all** $i \in V(G)$

for $i \in V(G)$ **do**

if $\neg d_i$ **then**

$c_j \leftarrow$ false **for all** $j \in V(G)$

 SEARCH (i)

end if

end for

terminate with output true

procedure SEARCH (i)

$d_i, c_i \leftarrow$ true

for $j \in \text{NEIGHBORS}(i)$ **do**

if $\alpha(\{i, j\}) = 0 \wedge c_j$ **then**

terminate with output false

else if $\alpha(\{i, j\}) = 1 \wedge \neg d_j$ **then**

 SEARCH (j)

end if

end for

3. Computing all the vertices of C_G

We conclude that it is computationally easy to check whether a given edge $\{0, 1\}$ -labeling, i.e., a given deterministic edge weighting, is classical. Nevertheless, determining the whole set of vertices of the classical polytope is computationally hard since the number of edge labelings to be tested grows exponentially with the number of edges of the graph.

It is interesting to note that for the complete event graph K_n of n vertices, the number of classical edge labelings, i.e., vertices of the classical polytope C_{K_n} , is given by a well-known sequence, the Bell or exponential numbers [69,70]. The n th Bell number is the number of partitions, or equivalence relations, of a set of size n . It is clear that edge $\{0, 1\}$ -labelings of K_n are in one-to-one correspondence with symmetric reflexive relations on the set of vertices $\{1, \dots, n\}$, where the label of an edge $\{v, w\}$ determines whether the pairs (v, w) and (w, v) are in the relation. Among these, the classical edge labelings correspond to the equivalence relations (which additionally satisfy transitivity), with the underlying vertex labeling determining a partition of the vertices. For a general graph G , it is still true that the classical edge labelings arise from partitions, or equivalence relations, on the set of vertices, determined by the underlying vertex labeling. The difference is that an edge labeling does not carry enough information to characterize a relation fully. So, in particular, different vertex partitions may give rise to the same classical edge labeling.

We can use this observation to propose a different method for generating all vertices of C_G by constructing vertex-labelings of G . The procedure is given below in pseudocode.

Input: graph G with $V(G) = \{1, \dots, N\}$.

Output: vertices of the polytope C_G .

global variable λ_i **for each** $i \in V(G)$

global variable α_e **for each** $e \in E(G)$

procedure MAIN ()

 GENERATE (1,1)

end procedure

procedure GENERATE ($i, next$)

if $i = N + 1$ **then**

output $(\alpha_e)_{e \in E(G)}$

else

for $x < next$ **do**

 UPDATE (i, x)

 GENERATE ($i + 1, next$)

end for

 UPDATE ($i, next$)

 GENERATE ($i + 1, next + 1$)

end if

end procedure

procedure UPDATE (i, x)

$\lambda_i \leftarrow x$

for $j < i$ **with** $\{i, j\} \in E(G)$ **do**

$\alpha_{\{i,j\}} \leftarrow$ **if** $\lambda_j = x$ **then** 1 **else** 0

end for

end procedure

The procedure above has the disadvantage that it might output the same vertex of the polytope multiple times. This

is because, as already discussed, different partitions of the vertices of G can give rise to the same edge labeling. The problem is especially noticeable for sparse graphs.

An alternative method for generating the vertices of C_G , which might be more efficient in the case of sparser graphs, is to directly search through $\{0, 1\}^{E(G)}$ while checking for consistency on the fly, in order to trim the search space so that only the realizable edge labelings are constructed. This can be done by keeping a representation of the current vertex partition (induced by the edges labeled 1 in the edge labeling being constructed), for example using a union-find data structure, together with a record of forbidden merges between partition components (induced by the edges labeled 0s in the edge labeling being constructed). The disadvantage is that the upkeep of this representation, necessary for checking consistency on the fly, cannot be done in constant time. This incurs an overhead at each step in the search.

APPENDIX B: CHARACTERIZING CLASSICAL POLYTOPES BY GRAPH DECOMPOSITIONS

In this Appendix, we prove some general facts that relate the classical polytopes of different graphs. In particular, we show that some methods of combining graphs to build larger graphs do not give rise to new classicality inequalities. Or, seen analytically rather than synthetically, that some graphs G can be decomposed into smaller component graphs in a way that reduces the question of characterizing C_G to that of characterizing the classical polytopes associated with these components. These observations help trim down the class of graphs that is worth analyzing in the search for new classicality inequalities. As a by-product, we characterize the class of graphs for which all edge weightings are classical as being that of trees, an analog of Vorob'ev's theorem [71] in this framework.

Proposition 3. Let G_1 and G_2 be graphs, and write $G_1 + G_2$ for their disjoint union. Then

$$C_{G_1+G_2} = C_{G_1} \times C_{G_2} = \{(r_1, r_2) \mid r_1 \in C_{G_1}, r_2 \in C_{G_2}\}.$$

Proof. Given vertex labelings $\lambda_i : V(G_i) \rightarrow \Lambda_i$ for each $i = 1, 2$, one obtains a function

$$\lambda_1 + \lambda_2 : V(G_1) \sqcup V(G_2) \rightarrow \Lambda_1 \sqcup \Lambda_2$$

which is a vertex labeling of $G_1 + G_2$ since $V(G_1 + G_2) = V(G_1) \sqcup V(G_2)$. The corresponding equality edge labeling, $\epsilon_{\lambda_1 + \lambda_2} : E(G_1 + G_2) \rightarrow \{0, 1\}$, is precisely the function

$$[\epsilon_{\lambda_1}, \epsilon_{\lambda_2}] : E(G_1) \sqcup E(G_2) \rightarrow \{0, 1\}$$

given by

$$e \mapsto \begin{cases} \epsilon_{\lambda_1}(e) & \text{if } e \in E(G_1), \\ \epsilon_{\lambda_2}(e) & \text{if } e \in E(G_2), \end{cases}$$

implying the result. \blacksquare

In particular, vertices of the polytope $C_{G_1+G_2}$ are in bijective correspondence with pairs consisting of one vertex from each of the polytopes C_{G_i} , while the facets of $C_{G_1+G_2}$ are in bijective correspondence with the union of the facets of C_{G_1} and the facets of C_{G_2} . That is, the inequalities defining $C_{G_1+G_2}$ are those defining C_{G_1} plus those defining C_{G_2} . Taking the disjoint union of event graphs thus creates no new classicality

inequalities. As a consequence, we might as well focus solely on studying the classical polytopes of connected graphs.

The result above considers the construction of a new graph by placing two graphs side by side. But similar results can be obtained for more complicated ways of combining graphs, namely gluing along a vertex or along an edge.

Definition 7 (Gluing). Given graphs G_1 and G_2 , and tuples of vertices

$$\begin{aligned} \mathbf{v}_1 &= (v_1^1, \dots, v_1^k) \in V(G_1)^k, \\ \mathbf{v}_2 &= (v_2^1, \dots, v_2^k) \in V(G_2)^k, \end{aligned}$$

the *gluing of G_1 and G_2 along \mathbf{v}_1 and \mathbf{v}_2* , written $G_1 +_{\mathbf{v}_1=\mathbf{v}_2} G_2$, is the graph obtained by taking the disjoint union $G_1 + G_2$ and identifying the vertices v_1^j and v_2^j for $j = 1, \dots, k$. Explicitly, its vertices are

$$V(G_1 +_{\mathbf{v}_1=\mathbf{v}_2} G_2) := O_1 \sqcup O_2 \sqcup N,$$

where $O_i := V(G_i) \setminus \{v_i^1, \dots, v_i^k\}$ is the set of vertices of G_i not being identified, and $N = \{v^1, \dots, v^k\}$ is a set of “new” vertices (i.e., not in either G_i); its edges are

$$E(G_1 +_{\mathbf{v}_1=\mathbf{v}_2} G_2) := E_1 \cup E_2,$$

where E_i is equal to $E(G_i)$ but with occurrences of v_i^j replaced by the new v^j .

Proposition 4. Let G_1 and G_2 be graphs, $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. Then $C_{G_1 +_{v_1=v_2} G_2} = C_{G_1} \times C_{G_2}$.

Proof. We proceed as in the proof of Proposition 3, using the same notation, but then we take a quotient of the merged alphabet $\Lambda_1 \sqcup \Lambda_2$ identifying two labels, one from each component: $\lambda_1(v_1) \in \Lambda_1$ with $\lambda_2(v_2) \in \Lambda_2$. This yields a well-defined labeling for $G_1 +_{v_1=v_2} G_2$ where the new vertex v is labeled by the element resulting from this identification. This does not affect the equality edge-labelings, and so we obtain the same result. ■

Read analytically, if G is a graph with a cut vertex v , i.e., a vertex whose removal disconnects the graph into two components with vertex sets V_1 and V_2 , then its polytope can be characterized in terms of the polytopes of the induced subgraph on $V_1 \cup \{v\}$ and $V_2 \cup \{v\}$. In particular, the facet-defining inequalities of C_G are those of each of these two components.

As an aside, this result is the missing ingredient for fully characterizing the event graphs that cannot display any non-classicality, i.e., for which all edge weightings $E(G) \rightarrow [0, 1]$ are classical. This could be seen as an analog of Vorob’ev’s [71] theorem in our framework.

Corollary 2. A graph G is such that $C_G = [0, 1]^{E(G)}$ if and only if it is a tree.

Proof. For the “only if” part, if G has a cycle, then any edge labeling $E(G) \rightarrow \{0, 1\}$ that restricts to $(1, \dots, 1, 0)$ on said cycle is not in C_G . For the “if” part, apply Proposition 4 multiple times, following the construction of a tree as a sequence of gluings along a vertex of copies of K_2 , whose classical polytope is $[0, 1]$. ■

We now move to consider gluing along an edge.

Proposition 5. Let G_1 and G_2 be graphs, $v_1, w_1 \in V(G_1)$ and $v_2, w_2 \in V(G_2)$, such that $e_i := \{v_i, w_i\} \in E(G_i)$. Writing

$$G := G_1 +_{(v_1, w_1)=(v_2, w_2)} G_2,$$

we have

$$\begin{aligned} C_G &= \{r \in [0, 1]^{E(G)} \mid r|_{E(G_1)} \in C_{G_1}, r|_{E(G_2)} \in C_{G_2}\} \\ &\cong \{(r, s) \mid r \in C_{G_1}, s \in C_{G_2}, r_{e_1} = s_{e_2}\} \\ &\cong (C_{G_1} \times [0, 1]^{E(G_2) \setminus \{e_2\}}) \cap ([0, 1]^{E(G_1) \setminus \{e_1\}} \times C_{G_2}), \end{aligned}$$

where for the last line we assume that C_{G_1} is written with e_1 as its last coordinate and C_{G_2} with e_2 as its first coordinate.

Proof. The proof is similar to that of Proposition 4, but now we are forced to make two identifications between elements of Λ_1 and of Λ_2 in $\Lambda_1 \sqcup \Lambda_2$. When λ_1 and λ_2 are such that $\epsilon_{\lambda_1}(e_1) = \epsilon_{\lambda_2}(e_2)$, i.e., such that

$$\lambda_1(v_1) = \lambda_1(w_1) \Leftrightarrow \lambda_2(v_2) = \lambda_2(w_2),$$

then this yields a well-defined vertex labeling of G and the result follows. ■

Note that the result is not quite as strong as Propositions 3 and 4. While the inequalities of C_{G_1} plus those of C_{G_2} form a complete set of inequalities for the classical polytope of the resulting graph $G_1 +_{(v_1, w_1)=(v_2, w_2)} G_2$, this is not necessarily a minimal set.

Finally, we consider what we can say in general about the classical polytopes of subgraphs.

Proposition 6. Let G be a graph and G' be a subgraph of G , i.e., $V(G') \subseteq V(G)$ and $E(G') \subseteq E(G)$. Then C_G is a subpolytope of $C_{G'} \times [0, 1]^{E(G) \setminus E(G')}$.

Proof. We need to show that the vertices of C_G constitute a subset of the vertices of $C_{G'} \times [0, 1]^{E(G) \setminus E(G')}$, i.e., that $\text{Eq}(G) \subseteq \text{Eq}(G') \times \{0, 1\}^{E(G) \setminus E(G')}$. Given a classical edge labeling of G , i.e., an edge labeling of the form ϵ_λ for some vertex labeling $\lambda : V(G) \rightarrow \Lambda$, we can restrict λ to a vertex labeling of G' and conclude that its equality labeling is simply the restriction of $\epsilon_\lambda : E(G) \rightarrow \{0, 1\}$ to the subset $E(G')$ of its domain. ■

In particular, C_{K_n} is a subpolytope of $C_G \times [0, 1]^{E(\bar{G})}$ for any event graph G with n vertices, where \bar{G} denotes the complement of G .

APPENDIX C: CLASSICAL POLYTOPE FACETS AND QUANTUM VIOLATIONS FOR SMALL GRAPHS

In this Appendix, we study the facet-defining inequalities of some small graphs. In particular, we analyze and classify the facet-defining inequalities for the classical polytopes C_G corresponding to complete event graphs of four and five vertices ($G = K_4$ and $G = K_5$, respectively). We also find quantum violations of these inequalities with pure states that are sampled from the set of quantum states. For sampling, we used the Python library QuTip [72].

Reference [32] gave a complete characterization of the classical polytope of the graph $K_3 = C_3$, the smallest graph with nontrivial inequalities, together with a characterization of its maximal quantum violations, as well as applications. More generally, Ref. [32] gave the complete set of inequalities for the classical polytope of the cycle graphs C_n , which take the very simple form in Eq. (1). Here, we move to consider graphs with more than three edges and which are not cycles.

TABLE I. Quantum violations for facet inequalities of C_{K_5} .

Class	Violation	Inequality Representative for the Class	Dimension
11–40	1/4	$-r_{12} + r_{15} + r_{25} \leq 1$	2
41–60	1/3	$+r_{15} + r_{25} + r_{35} - (r_{12} + r_{13} + r_{23}) \leq 1$	3
61–65	0.243	$+r_{12} + r_{13} + r_{14} + r_{15} - (r_{23} + r_{24} + r_{25} + r_{34} + r_{35} + r_{45}) \leq 1$	4
66–75	0.312	$+r_{12} + r_{14} + r_{15} + r_{23} + r_{34} + r_{35} - (r_{13} + r_{24} + r_{25} + r_{45}) \leq 2$	3
76–87	0.795	$+r_{12} + r_{15} + r_{23} + r_{34} + r_{45} - (r_{13} + r_{14} + r_{24} + r_{25} + r_{35}) \leq 2$	2
88–92	0.344	$+2r_{12} + 2r_{23} + 2r_{24} + 2r_{25} - (r_{13} + r_{14} + r_{15} + r_{34} + r_{35} + r_{45}) \leq 3$	4
93–152	0.688	$+r_{13} + r_{14} + 2r_{24} + r_{34} + 2r_{45} - (2r_{12} + 2r_{25} + 2r_{35}) \leq 3$	3
153–212	0.7306	$+2r_{12} + 2r_{14} + 2r_{15} + r_{23} + r_{35} - (2r_{13} + 2r_{24} + r_{25} + 2r_{45}) \leq 3$	2
213–242	0.855	$+2r_{13} + 2r_{14} + 2r_{23} + 2r_{24} + 3r_{35} + 3r_{45} - (2r_{12} + 4r_{15} + 4r_{25} + r_{34}) \leq 5$	3

1. Facet-defining inequalities for small complete graphs

The facet-defining inequalities of the classical polytope of the graph C_4 (the four-cycle) are those of the form given by the CHSH inequality mentioned in the main text. If we add one more edge to this graph, the corresponding polytope ends up being described by three-cycle inequalities alone. Therefore, the first interesting graph yielding nontrivial and noncycle inequalities is K_4 , the complete graph of four vertices. The classical polytope of this graph has facets defined by three- and four-cycle inequalities, together with facets defined by the new inequalities described in Eq. (2) in the main text, i.e., those of the form

$$(r_{12} + r_{13} + r_{14}) - (r_{23} + r_{34} + r_{24}) \leq 1.$$

This inequality has a structure that is present for all K_n graphs, as will be discussed in Appendix D. Since complete graphs have all possible edges, these are the graphs that impose the largest number of nontrivial constraints on edge assignments, as per Proposition 6. Therefore, it is natural to look at those graphs first.

We addressed the complete characterization of the classical polytopes of complete graphs, proceeding as far as the computational complexity of the problem allowed. In particular, we found complete sets of facet-defining inequalities for C_{K_5} and C_{K_6} . The polytope C_{K_5} has 52 vertices and 242 facets. These facets are divided into nine symmetry classes. Representative inequalities from each of these classes are shown in Table I. The polytope C_{K_6} has 203 vertices and requires 50 652 inequalities. A list of inequalities and PYTHON code used to obtain them can be found in Ref. [43].

2. Quantum violations

We looked for quantum violations of each inequality class of C_{K_5} obtained by pure states in Hilbert spaces of dimensions 2, 3, and 4. The violations found are included in Table I. The inequality in the third row is apparently not violated by either qubit or qutrit states. The largest violation found among all the inequalities was 0.855, for the inequality in the last row of the table. The sets of quantum states yielding the violations found are presented in Ref. [43].

For some classes of inequalities, we also found violations using pure qubit states that display interesting symmetries in the Bloch sphere. We present those violations in Fig. 2. For instance, consider the inequality in the fifth row of Table I. It

can be violated with the quantum states

$$|\psi_k\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi ik/5}|1\rangle) \quad (C1)$$

with $k = 0, \dots, 4$. This quantum realization attains a value of $\frac{5\sqrt{5}}{4}$ and hence a violation of $\frac{5\sqrt{5}}{4} - 2 \approx 0.79508$. Another interesting violation with qubits is for the inequality in the fourth row of the table. There, a maximal qubit violation is achieved by the states depicted in Fig. 2: choosing $|\psi_2\rangle, |\psi_4\rangle, |\psi_5\rangle$ equally distributed on the equator of the Bloch sphere, i.e., separated by angles of $\frac{2\pi}{3}$, implying that $r_{24} = r_{25} = r_{45} = \frac{1}{4}$, and choosing $|\psi_1\rangle = |0\rangle, |\psi_3\rangle = |1\rangle$, implying that $r_{13} = 0$ and all remaining overlaps are equal to $\frac{1}{2}$. This set of vectors attains the value $\frac{6}{2} - \frac{3}{4} = \frac{9}{4}$ and hence a violation of $\frac{9}{4} - 2 = \frac{1}{4}$. These symmetrically arranged qubit states are also the states used in the construction of the elegant joint measurement of Ref. [73]. However, we could find a higher violation of the same inequality using qutrits, as shown in the table.

We will see in Appendix D that the inequality in Eq. (2) generalizes to an infinite family of inequalities for the polytopes of K_n . The quantum violation found for this noncycle K_4 inequality used the following four qutrit states:

$$\begin{aligned} |\psi_1\rangle &= |0\rangle, \\ |\psi_2\rangle &= \sqrt{\frac{5}{9}}|0\rangle + \sqrt{\frac{4}{9}}|1\rangle, \\ |\psi_3\rangle &= \sqrt{\frac{5}{9}}|0\rangle - \sqrt{\frac{1}{9}}|1\rangle + i\sqrt{\frac{1}{3}}|2\rangle, \\ |\psi_4\rangle &= \sqrt{\frac{5}{9}}|0\rangle - \sqrt{\frac{1}{9}}|1\rangle - i\sqrt{\frac{1}{3}}|2\rangle. \end{aligned}$$

This set of states attains a value of $\frac{4}{3}$ and hence violation of $\frac{4}{3} - 1 = \frac{1}{3}$. This corresponds to the second class of inequalities of C_{K_5} in Table I.

We remark once more that the above violations are *not* necessarily optimal. They were not found using, e.g., techniques of semidefinite programming over the quantum set. We found this landscape of violations by sampling quantum states and calculating the value of the left-hand side of the inequality, which is suboptimal. An important remark is that the quantum violation for the three-cycle inequality class (first row in Table I) is *provably maximal*, as shown in Ref. [32].

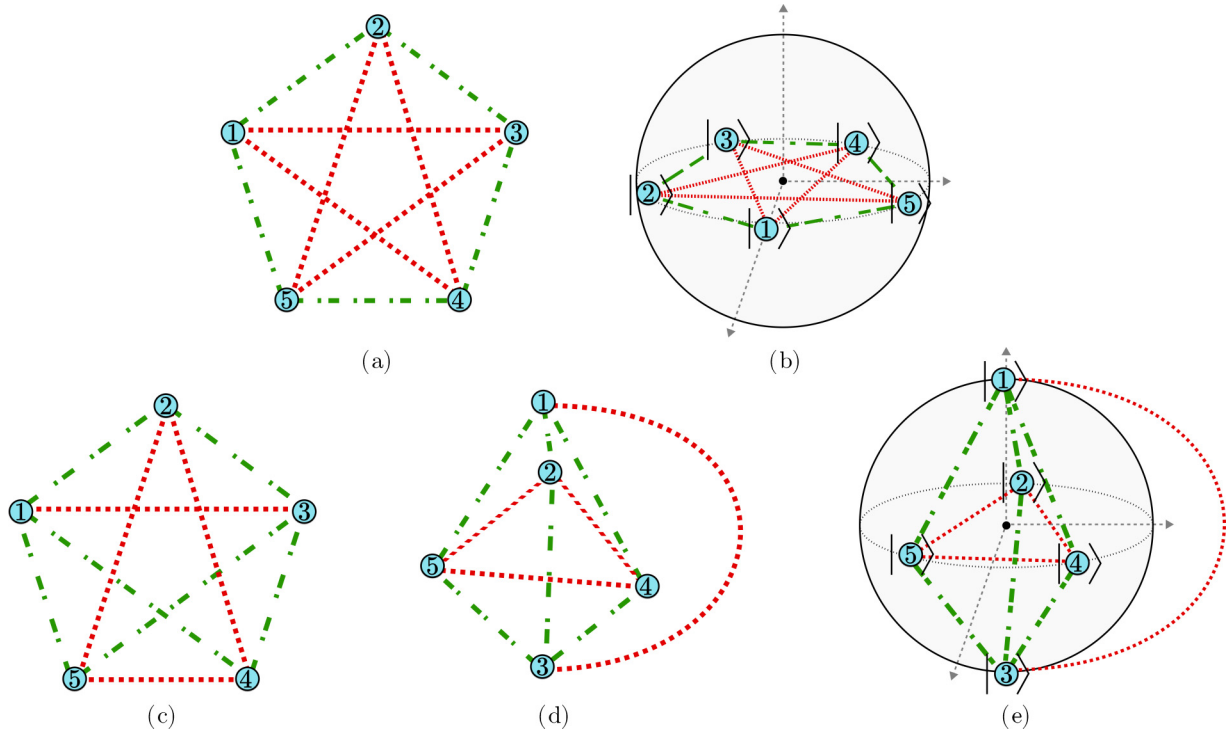


FIG. 2. Qubit states violating classicality inequalities. Part (a) depicts the classicality inequality $r_{12} + r_{23} + r_{34} + r_{45} + r_{15} - r_{13} - r_{14} - r_{24} - r_{25} - r_{35} \leq 2$ with edges corresponding to positive terms in green (dash-dotted lines) and to negative terms in red (dashed-only lines). Part (b) shows a set of five pure states equally spaced over a great circle of the Bloch sphere, which violates this inequality attaining a value of $5\sqrt{5}/4 > 2$. Part (c) depicts the classicality inequality $r_{12} + r_{14} + r_{15} + r_{23} + r_{34} + r_{35} - r_{13} - r_{24} - r_{25} - r_{45} \leq 2$ as in (a). Part (d) depicts the same inequality with the graph displayed in a different geometric configuration, mirroring that of a set of states in the Bloch sphere that largely violates it. Part (e) represents that set of five pure states in the Bloch sphere: three states equally spaced around the equator plus the two eigenstates of the Pauli matrix σ_z ; this set of states attains a value of $9/4 > 2$ for the inequality.

APPENDIX D: INFINITE FAMILY OF CLASSICAL POLYTOPE FACETS

Equation (2) in the main text shows a facet-defining inequality of the polytope C_{K_n} that is not of the previously known form of inequalities derived from cycles in Ref. [32] (which were enough, incidentally, to characterize the classical polytope of the graph $K_3 = C_3$). In this Appendix, we generalize it to an infinite family of new classicality inequalities. More concretely, we present a construction of a facet-defining inequality of the classical polytope C_{K_n} for any $n \geq 2$. Moreover, each inequality on this family cannot be obtained from combining prior members of the family. For $n = 4$, this recovers the just-mentioned inequality from Eq. (2), while for $n = 3$ it naturally reduces to the three-cycle inequality.

Fix a natural number $n \geq 2$. Write $V_n = \{1, \dots, n\}$ for the vertices of K_n , and let E_n denote the set of edges of K_n , i.e., all two-element subsets of V_n . Consider a partition of E_n into the subsets $G_n, R_n \subseteq E_n$ given as

$$G_n := \{\{1, i\} \mid i = 2, \dots, n\},$$

$$R_n := E_n \setminus G_n.$$

This is depicted in Fig. 3. The edges in R_n determine a complete subgraph of K_n with one fewer vertex, i.e., a subgraph isomorphic to K_{n-1} . In turn, the edges in G_n form a subgraph isomorphic to $K_{1,n-1}$, a star graph with n vertices. We use this specific partition of E_n to define a generalized version of the

inequality from Eq. (2):

$$h_n(r) := \sum_{e \in G_n} r_e - \sum_{e \in R_n} r_e \leq 1. \quad (\text{D1})$$

We first show that this is indeed a classicality inequality for the complete graph K_n .

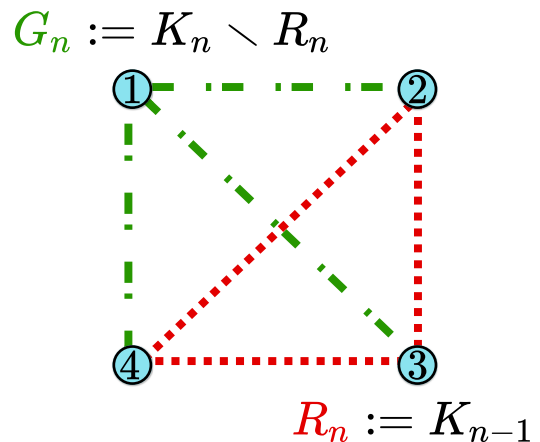


FIG. 3. Depiction of the sets R_n and G_n for a given complete graph K_n . The set R_n is always a complete subgraph (isomorphic to K_{n-1} of K_n). Here we considered $n = 4$ as an example.

Proposition 7. For any $n \geq 2$, the classical polytope C_{K_n} of the complete event graph K_n is contained in the half-space defined by the inequality h_n from Eq. (D1), i.e., all classical edge weightings of K_n satisfy the inequality.

Proof. It suffices to check that the inequality is satisfied by any vertex of the polytope C_{K_n} . Recall that the vertices of this polytope correspond to classical edge $\{0, 1\}$ -labelings of the graph K_n , that is, those realizable as the equality labeling of some vertex labeling.

So, let $\lambda : V_n \rightarrow \Lambda$ be any vertex labeling and $r \in [0, 1]^{E_n}$ be the vertex of the classical polytope corresponding to its equality edge labeling. That is, for all $e = \{i, j\} \in E_n$,

$$r_{ij} = \epsilon_\lambda(\{i, j\}) = \begin{cases} 1 & \text{if } \lambda(i) = \lambda(j), \\ 0 & \text{if } \lambda(i) \neq \lambda(j). \end{cases}$$

Consider the set of vertices in $\{2, \dots, n\}$ that are labeled the same as vertex 1,

$$\begin{aligned} S_\lambda &= \{i \in \{2, \dots, n\} \mid \lambda(i) = \lambda(1)\} \\ &= \{i \in \{2, \dots, n\} \mid r_{1i} = 1\}. \end{aligned}$$

By construction, an edge in G_n , which is of the form $\{1, i\}$, is labeled 1 or 0 depending on whether i is in S_λ or not. Moreover, by transitivity of equality, if $i, j \in S_\lambda$, then $\lambda(i) = \lambda(j)$, meaning that the edge $\{i, j\}$ is also labeled 1. Writing $k := |S_\lambda|$, one can therefore bound the left-hand side of Eq. (D1):

$$\begin{aligned} \sum_{e \in G_n} r_e - \sum_{e \in R_n} r_e &= \sum_{i \in S_\lambda} r_{1i} - \sum_{e \in R_n} r_e \\ &= k - \sum_{e \in R_n} r_e \\ &\leq k - \sum_{i, j \in S_\lambda} r_{ij} \\ &= k - \binom{k}{2} \\ &= 1 - \binom{k-1}{2} \\ &\leq 1, \end{aligned}$$

where for the corner case $k = 0$ this still holds putting $\binom{-1}{2} = 1$. ■

We now state the central result of this Appendix.

Theorem 1. The inequality h_n from Eq. (D1) defines a facet of the classical polytope C_{K_n} of the complete event graph K_n for any $n \geq 2$.

Proof. We establish this result by finding the set of vertices of the polytope C_{K_n} that belongs to—and therefore determines—this facet. In fact, it suffices to find a set of points F in the space (of edge weightings) such that (i) all the points in F belong to the polytope C_{K_n} , (ii) all the points in F saturate the inequality, i.e., belong to the hyperplane determined by it, (iii) the set F is affinely independent, and (iv) F contains as many points as the dimension D of the polytope, so that it generates an affine subspace of dimension $D - 1$. In our proof, the chosen points are moreover vertices of the polytope, as they are edge $\{0, 1\}$ -labelings.

We construct a set F of polytope vertices. This consists of two kinds of edge labelings: those that assign 1 to exactly

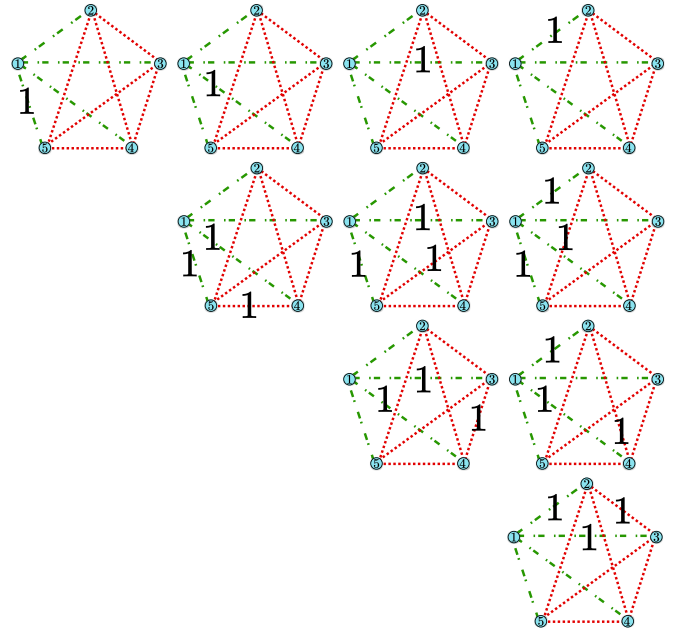


FIG. 4. The construction of the set F for the K_5 graph. Each edge is labeled 1 where explicitly noted, otherwise it is labeled 0 (to keep the figures easy to read). The first row shows the four labelings of the form $r^{(i)}$ with only one edge labeled 1 from G_5 . The remaining rows show the labelings of the form $r^{(i,j)}$, which assign label 1 to exactly one triangle consisting of two edges from G_5 and the connecting edge from R_5 .

one edge of G_n (and 0 to all other edges of E_n) and those that assign 1 precisely to a triangle consisting of two edges from G_n and another from R_n . More formally, we define a family of edge $\{0, 1\}$ -labelings indexed by subsets of size 1 or 2 of the vertex set $\{2, \dots, n\}$, as follows: for each $i = 2, \dots, n$, define the edge $\{0, 1\}$ -labeling $r^{(i)}$ with $r_{1i}^{(i)} = 1$ and $r_e^{(i)} = 0$ for all other edges e ; for each pair $i, j = 2, \dots, n$ with $i \neq j$, define the edge $\{0, 1\}$ -labeling $r^{(i,j)}$ with $r_{1i}^{(i,j)} = r_{1j}^{(i,j)} = r_{ij}^{(i,j)} = 1$ and $r_e^{(i,j)} = 0$ for all other edges e . The set F is then given by

$$F := \{r^{(i)} \mid i = 2, \dots, n\} \cup \{r^{(i,j)} \mid i, j = 2, \dots, n, i \neq j\}.$$

Figure 4 depicts the construction of the set F for the case of $n = 5$. We now check conditions (i)–(iv) to establish the desired result.

For condition (i), we use Proposition 1 to show that all the edge labelings in the set S are classical and thus vertices of the polytope C_{K_n} . Indeed, no cycle can have exactly one edge with label 0. In the case of the labelings of the form $r^{(i)}$, this is immediate as there is only one edge not labeled 0. For the labelings of the form $r^{(i,j)}$, no triangle (i.e., subgraph isomorphic to C_3) has exactly one edge labeled 0: if one chooses two edges labeled 1, then the remaining edge that completes the three-cycle also has label 1. Moreover, any larger cycle can have at most two edges labeled 1. Alternatively, we can show this by constructing an underlying vertex labeling: for $r^{(i)}$ pick $\lambda : V_n \rightarrow \Lambda$ with $\lambda(1) = \lambda(i)$ and all other vertices labeled differently; for $r^{(i,j)}$ pick λ with $\lambda(1) = \lambda(i) = \lambda(j)$ and the other vertices labeled differently.

Condition (ii) is directly checked: for each $i = 2, \dots, n$ we have

$$\sum_{e \in G_n} r_e^{(i)} - \sum_{e \in R_n} r_e^{(i)} = r_{1i}^{(i)} - 0 = 1 - 0 = 1,$$

and for each pair $i, j = 2, \dots, n$ with $i \neq j$,

$$\sum_{e \in G_n} r_e^{(i,j)} - \sum_{e \in R_n} r_e^{(i,j)} = r_{1i}^{(i,j)} + r_{1j}^{(i,j)} - r_{ij}^{(i,j)} = 2 - 1 = 1.$$

For condition (iii), affine independence can be verified by inspecting the matrix whose columns are the vectors corresponding to the edge-labelings in F . Ordering the components of each vector (corresponding to the edges of K_n) in lexicographic order and listing $r^{(i)}$ followed by $r^{(i,j)}$ also in that order, the matrix is arranged to be triangular with diagonal entries all equal to 1, hence its determinant is equal to 1, implying linear independence of the vectors.

Finally, for condition (iv), as all these labelings are distinct, one can count the number of elements of S from the way they were constructed:

$$|F| = \binom{n-1}{1} + \binom{n-1}{2} = \binom{n}{2} = \frac{n(n-1)}{2}.$$

We conclude that it is the same as the dimension of the ambient space (of edge labelings) where the polytope lives, and thus also of the polytope itself. ■

APPENDIX E: EVENT GRAPHS AND KOCHEN-SPECKER CONTEXTUALITY

In this Appendix, we establish a formal connection between our framework and Kochen-Specker contextuality. The central result (Theorem 2) shows how our event graph formalism recovers all noncontextuality inequalities obtainable from the Cabello-Severini-Winter (CSW) exclusivity graph approach [28].

To achieve this, we encode a contextuality setup, represented in CSW by an exclusivity graph H , by imposing exclusivity constraints on a related event graph H_\star . This process amounts to taking a cross-section yielding a subpolytope of the classical polytope C_{H_\star} . We show that the resulting facet inequalities bound noncontextual models for H .

In fact, we prove something *stronger*. We describe an explicit isomorphism between the noncontextual polytope associated by CSW with the exclusivity graph H and this cross-section subpolytope of the classical polytope C_{H_\star} associated by our approach with the event graph H_\star . In particular, these polytopes have the same nontrivial facet-defining inequalities. These are obtainable from the inequalities that define the full (unconstrained) classical polytope of the event graph H_\star by setting some coefficients to zero. Theorem 2 thus establishes a tight correspondence between our event graph approach and a broad, well-established framework for contextuality.

In what follows, we introduce the relevant definitions regarding the exclusivity graph approach, the associated event graphs, and the constraints to be imposed on them, before proving the new results.

1. The exclusivity graph approach

In the CSW framework from Ref. [28], contextuality scenarios are described by so-called exclusivity graphs. Hence this formalism is also known as the exclusivity graph approach; see also Ref. [31] (Chap. 3) for a recent and comprehensive discussion.

The vertices of an exclusivity graph H represent measurement events, and its edges indicate exclusivity between events, where two events are exclusive that can be distinguished by a measurement procedure.

Even though the CSW framework is theory-independent, it is helpful for clarity of exposition to consider its instantiation in quantum theory, in order to better convey the underlying intuitions. In quantum theory, measurement events are represented by projectors (PVM elements) on a Hilbert space, or equivalently, by closed subspaces of the Hilbert space. Exclusivity is captured by orthogonality, which characterizes when two projectors may appear as elements of the same PVM, i.e., events from *the same* measurement procedure. Given a set of projectors $\{\Pi_v\}_{v \in V}$ on a fixed Hilbert space, the corresponding contextuality scenario is thus described by its orthogonality graph. This graph has a set of vertices V and an edge $\{u, v\}$ if and only if the projectors Π_u and Π_v are orthogonal to each other, i.e., when $\Pi_u \Pi_v = 0$.

In this approach, a non-negative vertex weighting $\gamma : V(H) \rightarrow \mathbb{R}_{\geq 0}$ on the exclusivity graph H determines a noncontextuality inequality on the probabilities $P(v)$ of measurement events $v \in V(H)$:

$$\sum_{v \in V(H)} \gamma(v) P(v) \leq \alpha(H, \gamma),$$

where $\alpha(H, \gamma)$ is the independence number of the vertex-weighted graph. In the quantum case, this yields a noncontextuality condition on the statistics predicted by a given quantum state ψ :

$$\sum_{v \in V(H)} \gamma(v) \langle \psi | \Pi_v | \psi \rangle \leq \alpha(H, \gamma).$$

Such noncontextuality inequalities above determine the polytope of noncontextual behaviors for any exclusivity graph H . This polytope, known as the stable set polytope of H , $\text{STAB}(H)$, is most readily defined by its V-representation, which we now present, following Ref. [31] (Chap. 3).

Definition 8. Let H be a graph. A subset $S \subseteq V(H)$ of vertices is called a *stable set* if no two vertices of S are adjacent in H , i.e., for all $v, w \in S$, $\{v, w\} \notin E(H)$. Write $\mathcal{S}(H)$ for the set of stable sets of H .

To any subset of vertices $W \subseteq V(H)$ corresponds its characteristic map, the vertex $\{0, 1\}$ -labeling $\chi_W : V(H) \rightarrow \{0, 1\}$ given by

$$\chi_W(v) := \begin{cases} 1 & \text{if } v \in W, \\ 0 & \text{if } v \notin W. \end{cases}$$

Through the inclusion $\{0, 1\} \subseteq [0, 1]$, one regards a vertex $\{0, 1\}$ -labeling (equivalently, a subset of vertices) as a point in $[0, 1]^{V(H)} \subseteq \mathbb{R}^{V(H)}$. Those arising from stable sets $S \in \mathcal{S}(H)$ correspond to the deterministic noncontextual models, which determine the whole convex set of noncontextual behaviors.

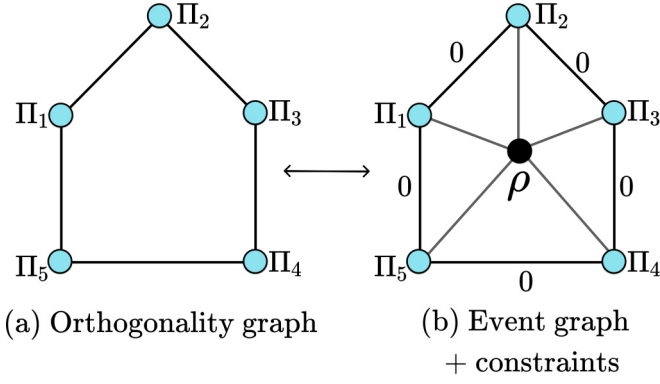


FIG. 5. Equivalence described by Theorem 2 linking contextuality in the manner of CSW to event graphs. The behaviors on an exclusivity graph are in bijective correspondence with edge weightings (overlap assignments) in the related event graph subject to constraints. In particular, the *noncontextual* behaviors for the exclusivity graph correspond bijectively to the *classical* edge weightings in the event graph with constraints.

Definition 9. The *stable set polytope* of a graph H , denoted $\text{STAB}(H)$, is the convex hull of the points $\chi_S \in [0, 1]^{V(H)}$ with S ranging over all stable sets of H ,

$$\text{STAB}(H) := \text{ConvHull}\{\chi_S \mid S \in \mathcal{S}(H)\}.$$

To get the intuition underlying this description, one may think of a vertex $\{0, 1\}$ -labeling $\chi_W : V(H) \rightarrow \{0, 1\}$ as a deterministic assignment of truth values to all measurement events (vertices of the exclusivity graph). In this interpretation, the subset of vertices $W \subseteq V(H)$ is the set of measurement events that are assigned *true*. The stability condition indicates that no two adjacent vertices of the exclusivity graph H are labeled with 1, that is, two exclusive measurement events cannot be simultaneously true. This captures the exclusivity condition at the deterministic level, thus yielding the deterministic noncontextual models.

2. From exclusivity graphs to constrained event graphs

We relate this approach to our framework by constructing a new (event) graph H_* from any (exclusivity) graph H . This is obtained by adding a new vertex ψ with an edge connecting it to all the vertices of H . See Fig. 5 for an instance of this construction for the KCBS scenario, and Fig. 6 for a more generic description. The construction is formally described in Definition 10 below.

The relevance of the new vertex ψ is well known; it is usually called the “handle” and it appears in the literature on the graph approaches [31,74,75]. Its name comes from the geometric arrangement of the vectors providing the maximal quantum violation of the KCBS inequality of Eq. (5): the quantum state resembles the handle of an umbrella made of the vectors that describe measurement events.

Definition 10. Let H be a graph. Define a new graph H_* by

$$\begin{aligned} V(H_*) &:= V(H) \sqcup \{\psi\}, \\ E(H_*) &:= E(H) \cup \{\{\psi, v\} \mid v \in V(H)\}. \end{aligned}$$

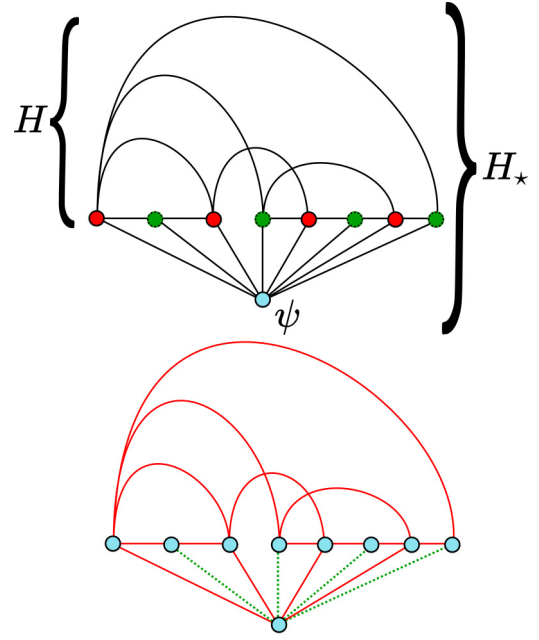


FIG. 6. Translation between vertex labelings of H that are characteristic maps of stable sets, hence vertices of $\text{STAB}(H)$, and constrained edge labelings of H_* that are classical, hence vertices of $C_{H_*}^0$. The top figure depicts a graph H , standing for a generic exclusivity graph, and its extension H_* by adjoining the handle ψ and new edges $\{\psi, v\}$ for all $v \in V(H)$. The vertices of H that are shown in green (dashed) form a stable set $S \in \mathcal{S}(H)$. Its characteristic map $\chi_S : V(H) \rightarrow \{0, 1\}$ assigns 1 to the green (dashed) vertices and 0 to the red (solid) vertices of H . The bottom figure shows how such a vertex $\{0, 1\}$ -labeling is translated to an edge $\{0, 1\}$ -labeling of H_* assigning 0 to all the edges of H (and vice-versa) as described in the proof of Theorem 2. Green (dashed) edges are labeled 1 and red (solid) edges are labeled 0, in accordance with the vertex labelings from χ_S , complemented by the labels induced by exclusivity constraints, $\mathbf{0}_H$, as described in the text. S being stable is equivalent to the resulting edge labeling of H_* being classical.

Moreover, define $C_{H_*}^0$ to consist of the classical edge weightings of H_* that assign value 0 to all edges in H ,

$$C_{H_*}^0 := \{r \in C_{H_*} \mid \forall e \in E(H), r_e = 0\}.$$

The set $C_{H_*}^0$ is, by construction, a cross-section of the classical polytope C_{H_*} of the event graph H_* , where its intersection with the $|V(H)|$ -dimensional subspace is defined by the equations $\bigwedge_{e \in E(H)} r_e = 0$. Moreover, it is a subpolytope of C_{H_*} , i.e., the convex hull of a subset of its vertices. These vertices are the classical edge $\{0, 1\}$ -labelings that assign label 0 to edges in H . In terms of the underlying vertex labelings (from which classical edge labelings arise as equality labelings), the requirement is that any two vertices adjacent in H must be labeled differently.

3. Recovering the noncontextual polytope

The edge set of the graph H_* can be partitioned into two sets: the edges already present in H and the new edges of the form $\{\psi, v\}$ for $v \in V(H)$. The latter are in one-to-one

correspondence with vertices of H . So, there is a bijection $E(H_\star) \cong E(H) \sqcup V(H)$.

When considering the polytope $C_{H_\star} \subseteq [0, 1]^{E(H_\star)}$, we adopt the convention of ordering the coordinates with the edges already in H listed first, so that

$$\mathbb{R}^{E(H_\star)} \cong \mathbb{R}^{E(H) \sqcup V(H)} \cong \mathbb{R}^{E(H)} \times \mathbb{R}^{V(H)}.$$

The subpolytope $C_{H_\star}^0$ is thus written as the set of points of C_{H_\star} of the form $(\mathbf{0}_H, r)$, where $\mathbf{0}_H$ is the zero vector in $\mathbb{R}^{E(H)}$ (corresponding to the edges inherited from H) and r is a weighting of the remaining (new) edges. In particular, the vertices of $C_{H_\star}^0$ are precisely the classical $\{0, 1\}$ -labelings of H_\star that assign the label 0 to all the edges in H .

We can now prove our main result, showing that C_{H_\star} is indeed (isomorphic to) the polytope of noncontextual behaviors for H .

Theorem 2. For any (exclusivity) graph H , there is an isomorphism of polytopes

$$C_{H_\star}^0 \cong \text{STAB}(H)$$

between the stable set polytope (of noncontextual models) of H and the subpolytope of the classical polytope of event graph H_\star constrained by the exclusivity conditions. More explicitly, this is given by the identification

$$C_{H_\star}^0 = \{\mathbf{0}_H\} \times \text{STAB}(H),$$

where $\mathbf{0}_H$ is the zero vector in $\mathbb{R}^{E(H)}$.

Proof. To establish the result, we consider the vertices of these polytopes. Per the above discussion, we have $E(H_\star) \cong E(H) \sqcup V(H)$. Consequently, there is a bijection between vertex $\{0, 1\}$ -labelings of H [equivalently, subsets of $V(H)$], on the one hand, and edge $\{0, 1\}$ -labelings of H_\star that assign label 0 to all the edges in $E(H)$, on the other. Explicitly, to each subset of vertices $W \subseteq V(H)$ corresponds the edge-labeling of H_\star ,

$$[\mathbf{0}_H, \chi_W] : E(H_\star) \cong E(H) \sqcup V(H) \longrightarrow \{0, 1\},$$

as depicted in Fig. 6.

We show that this bijection restricts to a bijection between the *classical* assignments in both cases. Concretely, a subset of vertices $S \subseteq V(H)$ is *stable*, hence (its characteristic map $\chi_S : V(H) \longrightarrow \{0, 1\}$ is) a vertex of the polytope $\text{STAB}(H)$, if and only if the corresponding edge labeling $[\mathbf{0}_H, \chi_S]$ of H_\star is classical, hence a vertex of the polytope C_{H_\star} and thus of $C_{H_\star}^0$.

We establish the two directions of this equivalence simultaneously, recalling the characterisation of classical edge labelings from Proposition 1. Consider H_\star with edge labeling $[\mathbf{0}_H, \chi_S]$. The labeling fails to be classical if and only if there is an edge with label 0 between two vertices linked by a path consisting of edges with label 1. Since all the edges between vertices in H have label 0, the only way to build such a path of 1-labeled edges is via the handle ψ : e.g., $\{u, \psi\}, \{\psi, v\}$, where both u and v must belong to S . So, two vertices u and v of H_\star are linked by a 1-labeled path if and only if they both belong to $S \cup \{\psi\}$. Therefore, the labeling is classical if and only if there is no edge with label 0 between vertices in this set $S \cup \{\psi\}$. To further simplify this condition, note that edges between ψ and a vertex from S have label 1 by construction of the second component of $[\mathbf{0}_H, \chi_S]$, while from

the first component, all edges between vertices in H have label 0. The classicality condition is thus equivalent to there being no edges in H between vertices in S , which is to say that S is stable. ■

4. Recovering all noncontextuality inequalities

We established Theorem 2 in terms of the vertices of the polytopes, i.e., by working with their V-representations. We now consider the relationship between their H-representations, i.e., their facet-defining inequalities [76].

Of course, there is also a bijection between the facets of $\text{STAB}(H)$ and those of $C_{H_\star}^0$. Given the particularly simple description of the isomorphism, whereby $C_{H_\star}^0$ is written as a product of polytopes, we can write this correspondence explicitly. It turns out that the facet-defining inequalities of the subpolytope $C_{H_\star}^0$ are precisely the same as the facet-defining inequalities of the stable polytope of H . Moreover, these can be obtained from the inequalities defining the (unconstrained) polytope C_{H_\star} of the event graph H_\star by setting some coefficients to zero. We thus recover the full set of noncontextuality inequalities from our event graph formalism.

To see this, recall that if P and Q are two convex polytopes with H-representations $P = \{x \mid A_1 x \preceq b_1\}$ and $Q = \{y \mid A_2 y \preceq b_2\}$, then their product has H-representation

$$P \times Q = \{(x, y) \mid A_1 x \preceq b_1 \text{ and } A_2 y \preceq b_2\}.$$

Here, the notation $Az \preceq b$ describes a set of linear inequalities on z in matrix form, with the symbol \preceq standing for componentwise inequality \leq between real numbers.

Applying this to

$$\begin{aligned} C_{H_\star}^0 &= \{\mathbf{0}_H\} \times \text{STAB}(H) \\ &= \{(x, y) \mid x \in \{\mathbf{0}_H\}, y \in \text{STAB}(H)\}, \end{aligned}$$

we obtain that the H-representation of $C_{H_\star}^0$ is the conjunction of the H-representations of $\{\mathbf{0}_H\}$ and of $\text{STAB}(H)$. The former consists simply of the equations $r_e = 0$ for each $e \in E(H)$, zeroing out the first components, which corresponds to the weights of edges already in H . Thus the nontrivial inequalities bounding $C_{H_\star}^0$ are thus the same as the inequalities bounding $\text{STAB}(H)$.

Since $C_{H_\star}^0$ is obtained from C_{H_\star} by intersecting with the subspace that zeroes the components corresponding to edges in $E(H)$, a complete set of inequalities for $C_{H_\star}^0$ can be obtained from the facet-defining inequalities of C_{H_\star} by disregarding those components, i.e., setting the corresponding coefficients to zero.

This process is illustrated by the derivation of the KCBS inequality presented in the main text. There, the exclusivity graph is the five-cycle, with neighboring vertices representing orthogonal projectors. The graph H_\star is then the six-vertex wheel graph W_6 of Fig. 1(e). As shown in the main text, the KCBS noncontextuality inequality $\sum_a \gamma_a |\langle \psi | a \rangle|^2 \leq \alpha(H, \gamma)$ arises as a $C_{H_\star}^0$ inequality, being obtained from a classicality inequality for the event graph W_6 (a facet-defining inequality of C_{H_\star}) by setting to zero the coefficients relating to edges already in H .

APPENDIX F: EVENT GRAPHS AND PREPARATION CONTEXTUALITY

In this Appendix, we relate our approach to Spekkens's notion of preparation contextuality. This may be understood as providing a *theory-independent* perspective on the use of our formalism to witness quantum coherence. There, the vertices of event graphs were interpreted as quantum states, and the edges as two-state overlaps. A similar treatment can be carried out for a certain class of operational theories which support a notion of confusability, with vertices interpreted as (abstract) preparation procedures.

1. Operational probabilistic theories

Spekkens's notion of generalized contextuality is associated with operational probabilistic theories [77–79]. The description of an operational theory starts with a set of basic (operational) physical processes: in the simplest scenarios, one considers preparations and measurements. One considers experiments consisting of a preparation P followed by a measurement M that returns an outcome k . A probability rule associates a probability $p(k | M, P)$ of obtaining outcome k when performing measurement M after the preparation P . More precisely, it associates a probability distribution over outcomes k to each choice of preparation P and measurement M . For a dichotomic measurement M , i.e., one with only two possible outcomes 0 and 1, we simplify notation and write $p(M | P)$ for $p(1 | M, P)$. A crucial—if sometimes overlooked—aspect is that the full set of procedures includes also classical probabilistic mixtures (i.e., convex combinations) of basic procedures, with the probability rule extended accordingly (i.e., linearly).

Given an operational theory, one defines an equivalence relation identifying indistinguishable procedures. Following Ref. [62], two preparation procedures are *operationally equivalent*, written $P \simeq P'$, if and only if for all measurements M and possible outcomes k ,

$$p(k|M, P) = p(k|M, P').$$

A similar definition applies to measurement procedures, but this will not be needed in what follows.

When one treats quantum theory as an operational theory, quantum states $|\phi\rangle$ correspond to equivalence classes of operational procedures. For instance, a state $|0\rangle$ may represent preparing a ground state of a nitrogen atom, or preparing the horizontal polarization in photonic qubits. We relax this terminology and refer to “the preparation P associated with a state $|\phi\rangle$,” even though, strictly speaking, P is only an instance of an equivalence class of procedures. Such relaxation is safe for our purposes. In effect, it corresponds to treating pure quantum states as the basic procedures. The interesting operational equivalences relevant for preparation contextuality go beyond these, holding between classical mixtures of basic procedures. For example, in quantum theory, the preparation procedure corresponding to an equal mixture of pure qubit states $|0\rangle$ and $|1\rangle$ is operationally equivalent to that corresponding to an equal mixture of states $|+\rangle$ and $|-\rangle$. Indeed, both these classical mixtures define the same qubit mixed state, the totally mixed state.

2. LSSS operational constraints

We wish to generalize the situation in which our graph-theoretic framework is used to witness quantum coherence. There, vertices of an event graph G are interpreted as representing vectors $\{|\phi_i\rangle\}_{i \in V(G)}$ in some Hilbert space \mathcal{H} , i.e., pure quantum states. Edge weights then correspond to two-state quantum overlaps, $|\langle\phi_i|\phi_j\rangle|^2$. Such overlaps can be accessed empirically by, e.g., measuring one of the states on a measurement basis that includes the other.

Abstracting from this, we consider a situation in which we associate a preparation procedure P_i with each vertex $i \in V(G)$ of a given graph G . But in order to emulate the setup above for more general operational theories, it is necessary to impose some additional operational constraints. These constraints distill the aspects of quantum theory that make this work, allowing (a theory-independent version of) two-state overlaps. We shall refer to them as the Lostaglio-Senno-Schmid-Spekkens (LSSS) operational constraints, after Refs. [63,64]. Note that these constraints apply to preparation procedures; we need not assume any operational equivalences for measurement procedures. Therefore, the scenarios under consideration aim to probe preparation contextuality only.

First, for any preparation P_i , we assume that there is a corresponding “test measurement” M_i with outcomes $\{0, 1\}$ satisfying the operational statistics $p(M_i | P_i) = 1$. In quantum theory, if P_i is the preparation associated with state $|\phi_i\rangle$, then M_i is realized by the projective measurement $\{|\phi_i\rangle\langle\phi_i|, \mathbb{1} - |\phi_i\rangle\langle\phi_i|\}$, where the first projector corresponds to the outcome $k = 1$.

Moreover, for any edge $\{i, j\} \in E(G)$, whose incident vertices have preparations P_i and P_j , we assume that there exists another pair of preparations $P_{i\perp}$ and $P_{j\perp}$ satisfying $p(M_i | P_{i\perp}) = 0$, $p(M_j | P_{j\perp}) = 0$, and the operational equivalence $\frac{1}{2}P_i + \frac{1}{2}P_{i\perp} \simeq \frac{1}{2}P_j + \frac{1}{2}P_{j\perp}$. In quantum theory, this is always satisfied: given a pair of pure states $|\phi_i\rangle$ and $|\phi_j\rangle$, one picks $|\phi_{i\perp}\rangle$ to be the vector orthogonal to $|\phi_i\rangle$ living in the two-dimensional space spanned by $\{|\phi_i\rangle, |\phi_j\rangle\}$, and similarly for $|\phi_{j\perp}\rangle$.

The probabilities $p(M_i | P_j)$ are usually called the *confusability* [7,64], because they may be interpreted as the probability of guessing incorrectly that the preparation performed had been P_i instead of P_j . These probabilities provide a theory-independent, operational treatment of two-state overlaps, which reduces to the familiar notion in the case of quantum theory viewed as an operational theory:

$$p(M_i | P_j) \stackrel{QT}{=} \text{Tr}(|\phi_i\rangle\langle\phi_i| |\phi_j\rangle\langle\phi_j|) = |\langle\phi_i|\phi_j\rangle|^2.$$

Therefore, we use these confusability probabilities to provide edge weights $r_{ij} = p(M_i | P_j)$ in our framework. In summary, an assignment of preparation procedures to the vertices of G , such that the LSSS operational constraints are satisfied for the pairs of preparations associated with each edge, determines an edge weighting $r : E(G) \rightarrow [0, 1]$.

3. Preparation noncontextuality

When faced with an operational theory, a natural question is whether it admits a (noncontextual) hidden-variable expla-

nation, that is, whether it can be realized by a noncontextual ontological model. In general, an ontological model consists of a measurable space $(\Lambda, \mathcal{F}_\Lambda)$ of *ontic* states equipped with ontological interpretations for preparation and measurement procedures: preparation procedures P determine probability measures μ_P on Λ , whereas measurement procedures M determine measurable functions ξ_M mapping each ontic state $\lambda \in \Lambda$ to a distribution on outcomes, i.e., Markov kernels from Λ to the space of outcomes. Note that the interpretation of classical mixtures of procedures must be determined linearly from that of basic procedures, e.g., $\mu_{\frac{1}{2}P + \frac{1}{2}Q} = \frac{1}{2}\mu_P + \frac{1}{2}\mu_Q$. The composition of the interpretations of a preparation and a measurement (going via the ontic space Λ) is required to recover the empirical or operational predictions, i.e.,

$$p(\cdot | M, P) = \int_{\Lambda} \xi_M d\mu_P,$$

or with variables,

$$p(k | M, P) = \int_{\Lambda} \xi_M(k | \lambda) d\mu_P(\lambda).$$

Such a realization by an ontological model is said to be noncontextual if operationally equivalent procedures are given the same interpretation. For preparations, the requirement is that two operationally equivalent preparation procedures determine the same probability measure on Λ . We refrain from going into detail on the general definition, as the characterization that follows suffices.

In Refs. [63,64], it was shown that the LSSS constraints imply that any preparation noncontextual model explaining preparation procedures P_i as probability measures μ_i on Λ must satisfy

$$p(M_i | P_j) = 1 - \|\mu_i - \mu_j\|_{\text{TV}}, \quad (\text{F1})$$

where $\|\cdot - \cdot\|_{\text{TV}}$ denotes the total variation distance between probability measures, given for an arbitrary measurable space $(\Lambda, \mathcal{F}_\Lambda)$ by

$$\|\mu_i - \mu_j\|_{\text{TV}} = \sup_{E \in \mathcal{F}_\Lambda} |\mu_i(E) - \mu_j(E)|.$$

In the case when Λ is discrete (which is effectively all we actually need), this distance is related to the l_1 norm [80]:

$$\|\mu_i - \mu_j\|_{\text{TV}} = \frac{1}{2} \|\mu_i - \mu_j\|_1 = \frac{1}{2} \sum_{\lambda \in \Lambda} |\mu_i(\lambda) - \mu_j(\lambda)|.$$

We can take that as a *definition* of preparation noncontextual edge weightings.

Definition 11. Let G be an event graph. An edge weighting $r : E(G) \rightarrow [0, 1]$ is said to be *preparation-noncontextual* if the edge weights are of the form in the right-hand side of Eq. (F1), i.e., $r_{ij} = 1 - \|\mu_i - \mu_j\|_{\text{TV}}$, for some choice of an (ontic) measurable space Λ and of probability measures μ_i on Λ for each vertex $i \in V(G)$.

4. Cycle inequalities witness preparation contextuality

We now show how in the case of cycle graphs the inequalities derived from our framework serve as witnesses of preparation contextuality for operational theories satisfying the LSSS constraints.

The technical result is stated in the following proposition; it follows from the triangle inequality.

Proposition 8. Any inequality bounding the set C_n cannot be violated by a preparation noncontextual edge weighting (Definition 11).

Proof. For simplicity, we use addition modulo n when labeling the vertices of the cycle graph C_n , meaning that $i = i + n$. From the triangle inequality of the norm $\|\cdot\|_{\text{TV}}$ it follows that

$$\begin{aligned} & \|\mu_i - \mu_{i+n-1}\|_{\text{TV}} \\ &= \|\mu_i - \underbrace{\mu_{i+1} + \mu_{i+1} - \cdots - \mu_{i+n-2} + \mu_{i+n-2}}_{n-2 \text{ zeros}} - \mu_{i+n-1}\|_{\text{TV}} \\ &\leq \|\mu_i - \mu_{i+1}\|_{\text{TV}} + \cdots + \|\mu_{i+n-2} - \mu_{i+n-1}\|_{\text{TV}}. \end{aligned}$$

Therefore, writing $\|\mu_{i,j}\|_{\text{TV}} := \|\mu_i - \mu_j\|_{\text{TV}}$ for clarity,

$$\|\mu_{i,i+n-1}\|_{\text{TV}} - \|\mu_{i,i+1}\|_{\text{TV}} - \cdots - \|\mu_{i+n-2,i+n-1}\|_{\text{TV}} \leq 0.$$

We must now add 1 to each term to recover the noncontextual overlaps of Eq. (F1). We have n terms, but since the first term has a different sign, two of these 1's will cancel, leaving $n - 2$ added to both sides of the inequality:

$$\begin{aligned} & -1 + \|\mu_{i,i+n-1}\|_{\text{TV}} + 1 - \|\mu_{i,i+1}\|_{\text{TV}} \\ &+ \cdots + 1 - \|\mu_{i+n-2,i+n-1}\|_{\text{TV}} \leq n - 2. \end{aligned}$$

Recalling that $r_{ij} = 1 - \|\mu_{i,j}\|_{\text{TV}}$, we recover a cycle inequality for any chosen vertex i :

$$-r_{i,i+n-1} + r_{i,i+1} + \cdots + r_{i+n-2,i+n-1} \leq n - 2. \quad \blacksquare$$

We may see this result from two perspectives. We can take a *theory-dependent perspective* and look for what information we can extract assuming quantum theory as the relevant operational theory; this proposition then shows that pure quantum states that violate the n -cycle inequalities can be used to construct a proof of quantum preparation contextuality. The construction is done by constructing states and measurements that represent a realization of the prepare-and-measure scenario described by the LSSS constraints. In summary, violations of these inequalities serve as *witnesses of quantum preparation contextuality*.

In light of this result, the experiment of Ref. [81] can be understood as an experimental test that witnessed preparation contextuality of quantum theory; however, since the purpose was not to witness preparation contextuality, the authors have not experimentally probed the relevant operational equivalences, and they have not ruled out loopholes for such a test.

We can also take a *theory-independent perspective*. If a given operational theory satisfying the LSSS constraints for some cycle graph admits a preparation noncontextual ontological model, then the confusabilities $r_{ij} = p(M_i | P_j)$ are bounded by the cycle inequalities. For instance, the Spekkens Toy Theory [33] satisfies the LSSS constraints for any pair of preparation procedures. Since it admits a noncontextual ontological model, it cannot violate the cycle inequalities.

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