A simple proof of uniqueness of the KCBS inequality

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Bell’s investigation into the foundations of quantum mechanics revealed that its completion can not be given by a local model. A related property, that of non-contextuality, requires the completion to assign values to each quantum observable without it depending on the context, i.e. the set of observables it is measured with. An interesting generalisation of the Bell non-locality statement is that the completion can not be non-contextual if we impose a notion of exclusivity, known as the E-principle. The KCBS inequality may be considered an analogue of Bell-inequality and is used to probe contextuality. We show that the KCBS inequality is the only non-trivial facet defining non-contextuality inequality in the odd n-cycle contextuality scenario within the exclusivity graph approach. This is in contrast with the exponential number of facet-defining inequalities one obtains using the compatibility hypergraph approach, another major graph theoretic technique applied in this area. Our result entails that the KCBS inequality can be thought of as the unique hyperplane cutting through the polytope of all E-principle behaviours (analogous to the no-signalling polytope) uniquely in two parts, namely non-contextual and contextual. We discuss how this drastic simplification has interesting consequences and is expected to pave the path for a deeper understanding of the topic.

I. INTRODUCTION

Contextuality is one of the most general ways of capturing the divergence of quantum mechanics from classical physics [1]. The celebrated Bell non-locality can be viewed as a special case of contextuality where the context is provided via space-like separation of the parties involved [2–4]. Bell non-locality, in addition to its fundamental importance, has found many applications in quantum key distribution [5], randomness certification [6], self-testing [7–9] and distributed computing [10], to name a few. Recently, contextuality has also been applied to quantum key distribution [11, 12], randomness certification [13] and uncovered to be the resource powering certain types of quantum computation [14, 15], among others. Bell inequalities—the linear inequalities which capture the Bell non-locality of a probabilistic model—in the simplest case reduce to a famous, unique inequality known as the Clauser-Horne-Shimony-Holt (CHSH) inequality [16]. In general, however, characterisation of Bell inequalities gets complicated rapidly as the range of the involved parameters is increased [17]. Correspondingly, non-contextuality inequalities—the linear inequalities which capture the contextual nature of a probabilistic model—in the simplest case reduce to the well known Klyachko-Can-Binicioğlu-Shumovsky (KCBS) inequality [18]. Sometimes generalisations can act as relaxations and lead to easier characterisations. Since Bell non-locality can be seen as a special case of contextuality, it is natural to ask if a general analysis of the latter offers any relative simplification. As a first step in this direction, we ask if the generalisation of the KCBS inequality [19, 20, p. 241] admits a simple characterisation. We answer this question in the affirmative. In fact, we prove that the characterisation is unique using a simple argument.

Einstein expressed his discomfort with the probabilistic nature of quantum mechanics by providing a striking argument against it [21] using a notion of realism (element of physical reality) for two spatially separated experiments. He believed that there must exist local hidden variables which, once supplied, make QM deterministic. Such completions are referred to as local hidden variable models. Bell constructed an inequality which is violated by QM and yet it can never be violated by any such completion [3], falsifying Einstein’s belief.

The set of probabilistic assignments, which admit a local hidden variable description, form a convex polytope (a bounded set whose boundaries are defined by hyperplanes). The facet-defining Bell inequalities are the characterising hyperplanes of the aforesaid polytope. Finding these facet-defining Bell inequalities has been an active area of research. Consider the bipartite scenario where there are two measurement settings (Δ = 2), each yielding binary outcomes (m = 2). The local polytope in this scenario was characterised by Fine [22] and Froissart [23]. They showed that the CHSH inequality is the only non-trivial facet-defining inequality. However, for arbitrary m and Δ the family of inequalities, referred to as $I_{m,m,Δ,m,Δ}$, is difficult to characterise (see Table I).

In the Bell scenario, there was a clear role of spatial separation and therefore there were at least two parties involved. It turns out that one can study non-classicality even for a single indivisible quantum system. To this end, one uses non-contextual completions of probabilistic assignments where the phrase non-contextual emphasises
that there is a precise value assigned to each observable by the completion. This is because it is possible to define completions where the value assigned depends on the context, i.e. the set of compatible observables it is measured with, and such completions can explain the predictions of quantum mechanics. This is why quantum mechanics is sometimes called contextual [28].

There are two principal graph theoretic approaches towards formalising the probabilistic assignments corresponding to non-contextual completions [2]. In both cases, the sets are convex polytopes and the KCBS inequality turns out to be one of the facets thereof. The first approach known as the compatibility hypergraph approach, focuses on the compatibility relations of a given finite set of observables. Consider a situation where there are $n$ observables, for $n$ odd, and their compatibility relation is given by an $n$-cycle graph. The edges denote compatibility and the vertices denote the observables. This situation is of interest because for $n = 5$ it matches the scenario assumed for the validity of the KCBS inequality and extends to its generalisations. In this approach, facet-defining non-contextuality inequalities for the $n$-cycle compatibility scenario were first discussed by Araújo et al. [29] and a total of $2^n - 1$ of them were found, including the generalised KCBS inequality. While this situation is easier than the typical Bell scenarios, it still requires the characterisation of exponentially many facets. Here we use the second approach, the exclusivity graph approach [4], to radically simplify the picture paving the path for exploring other scenarios. We show that the KCBS inequality, as well as its generalizations to odd $n$ cycle scenarios, is the unique non-trivial facet-defining inequality [30].

### II. PRELIMINARIES

We summarise the exclusivity graph approach here, following the work of Amaral and Cunha [2], deferring a more complete discussion to the appendix. An outcome, $a$, and its associated measurement, $M$, are together called a measurement event and denoted by $(a|M)$. Let $p_j(k)$ be the probability of getting an outcome $k$ given that a measurement $j$ was performed. Two events, $e_i$ and $e_j$, are exclusive if there exists a measurement $M$ such that $e_i$ and $e_j$ correspond to different outcomes of $M$ (see Definition 18). With a family of events $\{e_1, e_2 \ldots e_n\}$ we associate the exclusivity graph, $G := (V, E)$ where $V$ is the set of vertices and $E$ that of edges, whose vertices are the events and there’s an edge between the vertices if and only if the events are exclusive (see Definition 19). The probabilities assigned to these events are formally given by a behaviour which for $G$ is defined to be a map $p : V \rightarrow [0, 1]$ that assigns to each vertex $i$ a probability $p(i)$ such that $p(i) + p(j) \leq 1$ for all vertices that share an edge. The map $p$ can also be seen as a vector in $\mathbb{R}^{|V|}$ (see Definition 21). Behaviours which admit a non-contextual completion, i.e. there exists a non-contextual hidden variable assignment such that if the hidden variable is traced out we recover the given behaviour, are defined to be non-contextual behaviours (see Definition 22). The set of such behaviours is denoted by $B_{NC}(G)$. We can similarly define the set of quantum behaviours, $B_Q$, to be the those which can be obtained by at least one quantum state and corresponding observables (see Definition 23). The set of E-principle behaviours, $B_E(G)$, is one where the behaviours respect the exclusivity principle (also referred to as the E-principle), i.e. exclusive events must have their probability sum to at most one (see Definition 25). The central claim of this formalism is that $B_{NC}(G) \subseteq B_Q(G) \subseteq B_E(G)$ (see Corollary 1). This is a corollary of a powerful identification of each of the sets with geometrical objects studied by Lovász which we describe later. We can now define more precisely a facet-defining non-contextuality inequality to being a non-trivial facet of $B_{NC}(G)$ where the direction of the inequality is chosen to satisfy containment in $B_{NC}(G)$ (see Definition 26). An $n$-cycle graph is an $n$ vertex graph where every $i$th vertex is connected to the $(i+1)$th vertex (the addition is modulo $n$). The generalised KCBS inequality, corresponding to the $n$-cycle graph for $n$ odd, can be expressed as [2]

$$K_n := \sum_{i=1}^{n} p_i \leq \frac{n-1}{2}.$$ 

We recover the original KCBS inequality [18] in the special case of $n = 5$.

### III. RESULT

**Theorem 1.** Consider an odd $n$-cycle exclusivity graph. The associated KCBS inequality is a unique facet-defining non-contextuality inequality.

We will need the aforementioned powerful result connecting the behaviours to geometrically well-studied objects.

**Lemma 1.** [4] Let $e_1, e_2 \ldots e_n$ be the (exclusive) events
associated with an Exclusivity Graph \( G = (V, E) \). Then,

\[
\begin{align*}
B_{NC}(G) &= \text{STAB}(G) \\
B_Q(G) &= TH(G), \\
B_{E}(G) &= \text{QSTAB}(G).
\end{align*}
\]

The objects of interest to us are defined as follows. The definition of the incidence vector, \( \vec{p}_{(k)} \), and clique are standard (see Section D).

**Definition 1.** \( \text{STAB}(G) \) is defined as the convex hull of the vectors \( \vec{p}_{(k)} \) for all stable set \( k \) where \( \vec{p}_{(k)} \) is the incidence vector of the set \( k \).

**Definition 2.** \( \text{QSTAB} \)-inequalities for a graph \( G \) are defined to be the set of inequalities given by

\[
\sum_{i \in Q} x_i \leq 1
\]

for every clique \( Q \) of the graph.

**Definition 3.** \( \text{QSTAB}(G) \) is the set of vectors \( x \in \mathbb{R}^{|V|} \) such that \( x_i \geq 0 \), and the \( \text{QSTAB} \)-inequalities associated with \( G \) are satisfied.

Before we prove Theorem 1, note that the characterisation of \( \text{STAB}(G) \) was given in terms of its vertices and that of \( \text{QSTAB}(G) \) was in terms of its hyperplanes. The following (known) link, Lemma 2, between these representations is key to the radical simplification.

**Definition 4.** \( \text{STAB} \)-inequalities for a graph \( G = (V, E) \) are defined to be the set of inequalities given by \( (x_i + x_j) \leq 1 \) for every \( (i, j) \in E \).

**Lemma 2.** [31] \( \text{STAB}(G) \) is the convex hull of the integral solutions to the equations \( x_i \geq 0 \), and \( \text{STAB} \)-inequalities for \( G \).

**Proof of Theorem 1.** We will consider a 5 cycle graph but our techniques readily generalise to the odd \( n \) cycle case (unless stated otherwise). The \( \text{QSTAB} \) inequalities, together with the \( x_i \geq 0 \) condition, can be expressed as

\[
\begin{align*}
0 &\leq x_i \leq 1 \text{ for } i = \{1, 2 \ldots 5\} \quad (1) \\
x_i + x_{i+1} &\leq 1 \text{ for } i = \{1, 2 \ldots 5\} \quad (2)
\end{align*}
\]

where \( i + 1 \) is modulo 5. Note the \( \text{STAB} \) inequalities, together with \( x_i \geq 0 \), turn out to be exactly the same as the aforesaid for the 5 cycle graph. (The \( \text{STAB} \) inequalities are not enough to define the set \( \text{STAB} \). One must take their integral solutions. The set obtained by taking a convex hull of these solutions is \( \text{STAB} \).) Each inequality is characterised by a hyperplane. The vertices must lie on the intersection of (at least) five distinct hyperplanes. From this, we can already see that the integral (integer) solutions of \( \text{STAB} \) inequalities and the \( \text{QSTAB} \) inequalities are the same. The KCBS inequality is one of the facet defining non-contextuality inequality. To see this, it suffices to observe that there are exactly 5 vertices of \( \text{STAB} \), whose corresponding behaviours saturate the said inequality and remaining vertices satisfy the same inequality. For the 5 cycle case, the remaining argument is trivial and we defer the proof of the \( n \) cycle case to the end.

Note that, together with the aforementioned, if we can establish that there is only one non-integral solution of \( \text{QSTAB} \) inequalities then we have proven our result.

To this end, observe that there can only be the following three types of solutions: (1) all \( x_i \) are integers, (2) none of the \( x_i \) are integers or (3) neither all \( x_i \) are integers nor all \( x_i \) are non-integers (viz. at least one integer and at least one non-integer solution).

We are interested in the latter two cases. In case 2, we can’t use any of the \( \text{QSTAB} \) inequalities involving only one term (Equation (1)). This is because for a vertex, we saturate five distinct inequalities. In this case, saturation of any of these inequalities will yield integer solutions which we are not considering. Hence, the only possibility is to use Equation (2). Now we show that the solution is unique. Let \( x_1 = q \) for any \( 0 < q < 1 \). Saturating, we deduce \( x_2 = 1 - q, x_3 = q, x_4 = 1 - q, x_5 = q \) and finally \( x_1 = 1 - q \). This entails \( x_1 = 1 - q = q \) which means \( q = 1/2 \) uniquely.

To complete the argument, we must show that there are no solutions in case 3. We already ruled out considering all five one term inequalities (Equation (1)) as they yield integer solutions. Let us consider \( k \) two term inequalities (Equation (2)) and \( m \) one term inequalities such that \( m + k = 5 \). The \( m \) one term inequalities, when saturated (because we consider the intersection of hyperplanes to obtain the vertices), will force the corresponding \( x_i \) to be integers. This means that there are at least \( m \) integral \( x_i \). To analyse further, we consider the following game. Imagine the 5-cycle graph (see Figure 1). Select \( m \) vertices of the graph (not to be confused with the vertices of \( \text{QSTAB} \)) and \( k \) edges. The vertices correspond to the variables fixed by the one-term inequalities (saturated, so equalities). The edges correspond to the two-term inequalities (again, saturated so equalities). Two cases can arise in such an assignment. Either each of the \( k \) edges is connected to one the \( m \) vertices (possibly via other edges, if not directly) or there is at least one edge which is not connected to any of the \( m \) vertices (again, possibly via other edges, if not directly). These two cases are represented by the left and right graph in Figure 1. Consider the second case. The disconnected edge (in the sense described earlier) will correspond to a two-term equality involving two variables which have no other constraints. This means that the set of inequalities chosen do not uniquely determine a solution, i.e. at least one of the inequalities chosen is redundant. This case is therefore irrelevant. Consider the first case now. In this case, start with any one of the \( m \) vertices. This corres-
ponds to a one-term equality which fixes the associated variable as an integer (as was noted earlier). Now the edge (if there is one) connected to this vertex directly, will fix the value of the other vertex associated with the edge to be an integer. This reasoning can be repeatedly used to show that all the variables involved along the edges connected to the said initial vertex are integers. This can be repeated for every one of the \( m \) vertices. This means that all variables are assigned integer values. We have reached a contradiction which means there are no solution of the kind assumed by case 3.

![Figure 1](image1.png)

**Figure 1.** There are two possible scenarios corresponding to case where there’s at least one integer and one non-integer solution (case 3 in the proof). The two-term inequalities decide the values for two \( x_i \)s and have been represented as edges and nodes (highlighted as small circles) have been used to denote the values determined by the one-term inequalities. Depending on the way the combination of inequalities is selected, one gets either all \( x_i \)s as integers or a redundant set of inequalities leading to an undecidable value for \( x_i \)s.

We end by showing, a possibly known fact, that the (generalised) KCBS inequality is facet defining (in the exclusivity graph approach). All incidence vectors (we will restrict to the ones corresponding to the stable set of the \( n \) cycle graph, for this proof) will always satisfy the KCBS inequality because the cardinality of the stable set is bounded by the independence number (see Definition 32) of the graph, which for our case is \( (n-1)/2 \) \([19, 20, 32]\). We will now show that there are exactly \( n \) vertices of STAB, i.e. incidence vectors which saturate the said inequality. To saturate, the incidence vector must have \((n-1)/2\) components with entry 1, and the remaining \((n+1)/2\) components with entry 0. Note that each incidence vector satisfies the STAB inequalities, i.e. if a given component is 1 then its adjacent components are necessarily 0. One can convince themselves that any such vector, i.e. incidence vectors that saturate the KCBS inequality, must have two zeros adjacent (cyclically over \( n \)) while all other entries are alternatively one and zero. The total number of ways of placing two adjacent zeros, which is exactly \( n \), then gives us the total number of incidence vectors which saturate the inequality thereby proving that the KCBS inequality is indeed facet defining.

**IV. CONCLUSION AND DISCUSSION**

In conclusion, we have provided a simple proof of the uniqueness of the KCBS inequality, i.e. we proved that the generalised KCBS inequality is the only non-trivial facet defining non-contextuality inequality in the odd \( n \)-cycle scenario using the exclusivity graph approach. This is in contrast with the \( 2^n - 1 \) non-trivial facets which emerge if the compatibility hypergraph approach is used for the analogous \( n \)-cycle contextuality scenario. Geometrically, the KCBS inequalities can be thought of as the unique hyperplane cutting through QSTAB which separates all E-principle behaviours uniquely in two parts, namely non-contextual and contextual. Naively, we might imagine the QSTAB polytope and the KCBS inequality to geometrically be illustrated by the image on the left in Figure 2. However, numerical evidence suggests that all the facets of QSTAB are also the facets of STAB which means the naïve understanding is flawed. Since we already saw that all the vertices of STAB are also vertices of QSTAB, it means that the facet corresponding to the KCBS inequality does not pass through any of the edges of QSTAB. One way of achieving this is illustrated by the image on the right in Figure 2 which intuitively captures this exotic underlying geometrical structure of the QSTAB polytope and the KCBS facet. A deeper understanding of the cause of its appearance is left for future work.

![Figure 2](image2.png)

**Figure 2.** Two conceivable illustrations of the QSTAB polytope (light blue) and the KCBS inequality (black) separating the said polytope from the STAB polytope. In the left image, the vertices of both polytopes are the same (except one) but there are two facets of QSTAB which are not a facet of STAB. Numerically we observe that all the facets of QSTAB are also the facets of STAB. This rules out the first image. The second image illustrates an alternative which helps us intuitively understand the higher dimension underlying geometry.

Beyond the \( n \)-cycle scenario, it is important to study circulant graphs as \( n \)-cycle graphs can be seen as special cases thereof and for certain circulant graphs, such as \( C_{8} \) \([1, 4]\), it is known that some of the facet-defining non-contextuality inequalities correspond to previously known facet-defining Bell inequalities. The general connection between Bell inequalities and non-contextuality inequalities, however, is not very well understood. It is exciting for this approach might offer significant simplifications to an otherwise hard problem and considering graphs motivated by Lovász’s geometry, such as the Paley
and Kneser graphs, might provide new insights.

As for the n-cycle scenario itself, in some cases the corresponding measures of resource (in terms of a resource theory) become equivalent by using the aforesaid result and might help in unifying the various approaches, at least in this special but important n-cycle class. There may also be an interesting conservation law of coherence and contextuality in this class which is worth exploring.

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Appendix A: Probabilistic Models | States and measurement

The results discussed here are based on the work of Amaral and Cunha [2]. In any experimental scenario there are two types of interventions possible, either preparation or operation. Preparation is used in the intuitive sense of the word, that is preparing the system in a given state, for instance using a laser to initialise the state of an atom. More explicitly, we make the following assumptions about the theory.

- Interventions are of two types: Preparation and Operation.
- Experiments are reproducible: For each operation, there may be several different outcomes, each occurring with a well defined probability for a given preparation.

Definition 5 (State). Two preparations are defined to be equivalent if they give the same probability distribution for all available operations. We will refer to the equivalence class of preparations as state.
Definition 6 (State space). The set of all states is referred to as the state space of the system.

Remark 1. The state space is convex.

Definition 7 (Pure states). All extremal points of the state space are defined to be pure states.

Definition 8 (Measurements). Measurements are operations with more than one outcome.

Remark 2. Unitary evolution is an example of an operation which is not a measurement.

Definition 9 (Probabilistic model). We call any mathematical description of a physical system which provides the following, a probabilistic model.

1. Objects to represent
   - (a) state
   - (b) operations
   - (c) measurements

2. Rule to calculate the probabilities of the possible outcomes of any arbitrary measurement given any arbitrary state.

Definition 10 (Probability theory). A probability theory is a collection of probabilistic models.

Definition 11 (Outcome repeatable measurements). A measurement \( j \) is defined to be an outcome repeatable measurement if every time one performs this measurement on a system and an outcome \( k \) is obtained, a subsequent measurement of \( j \) on the same system gives the outcome \( k \) again with probability one.

Definition 12 \( (p_j(k)) \). The probability of getting an outcome \( k \) given that a measurement \( j \) has been performed will be denoted by \( p_j(k) \).

All the measurements henceforth will be assumed to be outcome-repeatable.

Definition 13 (Compatible measurements, refinement and coarse graining). A set of measurements \( \{j_1, j_2 \ldots j_n\} \) is compatible if there is another measurement \( j \) with outcomes \( \{1, \ldots m\} \) and functions \( \{f_1, f_2 \ldots f_n\} \) such that the possible outcomes of \( j \) is the same as \( \{f_s(1), f_s(2) \ldots f_s(m)\} \) for each \( s \) and

\[
p_j(l) = \sum_{k \in f_j^{-1}(l)} p_j(k)
\]

where \( j \) is called a refinement of \( \{j_1, j_2 \ldots j_n\} \) and each \( j_s \) is called a coarse graining of \( j \).

If a set of measurements is compatible it is called a set of compatible measurements.

Appendix B: Completion of a probabilistic model

Definition 14 (Context). A set of compatible measurements is defined to be a context.

Our objective now is to construct a general mathematical framework which can describe the completion of a probabilistic model, i.e. give a model which is no longer probabilistic but reduces to the same probabilistic model if certain variables are ignored.

Definition 15 (Completion). Consider a probabilistic model \( P \) where \( S \) represents the set of pure states and \( X \) represents the set of measurements. The completion of this probabilistic model, denoted by \( P' \), consists of a set of measurements \( X' \), which are in one-to-one correspondence with \( X \), and a set of pure states \( S' \), which are in one-to-one correspondence with \( \Lambda \times S \) for some set \( \Lambda \). \( P' \) must satisfy the following requirements. For all \( \rho \in S' \) and all contexts \( c = \{ j_1, j_2 \ldots j_n \} \), \( P' \) should specify a probability distribution over \( \Lambda \) given by \( p(\lambda) \) and a probability distribution \( p_{\rho,j_k}(\lambda, \rho, c, j_k) : \mathbb{R} \to \{0, 1\} \) for each \( \lambda, \rho, c, j_k \) such that

\[
p_{\rho,j_k}(i_1, i_2 \ldots i_m) = \sum_{\lambda \in \Lambda} p(\lambda) \prod_{k=1}^{m} p_{\rho,j_k}(\lambda, \rho, c, j_k)
\]

where \( p_{\rho,j_k}(i_1, i_2 \ldots i_m) \) is the probability assigned by \( P \) to the measurement of \( j_1, j_2 \ldots j_n \) (encoded in \( c \)) yielding the outcomes \( i_1, i_2 \ldots i_m \), respectively, for the state \( \rho \).

Remark 3. We expect the completion \( P' \) to specify \( S' \) as \( \{\lambda, \rho\} \) for all \( \lambda \in \Lambda \) and \( \rho \in S \). Let us assume for simplicity that \( X' = X \). Now for every context \( c = \{ j_1, j_2 \ldots j_n \} \) (i.e. set of compatible measurements from \( X \)) the completion \( P' \) will predict with certainty the outcome of measuring any \( j_i \in c \), for a given \( (\lambda, \rho) \). This prediction is allowed to depend on the set \( c \) itself to accommodate “contextual completions”. We will see later that non-contextual (and functionally consistent) completions contradict the predictions of quantum mechanics.

Let \( X \) be a set of measurements. Let \( \{j_1, j_2 \ldots j_m\} \subset X \) be a set of compatible measurements.

Definition 16 (Non-contextual completion). Let \( c_1 = \{j_1, j_2 \ldots j_m\}, c_2 = \{j_1', j_2' \ldots j_m'\} \) be two contexts (note that \( j_i \) and \( j'_k \) may not be compatible for \( i, k > 1 \)). A completion \( P'' \) of a probabilistic model \( P \) is called non-contextual if \( p_{\rho,j_i}^{(\lambda, \rho, c_1)}(i) = p_{j_i}^{(\lambda, \rho, c_2)}(i) \) for all contexts \( c_1 \) and \( c_2 \) of the aforesaid form.

Appendix C: Formalising Scenarios | The exclusivity graph approach

Definition 17 (Measurement event). The tuple \( (a|M) \) is defined to be a measurement event where \( a \) is a measurement outcome associated with the measurement \( M \).
For brevity, we will use the word event in lieu of measurement event whenever there is no ambiguity.

**Definition 18 (Exclusive event).** Two events $e_i$ and $e_j$ are defined to be exclusive if there exists a measurement $M$ such that $e_i$ and $e_j$ correspond to different outcomes of $M$, i.e. $e_i = (a_i | M)$ and $e_j = (a_j | M)$ such that $a_i \neq a_j$.

**Definition 19 (Exclusivity graph).** For a family of events $\{e_1, e_2, \ldots, e_n\}$ we associate a simple undirected graph, $G := (V, E)$, with vertex set $V$ and edge set $E$ such that two vertices $i, j \in V$ share an edge if and only if $e_i$ and $e_j$ are exclusive events. $G$ is called an exclusivity graph.

**Definition 20 (Probability vector).** For a given exclusivity graph $G = (V, E)$ and a probability theory, the probability vector is a vector $p \in \mathbb{R}^{|V|}$ such that $p_i = \text{prob}(e_i)$ where $\text{prob}(e_i)$ is the probability assigned by the probability theory to the event $e_i$.

**Definition 21 (Behaviour).** A behaviour for an exclusivity graph $G = (V, E)$ is a map $p : V \to [0, 1]$ which assigns to each vertex $i \in V$ a probability $p(i)$ such that $p(i) + p(j) \leq 1$, for all vertices that share an edge, i.e. $(i, j) \in E(G)$. Due to the isomorphism between the map $p : V \to [0, 1]$ and the vector $\vec{p} \in [0, 1]^{|V|}$ we will associate with the $i$th component of $\vec{p}$ the value $p(i)$, i.e. $\hat{p}(i) = p(i)$. (Sometimes we will even drop the vector sign.)

**Remark 4.** We don’t use $p_{(i)} = p_M(i)$ because $M$ is not explicitly, a priori known so cluttering the notation doesn’t help.

For a given exclusivity graph $G = (V, E)$ a probability theory assigns probability $p_{(i)} = \text{prob}(e_i)$ where $\text{prob}(e_i)$ denotes the probability of occurrence of the event $e_i$.

**Definition 22 (Non-contextual behaviour).** A behaviour $p$ is called a deterministic non-contextual behaviour if $p : V \to \{0, 1\}$, i.e. $p_{(i)} \in \{0, 1\}$ for all $i$ and there exists a non-contextual completion of the corresponding probabilistic model $P$. The set of non-contextual behaviour is defined to be the convex hull of deterministic non-contextual behaviours and is denoted by $B_{\text{NC}}(G)$.

**Remark 5.** Defining the behaviour this way implicitly imposes functional consistency. This is because we require a non-contextual completion of deterministic behaviours to start with and later take its convex combination. This imposes the exclusivity condition at the level of the hidden variable model which in turn is a manifestation of functional consistency.

**Definition 23 (Quantum behaviour).** A behaviour for an exclusivity graph $G$ is called a quantum behaviour if there exists a quantum state $\rho$ and projectors $\Pi_1, \ldots, \Pi_n$ acting on a Hilbert space $\mathcal{H}$ such that $p_{(i)} = \text{Tr}(\rho \Pi_i)$ for all $i \in V$ and $\text{Tr}(\Pi_i \Pi_j) = 0$ for vertices that share an edge, i.e. $(i, j) \in E$.

The convex set of all quantum behaviours is denoted by $B_Q(G)$.

**Definition 24 (The exclusivity principle).** Given a subset $\{e_i\}$ of events which are pairwise exclusive we say that the exclusivity principle is obeyed by a probabilistic model if $\sum_i \text{prob}(e_i) \leq 1$ for all such subsets. We will sometimes refer to this as the E-principle.

**Definition 25 (E-principle behaviour).** A behaviour $p$ for an exclusivity graph $G$ is said to be an E-principle behaviour if the associated probabilistic model satisfies the exclusivity principle, i.e. $\text{prob}(e_i) = p(i)$ satisfies the E-principle.

The set of E-principle behaviours will be denoted by $B_E(G)$.

**Remark 6.** The set $B_{\text{NC}}(G)$ is a (convex) polytope, i.e. can be expressed as a solution of a finite number of linear inequalities.

**Definition 26 (Non-contextuality inequality, facet-defining).** Let $p$ be a behaviour and $\gamma_i, \beta \in \mathbb{R}$. A linear inequality, $\sum_i \gamma_i p_{(i)} \leq \beta$, is called a non-contextuality inequality of its satisfaction is a necessary condition for membership to the set $B_{\text{NC}}(G)$. Equivalently, to claim non-membership in the set $B_{\text{NC}}(G)$, it is sufficient to show a violation of the said linear inequality.

A non-contextuality inequality is called facet-defining if it defines a non-trivial facet of $B_{\text{NC}}(G)$.

### Appendix D: Lovász Geometry

At the risk of causing frustration by redundancy, we state the following for clarity.

**Definition 27.** Graph: $G = (V, E)$ defined by the set of vertices and the set of edges

**Definition 28.** Orthonormal representation w.r.t. a graph $G$ is defined as follows. For all $i \to |v_i\rangle$ in $\mathbb{R}^d$ such that $\langle v_i | v_j \rangle = 0$ whenever $(i, j) \notin E$.

**Definition 29.** For a vector $|v_i\rangle$ in an orthonormal representation, the cost is defined as

$$c_i = |\langle \psi | v_i \rangle|^2$$

where $|\psi\rangle \equiv (1, 0, \ldots, 0)$ is a vector in $\mathbb{R}^d$.

**Definition 30.** The theta body corresponding to a graph $G$ is defined to be

$$\text{TH}(G) = \left\{ p \in \mathbb{R}^{|V|} : p_{(i)} = c_i \right\}$$

where $c_i$ is the cost (see Definition 29) corresponding to $G := (V, E)$.
Definition 31. Stable set/Independent set is a subset of vertices $K \subseteq V$ such that for all $i, j \in K$ there’s no edge between $i$ and $j$, viz. $(i,j) \notin E$.

Definition 32. Independence number of a graph $G$ is defined to be the cardinality of the largest independent set of $G$.

Definition 33. Clique is a subset of vertices $K \subseteq V$ such that for all $i,j \in K$ there’s an edge between $i$ and $j$, viz. $(i,j) \in E$.

Definition 34. Incidence vector of a set is defined to be a vector $\vec{p}$ (of size $|V|$) for $K \subseteq V$ such that $p(i) = \begin{cases} 1 & \text{if } i \in K \\ 0 & \text{else} \end{cases}$.

Example 1. Consider the 5-cycle graph $V = \{1, 2, 3, 4, 5\}$, $E = \{(1,2), (2,3), (3,4), (4,5), (5,1)\}$. $K = \{1,3\}$ is an example of a stable set. $K' = \{1,2\}$ is an example of a clique. The incident vector corresponding to $K$ is $p = (1,0,1,0,0)^T$.

Definition 35. STAB($G$) (not to be confused with the stable set) is defined as the convex hull of the vectors $\vec{p}_{(k)}$ for all stable sets $k$ where $\vec{p}_{(k)}$ is the incidence vector of the set $k$. (Note: if $k$ were an index, $\vec{p}_{(k)}$ would refer to the $k$th component of the vector $\vec{p}$; here $k$ is a set).

Definition 36. QSTAB($G$) is the set of vectors $x \in \mathbb{R}^{|V|}$ such that $x_i \geq 0$, $\sum_{i \in Q} x_i \leq 1$ for every clique $Q$.

Lemma 3. [31] STAB($G$) is the convex hull of the integral solutions to the equations $x_i \geq 0$, $(x_i + x_j) \leq 1$ for every $(i,j) \in E$, where $G = (V,E)$.

Remark 7. Every set of indices which is an edge is also a clique (the other way is not necessary, obviously). This means that the inequalities listed in Definition 36 (viz. $\sum_{i \in Q} x_i \leq 1$ for every clique $Q$) contain the inequalities listed in Lemma 3 (viz. $x_i + x_j \leq 1$ for every $(i,j) \in E$).

Lemma 4. [32] STAB($G$) $\subseteq$ TH($G$) $\subseteq$ QSTAB($G$).

Appendix E: Impossible Completions | Linking geometry and quantum mechanics

Lemma 5. [4] Let $e_1, e_2 \ldots e_n$ be the (exclusive) events associated with an Exclusivity Graph $G = (V,E)$. Then,

\[
\begin{align*}
B_{NC}(G) &= \text{STAB}(G), \\
B_{Q}(G) &= \text{TH}(G), \\
B_{E}(G) &= \text{QSTAB}(G).
\end{align*}
\]

Corollary 1. For a given Exclusivity Graph $G$ we have

\[
B_{NC}(G) \subseteq B_{Q}(G) \subseteq B_{E}(G).
\]