Graphical Non-contextual Inequalities for Qutrit Systems

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One of the interesting topics in quantum contextuality is the construction for various non-contextual inequalities. By introducing a new structure called hyper-graph, we present a general method, which seems to be analytic and extensible, to derive the non-contextual inequalities for the qutrit systems. Based on this, several typical families of non-contextual inequalities are discussed. And our approach may also help us to simplify some state-independent proofs for quantum contextuality in one of our recent works.

I. INTRODUCTION

It is well known that a violation of a Bell inequality\cite{1} can be used for refuting the local realism assumption of quantum mechanics. More generally, any quantum violation for a non-contextual inequality\cite{2,3,4,5,6,7} can be used to disprove the non-contextual assumption for quantum mechanics, and can be considered as another version of the proof for quantum contextuality or the Kochen-Specker(KS) theorem\cite{9,10,11}. One of the proofs for the KS theorem is to find a contradiction of a KS value assignment — which claims that the value assignment to an observable (can only be assigned to one of its eigenvalues) is independent of the context it measured alongside — to a set of chosen rays. And a non-contextual inequality can be considered as a bridge to connect a logical proof of the KS theorem and a corresponding experimental verification\cite{12,13,14,15}.

Recently, to give a universal construction for the state-independent proof for quantum contextuality, we introduced a (6\textsubscript{n} + 2)-ray model\cite{17}. As a kind of special state-dependent proofs for quantum contextuality, this family of models, can induce a type of basic non-contextual inequalities. Based on this, we can analytically derive numerous non-contextual inequalities.

In this paper, starting with the (6\textsubscript{n} + 2)-ray model, we introduce a kind of generalized graph which is called a “hyper-graph”. Then we give several interesting families of non-contextual inequalities from each kind of hypergraphs. Finally, we give a rough analysis for the possible quantum violations for these non-contextual inequalities and find that our graphical KS inequality approach may help us to improve some state-independent proofs for the Kochen-Specker theorem in our anther work\cite{17}.

II. DESCRIPTION OF THE (6\textsubscript{n} + 2)-RAY MODEL

Conventionally, the notation of a ray(normalized unless emphasized) in the topic of quantum contextuality is more commonly used than its two alternatives: a complex vector in the Hilbert space and a normalized rank-1 projector on the vector. To be specific, a ray $|\psi_i\rangle = \alpha_i|0\rangle + \beta_i|1\rangle + \gamma_i|2\rangle$ ($\alpha_i, \beta_i, \gamma_i \in \mathbb{C}$) can represent $r_i = (\alpha_i, \beta_i, \gamma_i)$ or or $P_i = |\psi_i\rangle\langle\psi_i|$. Accordingly, the orthogonality and normalization, $\langle\psi_i|\psi_j\rangle = \delta_{ij}$, can be written as $r^*_i r_j = \delta_{ij}$.

For any two rays $P_\phi = |\phi\rangle\langle\phi|$ and $P_\psi = |\psi\rangle\langle\psi|$, if $|\langle\psi|\phi\rangle| \leq \frac{n}{\pi^2}$, we can always add $2n$ complete orthonormal bases to build a $(6\textsubscript{n} + 2)$-ray model\cite{17}. The graphical representation for this model is shown in FIG.1 where $p_n$ and $q_n$ stand for the rays $P_{p_n}$ and $P_{q_n}$ respectively. And one can easily see the orthogonal relations for all these rays from this graph. Clearly, this model can be considered as a generalization of the Clifton’s 8-ray model\cite{15} as the latter is exactly the case for $n = 1$.

Analogous to the Clifton’s 8-ray model, if we assign value 1 to two rays $p_n$ and $q_n$ simultaneously by the non-contextual hidden variable theory, it is not difficult for us to get a contradiction that two orthogonal rays $p_n$ and $q_n$ should also be assigned to value 1. This is why the $(6\textsubscript{n} + 2)$-ray model can be considered as a proof for quantum contextuality, although in a state-dependent manner.

We can also get a non-contextual inequality from the $(6\textsubscript{n} + 2)$-ray model. For some systems with complicated algebraic structures, a regular method to get the upper bounds for the non-contextual inequalities is by the computer search\cite{15}. Though the $(6\textsubscript{n} + 2)$-ray model is somewhat complicated, we have already derived the upper bound in Ref.\cite{17} by an exact algebraic approach rather...
We can get the value assignment upper bound for \( \langle A_{2} \rangle \) with the help of \( \langle A_{2} \rangle \). For \( \sum_{i=1}^{3} p_{i} \leq 1 \), we can see clearly that \( \langle A_{2} \rangle \leq 1 \) from its expansion in Eq. (2), and for \( \sum_{i=1}^{3} p_{i} \geq 2 \), we can also get the same conclusion from \( \langle A_{2} \rangle = 3 \langle A_{2} \rangle - \sum_{i=1}^{3} p_{i} \leq 3 - 2 = 1 \).

Note that here \( 3 \langle A_{2} \rangle = \langle A_{2} \rangle_{1} + \langle A_{2} \rangle_{2} + \langle A_{2} \rangle_{3} \), where \( \langle A_{2} \rangle_{i} = p_{i} + p_{i+1} - p_{i} p_{i+1} \), \( i = 1, 2, 3 \) and \( p_{4} = p_{1} \). In what follows, the similar notations will be used unless specified.

Before discussing the KS value assignment inequality for the \((6n+2)\)-ray model, we would like to introduce a special observable, which will be considered as a “hyper-edge” operator in the following text and can be defined as

\[
C(p_{n}, q_{n}) = \sum_{i \in V} v_{i} - \sum_{i<j, (i,j) \in E} v_{i} v_{j} - p_{n} - q_{n},
\]

where \( V \) is the index set for all the vertices of the graph in Fig. 2 (c) and \( E \) is an index representation for the edge set. In other words, \((i,j) \in E\) indicates that \((v_{i}, v_{j})\) is in the edge set of the graph. Then we can get the following value assignment inequality

\[
(C(p_{n}, q_{n})) \leq 2n.
\]

This can be derived from another form of \( (C(p_{n}, q_{n})) \), namely,

\[
(C(p_{n}, q_{n})) = 2n \langle A_{\Delta} \rangle - \sum_{i=1}^{n} p_{i}(\alpha_{i}^{+} + \alpha_{i}^{-}) - \sum_{i=1}^{n} q_{i}(\beta_{i}^{+} + \beta_{i}^{-}) - p_{0} q_{0} \leq 2n.
\]

Let us return to the \((6n+2)\)-ray model in Fig. 2 (c). Lemma. — The KS value assignment inequality for the \((6n+2)\)-ray model can be given by

\[
(B_{n}) = \sum_{i \in V} v_{i} - \sum_{i<j, (i,j) \in E} v_{i} v_{j} \leq 1 + 2n.
\]

Proof. — Here we give a proof which is different from the approach in Ref. [17].

First, Eq. (6) holds for \( n = 0 \) since \( (B_{0}) = \langle A_{2} \rangle \).

Assume that the statement is also true for \( n-1 \) (\( n \geq 1 \)), namely, \( (B_{n-1}) \leq 2n - 1 \). Then we should prove that it holds for \( n \). Notice that \( (B_{n}) \) can also be written as

\[
(B_{n}) = (B_{n-1}) + \alpha_{n}^{+} + \alpha_{n}^{-} + \beta_{n}^{+} + \beta_{n}^{-} + p_{n} + q_{n} - p_{n-1}(\alpha_{n}^{+} + \beta_{n}^{+}) - q_{n-1}(\alpha_{n}^{-} + \beta_{n}^{-}) - p_{n}(\alpha_{n}^{+} + \alpha_{n}^{-}) - q_{n}(\beta_{n}^{+} + \beta_{n}^{-}) - \alpha_{n}^{+} \beta_{n}^{-} - \alpha_{n}^{-} \beta_{n}^{+},
\]

or

\[
(B_{n}) = (B_{n-1}) + 2(\langle A_{\Delta} \rangle + 4 \langle A_{2} \rangle)
\]

\( - (\alpha_{n}^{+} + \alpha_{n}^{-} + \beta_{n}^{+} + \beta_{n}^{-} + p_{n} + q_{n})
\]

\( - (p_{n-1} + q_{n-1})
\]

\( = (C(p_{n-1}, q_{n-1})) + 2 \langle A_{\Delta} \rangle + 4 \langle A_{2} \rangle
\]

\( - (\alpha_{n}^{+} + \alpha_{n}^{-} + \beta_{n}^{+} + \beta_{n}^{-} + p_{n} + q_{n}).
\]
\[\text{FIG. 3: (a) The hyper-graph associating with the } (6n+2)\text{-ray model. (b) Graphical representation for a hyper-edge.}\]

(i) For the case of \(\alpha_n^+ + \alpha_n^- + \beta_n^+ + \beta_n^- + p_n + q_n \leq 2\), we have \(\langle B_n \rangle \leq \langle B_{n-1} \rangle + 2 \leq 2n+1\) by Eq.\(8\); (ii) and when \(\alpha_n^+ + \alpha_n^- + \beta_n^+ + \beta_n^- + p_n + q_n \geq 3\), according to Eq.\(9\), we can get \(\langle B_n \rangle \leq 2(n-1) + 2 + 4 - 3 = 2n+1\).

Therefore, \(\langle B_n \rangle \leq 2n+1\) holds for any non-negative integer \(n\).

Next, some definitions from graph theory should be given before discussing our main results.

\section{III. AN INTRODUCTION TO THE HYPER-GRAPHS}

It is known that one of the original constraints for the KS value assignment requires that two mutually orthogonal rays cannot be assigned to value 1 simultaneously. This constraint can be generalized to two ordinary rays by the \((2n+6)\)-ray model. To be specific, if two rays \(|\phi\rangle\) and \(|\psi\rangle\) satisfy \(\langle \psi | \phi \rangle \leq \frac{2}{n+2}\), they can always generate a \((2n+6)\)-ray model by adding 2\(n\) auxiliary complete orthonormal bases, such that \(|\phi\rangle\) and \(|\psi\rangle\) cannot be both assigned to value 1. This motivates us to define a new graphical structure to enrich the original graphical representation. Later we will see that this structure will facilitate us to analytically derive the upper bounds for various non-contextual inequalities.

Notice that we have already presented a systematic and programmable approach to construct a state-independent proof of the KS theorem for the first time in Ref.\[17\] based on the \((6n+2)\)-ray model. Actually, a state-dependent proof which seems much simpler, can also be constructed by the same method via reducing some constraints. Next we give a brief review on this approach.

First, we choose several nonspecific (usually nonparallel or nonorthogonal) rays as a fundamental ray set \(F = \{|\psi_i\rangle\}_{i \in I}\) (or \(F = \{P_i|P_i = |\psi_i\rangle\langle\psi_i|\}_{i \in I}\), where \(I\) is an index set and the number of rays in \(F\) is \(|I|\). Then for a fixed \(N (N > 0, N \in \mathbb{Z})\), considering any two rays \(|\psi_k\rangle\) and \(|\psi_l\rangle\) from \(F\), if they satisfy \(\langle \psi_k | \psi_l \rangle \in \left(\frac{n}{n+1}, \frac{n}{n+2}\right)\) \((0 < n \leq N, n \in \mathbb{Z})\), we can economically build a \((6n+2)\)-ray model by adding 2\(n\) extra complete orthonormal bases. Take FIG.\[1\] or FIG.\[2\] (c) for example, what we need to do is just to replace \(p_n\) and \(q_n\) with \(P_k = |\psi_k\rangle\langle\psi_k|\) and \(P_l = |\psi_l\rangle\langle\psi_l|\) respectively. And an \(n\)-weighted hyper-edge linking the two rays can be defined as all the rays from the complete orthonormal bases together with all the edges from the original graphical representation for this \((6n+2)\)-ray model, see FIG.\[3\] (b), where each orange line represents a hyper-edge. Repeat this operation to other pairs of rays in \(F\), and we can construct a proof for the KS theorem and get the corresponding hyper-graph \(G\). Clearly, the simplest nontrivial hyper-graph is exactly the representation for the \((6n+2)\)-ray model (FIG.\[3\] (a)).

We denote by \(V\) and \(E\) the vertex set and the hyper-edge set of a hyper-graph \(G\) respectively. Without loss of generality, we denote \(V = F = \{P_i|i = 1, 2, ..., |V|\}\) and we have \(|V| = |I|\). Note that a 0-weighted hyper-edge between two vertices is an edge of a normal graph. And do not confuse two unconnected vertices with a two-vertex hyper-graph whose hyper-edge is 0-weighted. From this point of view, a normal graph is only a special case of a hyper-graph. This is why we use the same notation \(G\) to denote them for simplicity.

For each hyper-graph \(G\), we can associate with the following KS observable with respect to the non-contextual inequality\[17\]

\[G = \sum_{i=1}^{|V|} P_i + \sum_{i=1}^{|V|} \sum_{j \in N_i, j > i} C(P_i, P_j),\]

where \(C(P_i, P_j)\) defined by Eq.\[3\] can be referred to as a hyper-edge observable, and \(N_i\) stands for index set for the neighborhood of the vertex \(P_i\), i.e., if \(j \in N_i\), then \((P_i, P_j) \in E\). For our optimal construction of a proof for the KS theorem (by adding the minimum number of complete orthonormal bases between any two rays in \(V\)), \(C(P_i, P_j)\) vanishes if \(\langle \psi_i | \psi_j \rangle > \frac{N}{N+2}\) and involves 2\(n\) complete orthonormal bases where

\[n_{ij} = \left[\frac{2|\langle \psi_i | \psi_j \rangle|}{1 - |\langle \psi_i | \psi_j \rangle|^2}\right].\]

From Eq.\[1\], we can get \(\langle C(P_i, P_j) \rangle \leq 2n_{ij}\). But for a non-optimal construction, the number of the orthonormal bases corresponding to \(C(P_i, P_j)\) is usually larger than \(n_{ij}\) and \(C(P_i, P_j)\) vanishes if \((P_i, P_j) \notin E\). In what follows, we only care about the non-contextual inequality from a given hyper-graph rather than the construction of a proof for KS theorem. Hence other problems such as the optimization for \(n_{ij}\) will be ignored.

A vertex set \(U (U \subset V\) is called a maximal unconnected vertex set of a hyper-graph \(G\) if, (i) for any two vertices \(P_i\) and \(P_j\) in \(U\), \((P_i, P_j) \notin E\); (ii) for any other set \(U' \subset V\) satisfies (i), the vertex number \(|U'|\) \leq |\(U\)|. Usually, this set is not unique. Such an example is given in FIG.\[4\].
Let us return to the case of normal graphs. A subgraph $G'$ of a graph $G$ is also a graph whose vertex set satisfies $V' \subset V$ and whose edge set $E'$ consists of all of the edges in $E$ that have both endpoints in $V'$. But here $V$ and $E$ only stand for the vertex set and the edge set of the normal graph $G$, which is different from the notations referred above. This definition can be easily generalized to the hyper-graph case replacing the edge with hyper-edge. And we are supposed to call it “subgraph”. FIG. 4 gives us an example for all the five-vertex subgraphs from a six-vertex hyper-graph.

If we denote by $G'$ the subgraph obtained by removing the vertex $P_i$ and all the edges with one of the endpoint $i$, then it holds

$$
\langle G \rangle = \langle G' \rangle + \langle P_i \rangle + \sum_{j \in N_i} \langle C(P_i, P_j) \rangle.
$$

(10)

And we can get

$$
|V|\langle G \rangle = \sum_{i=1}^{V_1} \langle G' \rangle + \sum_{i=1}^{V_1} \langle P_i \rangle + \sum_{i=1}^{V_1} \sum_{j \in N_i} \langle C(P_i, P_j) \rangle
$$

$$
= \sum_{i=1}^{V_1} \langle G' \rangle - \sum_{i=1}^{V_1} \langle P_i \rangle + 2\langle G \rangle
$$

(11)

or a more compact form

$$
(|V| - 2)\langle G \rangle = \sum_{i=1}^{V_1} \langle G' \rangle - \sum_{i=1}^{V_1} \langle P_i \rangle.
$$

(12)

This can be considered as a relation of the subgraph decomposition.

IV. THREE TYPICAL NON-CONTEXTUAL INEQUALITIES

Let us consider some typical hyper-graphical structures and the related non-contextual inequalities. Here we mainly discuss three different families of hyper-graphs. Based on the hyper-graphical representation for the $(6n+2)$-ray model or Lemma, i.e., $\langle CP_2 \rangle = \langle L_2 \rangle = (B_n) \leq 2n + 1$ (see FIG. 5), we can derive the non-contextual inequalities analytically from the hyper-graphs with more vertices in FIG. 6.

A. Complete hyper-graphs

Analogous to the definition of a complete graph in graph theory, a complete hyper-graph is a hyper-graph in which every pair of vertices is connected by a hyper-edge. Then we can get the following theorem.

**Theorem 1.**— The non-contextual inequality associated with a $k$-vertex complete hyper-graph $(k \geq 2)$ can be written as

$$
\langle CP_k \rangle = \sum_{i=1}^{k} p_i + \sum_{i=1}^{k-1} \sum_{j=2, j>i}^{k} \langle C(p_i, p_j) \rangle \leq 2 \sum_{i=1}^{k(k-1)/2} n_i + 1,
$$

(13)

where $p_i$ is the $i$-th ray (vertex) and $n_i$ stands for the weight for the $i$-th hyper-edge in FIG. 6(a).

**Proof.**— Clearly the statement is true for $k = 2$.

Assume that Eq. (13) holds for any $\langle CP_{k-1} \rangle$ $(k \geq 3)$. We should prove that Eq. (13) also holds for $\langle CP_k \rangle$. From Eq. (12), we have

$$
(k - 2)\langle CP_k \rangle = \sum_{i=1}^{k} \langle CP_k \rangle - \sum_{i=1}^{k} p_i
$$

FIG. 6: (a)The family of complete hyper-graphs $\{CP_i, i = 2, 3, \ldots, k\}$. (b) A $k$-vertex linear hyper-graph $L_k$ (c) A $k$-vertex cyclic hyper-graph $C_k$.
(i) If \( \sum_{i=1}^{k} p_i \leq 1 \), we can see that Eq. \([13]\) still holds from Eq. \([4]\) and the expansion for \( \langle CP_k \rangle \) in Eq. \([13]\). 

(ii) If \( \sum_{i=1}^{k} p_i \geq 2 \), from another form of \( \langle CP_k \rangle \) referred above, we have

\[
(k - 2)\langle CP_k \rangle \leq k + (k - 2) \cdot 2 \sum_{i=1}^{k(k-1)} n_i - 2,
\]

namely,

\[
\langle CP_k \rangle \leq 2 \sum_{i=1}^{k(k-1)} n_i + 1.
\]

Therefore, Eq. \([13]\) holds for any \( \langle CP_k \rangle \) \( (k \geq 2) \).

**B. Linear hyper-graphs**

Likewise, for the linear hyper-graph shown in FIG. 6 (b), we have the following theorem.

**Theorem 2.**— For a \( k \)-vertex linear hyper-graph, the non-contextual inequality can be given by

\[
\langle L_k \rangle = \sum_{i=1}^{k} p_i + \sum_{i=1}^{k-1} (C(p_i, p_{i+1})) \leq 2 \sum_{i=1}^{k-1} n_i + \left\lfloor \frac{k}{2} \right\rfloor + \sum_{i=1}^{k} p_i - 1,
\]

where \( n_i \) is the weight for the relevant hyper-edge in FIG. 6 (b).

**Proof.**— Clearly, Eq. \([14]\) holds for \( k = 2 \). Assume that it is also true for \( \langle L_{k-1} \rangle \) \( (k \geq 3) \). Next let us prove that Eq. \([14]\) holds for \( \langle L_k \rangle \).

(i) From the expansion of \( \langle L_k \rangle \) in Eq. \([14]\), it is clear that the inequality holds for the case \( \sum_{i=1}^{k} p_i \leq \left\lfloor \frac{k}{2} \right\rfloor \).

(ii) If \( \sum_{i=1}^{k} p_i \geq \left\lfloor \frac{k}{2} \right\rfloor + 1 \), we can use another form of \( \langle L_k \rangle \), which reads

\[
\langle L_k \rangle = (k - 1)\langle CP_2 \rangle + p_k + \sum_{i=1}^{k} p_i.
\]

Therefore,

\[
\langle L_k \rangle \leq 2 \sum_{i=1}^{k-1} n_i + k - 1 + 1 - \sum_{i=1}^{k} p_i
\]

\[
\leq 2 \sum_{i=1}^{k-1} n_i + k - 1 - \left\lfloor \frac{k}{2} \right\rfloor
\]

\[
\leq 2 \sum_{i=1}^{k-1} n_i + \left\lfloor \frac{k}{2} \right\rfloor.
\]

Hence Theorem 2 holds for all possible KS value assignments to the related rays.

**C. Cyclic hyper-graphs**

Another non-contextual inequality from the cyclic hyper-graph in FIG. 6 (c) is shown in below.

**Theorem 3.**— For a \( k \)-vertex cyclic hyper-graph, the non-contextual inequality can be given by

\[
\langle C_k \rangle = \sum_{i=1}^{k} p_i + \sum_{i=1}^{k} C(p_i, p_{i+1}) \leq 2 \sum_{i=1}^{k} n_i + \left\lfloor \frac{k}{2} \right\rfloor,
\]

where \( n_i \) represents the weight for the hyper-edge linking the rays \( p_i \) and \( p_{i+1} \), and \( p_{k+1} = p_1 \).

**Proof.**— Similar to the proof in Theorem 2, we can also write \( \langle C_k \rangle \) in another form

\[
\langle C_k \rangle = k \langle CP_2 \rangle - \sum_{i=1}^{k} p_i.
\]

(i) By the original expression for \( \langle C_k \rangle \) in Eq. \([15]\), it is clear that the inequality holds for the case \( \sum_{i=1}^{k} p_i \leq \left\lfloor \frac{k}{2} \right\rfloor \).

(ii) If \( \sum_{i=1}^{k} p_i \geq \left\lfloor \frac{k}{2} \right\rfloor + 1 \), we can use the above second form of \( \langle C_k \rangle \). That is

\[
\langle C_k \rangle \leq 2 \sum_{i=1}^{k} n_i + k - \sum_{i=1}^{k} p_i
\]

\[
\leq 2 \sum_{i=1}^{k} n_i + k - \left\lfloor \frac{k}{2} \right\rfloor
\]

\[
\leq 2 \sum_{i=1}^{k} n_i + \left\lfloor \frac{k}{2} \right\rfloor.
\]

Therefore, Theorem 3 holds for any KS value assignment.

**V. NON-CONTEXTUAL INEQUALITY FOR AN ORDINARY HYPER-GRAph**

For any ordinary hyper-graph, we give a theorem which is equivalent to a conclusion in Ref. [17] to describe the non-contextual inequality.

**Theorem 4.**— For a \( k \)-vertex hyper-graph \( G_k \), we can always find at least one maximal unconnected vertex set \( U \). If we denote by \( p_i \) and \( n_j \) the \( i \)-th vertex and the weight for the \( j \)-th hyper-edge, then we have the following non-contextual inequality

\[
\langle G_k \rangle = \sum_{i=1}^{k} p_i + \sum_{i=1}^{k-1} \sum_{j \in N_i, j > i} C(p_i, p_j) \leq 2 \sum_{i=1}^{k} n_i + |U|,
\]

where \( E \) is the hyper-edge set.

**Proof.**— Equivalently, we can prove it by verifying another proposition. That is, if such an inequality can be
proved to be true for all the possible hyper-graphs with a fixed maximal unconnected vertex set \( U \) (\( |U| < k \), then it also holds for a hyper-graph with \( k \) vertices.

We denote by \( V \) the vertex set of the hyper-graph \( G_{|V|} \), and label the vertices in \( U \) by \( p_1, p_2, \ldots, p_{|U|} \).

The case for \( |V| = |U| \) is trivial.

For \( |V| = |U| + 1 \), at least one hyper-edge with endpoints \( p_{|U|+1} \) and some vertex in \( U \) can be found by the definition of the maximal unconnected vertex set. If \( E = \{(p_{|U|+1}, p_{\alpha_1}), (p_{|U|+1}, p_{\alpha_2}), \ldots, (p_{|U|+1}, p_{\alpha_l})\} \). Then we have

\[
\langle G_{|U|+1} \rangle = \sum_{i=1}^{1, i \neq \alpha_1} p_i + \langle CP_2 \rangle_{p_{|U|+1}, p_{\alpha_1}} + \sum_{i=2}^l \langle C(p_{|U|+1}, p_{\alpha_i}) \rangle \\
\leq |U| - 1 + 2n_1 + 1 + 2\sum_{i=2}^l n_i = 2\sum_{i=1}^l n_i + |U|.
\]

Assume that Eq. (16) holds for all the hyper-graphs with \( |V| = |U|+m \) (\( m > 1 \)). Then for \( |V| = |U| + m+1 \), if \( \sum_{i=1}^{U|+m+1} p_i \leq |U| \), it is clear that Eq. (16) is true. Therefore, we only need to check the case for \( \sum_{i=1}^{U|+m+1} p_i \geq |U| + 1 \). From the subgraph decomposition relation Eq. (12), we have

\[
\sum_{i=1}^{U|+m+1} p_i = |(U|+m+1) - 2\langle G_{|U|+m+1} \rangle \\
= \sum_{i=1}^{U|+m+1} p_i - \sum_{i=1}^{U|+m+1} p_i \\
\leq (|U| + m + 1)|U| + 2(|U| + m + 1 - 2)\sum_{i=1}^{E} n_i \\
- (|U| + 1) \\
\leq (|U| + m - 1)(|U| + 2\sum_{i=1}^{E} n_i) + (|U| - 1).
\]

Thus \( \langle G_{|U|+m+1} \rangle \leq 2\sum_{i=1}^{E} n_i + |U| + \frac{|U| - 1}{|U| + m - 1} \). Since for any value assignment, \( \langle G_{|U|+m+1} \rangle \) should be an integer, and \( \frac{|U| - 1}{|U| + m - 1} \) < 1, then \( \langle G_{|U|+m+1} \rangle \leq 2\sum_{i=1}^{E} n_i + |U| \). Hence the Eq. (16) holds for any hyper-graph with a maximal unconnected vertex set \( U \). As a special case, it also holds for \( G_k \).

By Theorem 4, one can also derive the Eqs. (13)–(14)–(15) by counting the number of the vertices in their maximal unconnected vertex sets.

VI. NON-CONTEXTUAL INEQUALITIES FOR SOME FRACTAL STRUCTURES

If the vertex number of an ordinary hyper-graph is large, then for any KS value assignment, the upper bound for its non-contextual inequality is very difficult to calculate. But in some special cases, analytical formulas for the upper bounds can be recursively derived. We have already given three families of such examples in previous sections. Here we present two more examples, which come from the fractal hyper-graphs.

Considering a fractal hyper-graph family, e.g. FIG 7 (a), it is not difficult for us to notice that some former methods to derive the upper bound of a non-contextual inequality may not work effectively in this scenario, e.g., the way used in Theorem 2 and Theorem 3. But fortunately another approach by Theorem 4 seems to be a nice choice. As for some fractal hyper-graph structures, it is easy to find out their maximal unconnected vertex sets.

For the fractal hyper-graph families \( \{F_L \}_{k \in \mathbb{N}} \) and \( \{F_C \}_{k \in \mathbb{N}} \) FIG 7 if we denote by \( U_{F_L}^k \) (\( U_{F_C}^k \)) the maximal unconnected vertex set for the \( k \)-th graph in \( \{F_L \}_{k \in \mathbb{N}} \) (\( \{F_C \}_{k \in \mathbb{N}} \)), then

\[
|U_{F_L}^k| = 2^k \cdot \frac{1 - (\frac{1}{4})^{\frac{k}{2}+1} + \frac{1}{4} - 4}{\frac{k}{2} + 1} = \frac{1}{3} \cdot (2^k - 2^k \text{ mod } 2-2),
\]

\[
|U_{F_C}^k| = 2^k - 1.
\]

Therefore, we have

\[
\langle F_L \rangle_k = \sum_{i=1}^{2^k-1} p_i + \sum_{i=1}^{2^k-1} \langle C(p_i, p_{2i}), p_{2i+1} \rangle \\
\leq 2\sum_{i=1}^{2^k-1} n_i + |U_{F_L}^k|,
\]

(17)
and

\[
\langle FC_k \rangle \\
3(2^k-1) \\
= \sum_{i=1}^{3(2^k-1)} p_i + \langle C(p_1, p_2) \rangle + \langle C(p_1, p_3) \rangle + \langle C(p_2, p_3) \rangle \\
+ \sum_{i=1}^{3(2^k-1)} \langle C(p_1, p_{2i+2}) \rangle + \langle C(p_1, p_{2i+3}) \rangle \\
+ \langle C(p_{2i+2}, p_{2i+3}) \rangle \\
\leq 2 \sum_{i=1}^{9(2^k-1)+3} n_i + |U_{FC}|. \quad (18)
\]

Then, from Theorem 4, the non-contextual inequality for the square lattice hyper-graph can be given by

\[
\langle SL_{m_x, m_y} \rangle = \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} n_{i, j} + \sum_{i=1}^{m_x-1} \sum_{j=1}^{m_y} \langle C(p_{i, j}, p_{i+1, j}) \rangle \\
+ \sum_{i=1}^{m_x} \sum_{j=1}^{m_y-1} \langle C(p_{i, j}, p_{i, j+1}) \rangle \\
\leq 2 \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} n_{i, j,i+1,j} + \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} n_{i, j,i,j+1} \\
+ |U_{SL_{m_x, m_y}}|, \quad (19)
\]

where \(p_{i, j}\) is the vertex on the site \((i, j)\) and \(n_{i, j,i+1,j}\) (\(n_{i, j,i,j+1}\)) is the weight of the hyper-edge \((p_{i, j}, p_{i+1, j})\) (\((p_{i, j}, p_{i, j+1})\)).

Likewise, for the torus lattice hyper-graph, as \(m_x, m_y \geq 3\), we can get the following non-contextual inequality

\[
\langle TL_{m_x, m_y} \rangle = \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} n_{i, j} + \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} \langle C(p_{i, j}, p_{i+1, j}) \rangle \\
+ \sum_{i=1}^{m_x} \sum_{j=1}^{m_y-1} \langle C(p_{i, j}, p_{i, j+1}) \rangle \\
\leq 2 \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} n_{i, j,i+1,j} + \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} n_{i, j,i,j+1} \\
+ |U_{TL_{m_x, m_y}}|, \quad (20)
\]

where \(p_{m_x+1, j} \equiv p_{1, j}\) (\(p_{i, m_y+1} \equiv p_{i, 1}\)) and \(n_{m_x,j,m_{x+1},j} \equiv n_{m_x,j,j+1}\) (\(n_{i,m_y,i,m_y+1} \equiv n_{i,m_y,i,1}\)).

Other models such like cubic lattice hyper-graphs can also be discussed by using the same method.

VII. NON-CONTEXTUAL INEQUALITIES FOR SOME LATTICE HYPER-GRAPHS

In the end, let us consider two typical lattice hyper-graph families, see FIG. 8. We denote by \(SL_{m_x, m_y}\) and \(TL_{m_x, m_y}\) the square lattice hyper-graph and the torus lattice hyper-graph of \(m_x \times m_y\) vertices respectively. We can get the classical upper bounds of their non-contextual inequalities by calculating the numbers of vertices, \(|U_{SL_{m_x, m_y}}|\) and \(|U_{TL_{m_x, m_y}}|\), in their maximal unconnected vertex sets \(U_{SL_{m_x, m_y}}^r\) and \(U_{TL_{m_x, m_y}}^r\). It is clear that \(|U_{SL_{m_x, m_y}}^r|\) and \(|U_{TL_{m_x, m_y}}^r|\) can be written as

\[
|U_{SL_{m_x, m_y}}^r| = \left\lfloor \frac{m_x m_y}{2} \right\rfloor; \\
|U_{TL_{m_x, m_y}}^r| = \left\lfloor \min\{m_x, m_y\} \right\rfloor \cdot \max\{m_x, m_y\}.
\]

VIII. QUANTUM VIOLATIONS

To see the quantum violation for the non-contextual inequality for a \(k\)-vertex ordinary hyper-graph \(G_k\), the key is to calculate the range of the eigenvalues for \(\sum_{i=1}^{k} p_i\). As for any hyper-edge observable \(C(p_i, p_j)\), from the view of the complete orthonormal bases, the quantum expectation is strictly equal to \(2n_{ij}\), where \(n_{ij}\) is the corresponding hyper-edge weight. We denote by \(\lambda_{\min}\) the minimal eigenvalue for \(\sum_{i=1}^{k} p_i\). Then We have \(\langle G_k \rangle_{\min} = 2 \sum_{i=1}^{k} n_i + \lambda_{\min}\), where the expression for \(\langle G_k \rangle\) can be found in Eq. 10 and the notation \(\langle \cdot \rangle_q\) represents the quantum expectation. If \(\lambda_{\min} > |U|\), then Eq. 10 provide us a state-independent non-contextual inequality. An equivalent conclusion can also be found in Ref. 17. For other cases, it is at best a state-dependent non-contextual inequality.
Besides calculating the eigenvalue for the sum of all the vertices in a hyper-graph, it seems that the relative size (compared with the vertex number of the hyper-graph) for a maximal unconnected vertex set of a hyper-graph may be one of the key factors in testing the quantum violation for the non-contextual inequality. Although sometimes it may not works very well, it can help us to get a preliminary estimation for the possibility of a quantum violation. From this point of view, the non-contextual inequality for the complete hyper-graph family in FIG.6 (a) seems to be the most possible case for a quantum violation. As the maximal unconnected vertex set is just a single vertex, and \((\sum_{i=1}^{7} p_i)q \geq \lambda_{\text{min}} \geq 1\) is easy to be satisfied. But the main shortcoming is that the number of the hyper-edges might be too large. To balance that, we try to choose the hyper-graphs with less hyper-edges, but might still have a state-independent quantum violation. Here we give an example in FIG.9.

From Theorem 4, as \(|U| = 2\), the non-contextual inequality can be given by

\[
\langle W_7 \rangle = \sum_{i=1}^{7} p_i + \sum_{i=1}^{7} \langle C(p_i, p_{i+1}) + C(p_i, p_{i+3}) \rangle \\
\leq 2 \sum_{i=1}^{14} n_i + 2,
\]

where \(p_{8,9,10} \equiv p_{1,2,3}\) and \(n_i\) is the weight for the \(i\)-th hyper-edge. To see the quantum violation, we choose \(\{p_1, p_2, p_3, p_4\}\) to be the 4 core rays (vertices) of the Yu-Oh model \[5\], namely, \(p_1, p_2, p_3, p_4\) are orienting to 4 vertices of a regular tetrahedron, and let \(\{p_5, p_6, p_7\}\) be an approximate orthonormal basis (e.g. with an error of \(\delta < 0.01\)), and also make sure that there are no parallel or antiparallel relationships for these rays, then \(\langle \sum_{i=1}^{7} p_i \rangle_q = \frac{4}{3} + 1 + O(\delta) \approx \frac{7}{3} > |U|\). And we can get a state-independent non-contextual inequality Eq. \[21\], with a reduction of 7 hyper-edges compared with the extreme case of a 7-vertex complete hyper-graph.

We can see that the inequality approach based on hyper-graphs sometimes may help us to optimize the method for construction of a state-independent proof for quantum contextuality in Ref. \[17\] from the above example. In other words, by this method we may get a more economical proof for quantum contextuality with less auxiliary complete orthonormal bases (hyper-edges) but still in a state-independent manner.

Constraints for state-dependent non-contextual inequalities by other models referred in previous sections are listed in the following table,

| Models | Constraints for \(\lambda_{\text{max}}\) |
|--------|----------------------------------|
| \(L_k\) | \(\lambda_{\text{max}} > |\frac{2}{7}|\) |
| \(C_k\) | \(\lambda_{\text{max}} > |\frac{1}{4}|\) |
| \(\mathcal{F}L_k\) | \(\lambda_{\text{max}} > |\frac{4}{7} \cdot (2^k - 2^k \mod 2 - 2)|\) |
| \(\mathcal{F}C_k\) | \(\lambda_{\text{max}} > |\frac{2k - 1}{2}|\) |
| \(\mathcal{S}L_{m_1, m_2}\) | \(\lambda_{\text{max}} > |\frac{m_1, m_2}{2} \cdot \max\{m_{x}, m_{y}\}|\) |
| \(T_{m_1, m_2}\) | \(\lambda_{\text{max}} > |\frac{\min\{m_{x}, m_{y}\}}{2} \cdot \max\{m_{x}, m_{y}\}|\) |

where \(\lambda_{\text{max}}\) is the maximal eigenvalue for the corresponding \(\sum_{i=1}^{\vert V \vert} p_i\) (or \(\sum_{i=1}^{3} \sum_{j=1}^{3} p_{i,j}\)) term.

IX. CONCLUSION AND DISCUSSION

We have discussed a general method for deriving the non-contextual inequalities based on the hyper-graphs for the qutrit systems. Several interesting families of non-contextual inequalities are given. Our method can be applied to any hyper-graph by a subgraph decomposition relation. This relation might be very useful in looking for further interesting relations from other possible correlated structures. We also give the conditions for quantum violations of different types of non-contextual inequalities. Besides, our graphical methods might be helpful to improve the construction for state-independent proofs for quantum contextuality in our anther recent work \[17\]. Moreover, we notice that the mathematical structures of certain non-contextual inequalities and the Hamiltonians for some systems in condensed matter physics are similar. This might motivate us to give a further research on the link between them and try to look for a new method to learn some many-body physical systems.

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