Dimension-dependent noncontextuality inequalities with large contexts

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Quantum theory shows a striking nonclassical feature of contextuality, which is also a crucial resource for quantum information processing. In this paper, we study the dependence of violating noncontextuality inequalities against the dimension of quantum systems. To this end, we consider the restrictions imposed on relations among measurements by limitation of dimensions. Based on the graph-theoretic approach to quantum contextuality, we construct noncontextuality inequalities using multiple mutually orthogonal projectors which are unique to high-dimensional quantum systems. We report two typical classes of dimension-dependent noncontextuality inequalities for one of which a violation implies the dimension of the quantum system is higher than a threshold, and for the other, different amounts of violations correspond to different thresholds of dimension. Our paper is expected to inspire more dimension-dependent noncontextuality inequalities.

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I. INTRODUCTION

Contextuality is a striking feature of quantum theory (QT) [1,2] and is being recognized as the crucial resource for various quantum information processes [3–7]. Since contextuality was originally proposed [8], physicists have spent decades to test it using fewer measurements and lower-dimensional system [1,2]. This goal was accomplished by a contextuality experiment using a three-dimensional system [9,10] and further investigated with two-level systems but in different scenarios [11–14]. In this paper, we investigate an interesting and seemingly opposite target that is to test contextuality using higher-dimensional systems. More precisely, we focus on the contextuality that can be tested only by the system with a dimension higher than a threshold, i.e., dimension-dependent contextuality.

An efficient method for testing contextuality in an experiment is testing noncontextuality (NC) inequalities [2]. In these contextuality experiments, a set of measurements are implemented in different contexts where a context is the joint measurement of a subset of measurements that are jointly measurable. After that, measurement statistics show contextuality by a violation of the NC inequality of which the bound is predicted by NC hidden variable (NCHV) theory.

The violations of NC inequalities always depend on the dimension of the quantum system [15–18]. For example, the Klyachko-Can-Binicioğlu-Shumovsky (KCBS) inequality [9] can only be violated by a system with dimension, at least, 3. Moreover, multipartite nonlocality inequalities [19] are NC inequalities that can be violated by a special high-dimensional system when considering locality as a special case of NC [20,21]. In 2014, Gühne *et al.,* showed that the NC inequality can be used to witness the lower bounds on the dimension of a quantum system accessed by the measurements [15].

To single out new NC inequalities, Cabello, Severini, and Winter (CSW) proposed a modern and elegant approach based on graph theory [22]. CSW approach associates an exclusive graph to a contextuality experiment and then addresses the issue of NC inequality using graph properties. Based on CSW approach, Ray *et al.,* developed the idea in Ref. [15] and presented a numerical method to calculate the maximum violation of NC inequality in a certain dimensional quantum system [18].

In this paper, we study the relation between the violation of NC inequality and the dimension of a quantum system. We consider a situation where the finite system dimensions impose additional restrictions on the relationship between measurements. As examples, we consider NC inequalities with large contexts by introducing a basic property of high-dimensional systems that is the existence of multiple mutually orthogonal states. Within those examples, we analyze two typical dimension-dependent classes of NC inequalities.

This paper is organized as follows. Section II introduces the CSW approach to contextuality. In Sec. III, we discuss the effect of dimension restriction on the violation of NC inequality. In Sec. IV, we analysis analyze some examples of dimension-dependent NC inequalities. All results are summarized and discussed in Sec. V.

II. CSW APPROACH TO NC INEQUALITY

In a contextuality experiment, measurements are ideal and each measurement M_j is compatible (jointly measurable) with some other measurements M_k, i.e., $p(a_j|M_j) = \sum_{a_k} p(a_j, a_k|M_j, M_k)$. As in Ref. [18], a measurement is ideal when it yields the same outcome when repeated on the same physical system and does not disturb any compatible

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observable. In this paper, we consider a special but widely considered case where each measurement has two outcomes $a_j \in \{0, 1\}$, and two events $e_j = (1|M_j)$ and $e_k = (1|M_k)$ of obtaining outcome 1 for two measurements M_j and M_k are exclusive if the two measurements are jointly measurable. In QT, such measurements can be realized as projective (sharp) measurements, $M_j = |\psi_j\rangle\langle\psi_j|$, and two measurements M_j and M_k are jointly measurable if and only if $\langle\psi_j \mid \psi_k\rangle = 0$. With these measurements, contextuality correlation is quantified as a positive linear combination of probabilities of events $e_j = (1|M_j)$,

$$S = \sum_j p(e_j),$$

where we consider weights of all events as 1 [22].

Given a set of events $\{e_j\}$ with certain exclusive relation, CSW associates an exclusivity graph G to these events [22]. In this graph G, each vertex $j \in V(G)$ represents the event e_j and two vertices are adjacent, $\{j, k\} \in E(G)$ if two corresponding events e_j and e_k are exclusive. The maximum value of S predicted by NCHV theory is the independence number $\alpha(G)$ of the graph [22], which gives the NC inequality as

$$S \overset{\text{NCHV}}{\leqslant} \alpha(G). \tag{1}$$

Here, the independence number $\alpha(G)$ is simply the maximum order of all sets of nonadjacent vertices of G.

In QT, the maximum value of S is exactly the Lovász theta of graph $\vartheta(G)$, $S \overset{\text{QT}}{\leqslant} \vartheta(G)$ [22,23]. The Lovász theta $\vartheta(G)$ can be exactly achieved by QT [18,22] implies that $\vartheta(G) = \max(S_Q)$ with $S_Q = \sum_{i\in V(G)} |\langle\phi \mid \psi_i\rangle|^2$, where the maximization is over all normalized pure states $|\phi\rangle$ and $|\psi_i\rangle$ and subject to the orthogonal restriction represented by G that $\langle\psi_j \mid \psi_k\rangle = 0$ for all $\{j, k\} \in E(G)$. Moreover, for arbitrary graph G, there is a sandwich relation [22] $\alpha(G) \leqslant \vartheta(G) \leqslant \alpha^*(G)$, where $\alpha^*(G)$ is the fractional packing number defined as $\alpha^*(G) = \max \sum_{i\in V(G)} p_i$ where the maximization subject to the restriction that sum of probabilities of events within arbitrary clique is no larger than 1.

Through the CSW approach, singling out a NC inequality is to construct a graph G that satisfies $\vartheta(G) > \alpha(G)$. Following Ref. [24], we call these graphs quantum contextual graphs (QCG).

It is not difficult to find a QCG [24,25]. For example, any graph with a noninteger Lovász theta is a QCG since the independence number is always an integer $\alpha(G) \leqslant \lfloor\vartheta(G)\rfloor$. What is difficult is to construct a QCG for specific demands, e.g., a graph with a large ratio of Lovász theta to independence number [26]. This difficulty is partially due to that the number of graphs grows exponentially with the order of graphs and computing the independence number of an arbitrary graph is nondeterministic polynomial (NP) complete.

III. DIMENSION-DEPENDENT NC INEQUALITY

During the calculation of Lovász theta, one does not impose any restriction to the dimension of states. When a dimensional restriction is imposed, the maximum value of S_Q might be less than $\vartheta(G)$. A simple example is that the maximum value of S_Q in the KCBS inequality is 2 with a two-dimensional system.

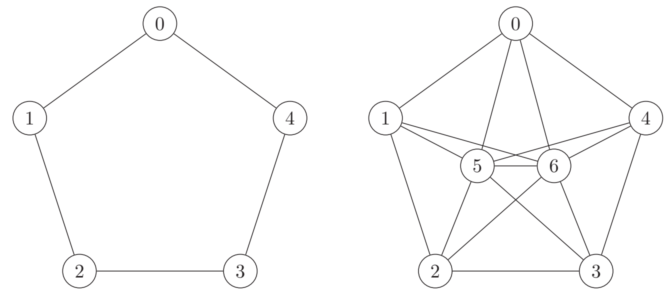

FIG. 1. Exclusive graph for the KCBS inequality C_5 (left) and the graph $K_2 \vee C_5$ (right).

It is defined as rank-constrained Lovász theta $\vartheta^d(G)$ that the maximum value of S_Q one can obtain from an experiment using d-dimensional quantum system [18]. For $d' > d$, the d-dimensional quantum system is a subsystem of the d'-dimensional one, so the rank-constrained Lovász theta satisfies $\vartheta^d(G) \leqslant \vartheta^{d'}(G) \leqslant \vartheta(G)$.

Given a graph G with the rank-constrained Lovász theta as $\vartheta^d(G) > \vartheta^{d-1}(G)$, the corresponding NC inequality is a dimension-dependent one. We call these graphs d-QCG. Given a graph that is d-QCG, once one obtains a value $S > \vartheta^{d-1}(G)$, the experimental system is contextual, and if the system is quantum its dimension is, at least, d (Noting that there are theories that are contextual but not quantum [27,28]). For example, C_5 is a d-QCG if and only if $d = 3$. Therefore, a dimension-dependent NC inequality simultaneously provides a contextuality sensor and a quantum dimension witness [18].

It is to be noted that when calculating rank-constrained Lovász theta, the states should not be restricted to nonzero ones. Otherwise, the NC inequality corresponding to the graph $K_n \vee C_5$, which is the join of graphs K_n and C_5, would be a trivial dimension-dependent one. For example, the graph $K_2 \vee C_5$ as shown in Fig. 1 has the same independence number and Lovász theta as these of C_5. If all states are required to be nonzero, a system that realizes these measurements has a dimension, at least, 4. However, using the same three-dimensional states $|\phi\rangle$ and $|\psi_i\rangle$ for $i \in [0\cdots4]$ as those for the maximum violation of KCBS inequality and choosing $|\psi_5\rangle = |\psi_6\rangle = 0$, the maximum violation is obtained. These zero states correspond to null measurements that extract no information from the system.

Given a set of d-dimensional quantum states $|\psi_i\rangle$ for $i \in V(G)$, with $\langle\psi_i \mid \psi_i\rangle = 0, 1$, we call it a *$d$-dimensional quantum representation* (d-DQR) of graph G if those states satisfy the orthogonal restriction $\langle\psi_i|\psi_j\rangle = 0$ for all adjacent vertices $\{i, j\} \in E(G)$.

With limited dimension, choosing a d-DQR of a graph might introduce additional restrictions to the states other than the orthogonal restriction by the graph. A typical situation is that some of the states must be chosen as zero ones. In this case, the nonzero states is a d-DQR of graph H, where H is a subgraph of G induced by the vertices that corresponding to nonzero states. Therefore, we have $S_Q \leqslant \vartheta^d(H)$. We call such a graph H as the *nonzero graph* of the d-DQR of G. Another situation is that some states corresponding to nonadjacent vertices being orthogonal. In this case, let us associate an *orthogonal graph* G_o to these states as each vertex represents a state and two vertices are adjacent if two corresponding states are orthogonal. Therefore, we have $V(G_o) = V(G)$ and $E(G) \subseteq E(G_o)$ due to these states are the d-DQR of graph G. Since these states are also a d-DQR of G_o, we have $S_Q \leqslant \vartheta^d(G_o)$. Therefore, we have the following theorem.

Theorem 1. Given a graph G, the rank-constrained Lovász theta satisfies that

$$\vartheta^d(G) \leqslant \max_H[\vartheta^d(H)] \leqslant \max_H[\vartheta(H)], \tag{2}$$

and

$$\vartheta^d(G) \leqslant \max_{G_o}[\vartheta^d(G_o)] \leqslant \max_{G_o}[\vartheta(G_o)],$$

where the maximization $\max_H$ is over all nonzero graphs of all d-DQR of G, and the maximization $\max_{G_o}$ is over all orthogonal graphs of d-DQR of G.

This theorem provides a way to estimate the upper bound of rank-constrained Lovász theta $\vartheta^d(G)$ through Lovász theta $\vartheta(H)$. Moreover, these graphs H and G_o have the following properties.

Lemma 1. (i) If G_o is a graph with $V(G_o) = V(G)$ and $E(G) \subseteq E(G_o)$, then $\vartheta^d(G_o) \leqslant \vartheta^d(G)$ and $\vartheta(G_o) \leqslant \vartheta(G)$. (ii) If H is an induced subgraph of G, then $\vartheta^d(H) \leqslant \vartheta^d(G)$ and $\vartheta(H) \leqslant \vartheta(G)$.

Proof. (i) Since states $E(G) \subseteq E(G_o)$, every state satisfies the orthogonal restriction of graph G_o must also satisfy the orthogonal restriction of graph G but not vice versa. Hence, $\vartheta^d(G_o) \leqslant \vartheta^d(G)$ and $\vartheta(G_o) \leqslant \vartheta(G)$.

(ii) For rank-constrained Lovász theta, suppose $\vartheta^d(H) = \sum_{i\in V(H)} |\langle\phi' \mid \psi_i'\rangle|^2$, where the d-dimensional states $|\phi'\rangle$ and $|\psi_i'\rangle$ are d-DQR of graph H. One can construct a set of states $|\psi_i''\rangle$ for $i \in V(G)$ as $|\psi_i''\rangle = |\psi_i'\rangle$ for $i \in V(H)$ and $|\psi_i''\rangle = 0$ for $i \notin V(H)$. These states $|\psi_i''\rangle$ are d-DQR of graph G. Therefore, the rank-constrained Lovász theta of G is $\vartheta^d(G) \geqslant \sum_{i\in V(G)} |\langle\phi' \mid \psi_i''\rangle|^2 = \sum_{i\in V(H)} |\langle\phi' \mid \psi_i'\rangle|^2 = \vartheta^d(H)$.

For the Lovász theta, the proof is similar, where the new states $|\psi''\rangle$ for $i \notin V(H)$ are chosen as $\langle\phi \mid \psi_i\rangle = 0$ and $\langle\psi_j \mid \psi_i\rangle = 0$ for all $j \in V(H)$. This choice is always possible because the dimension of state can be arbitrarily high. ■

For a special case that $\alpha(H) = \alpha(G)$, Lemma 1 implies that if the NC inequality corresponding to H can be violated by a d-dimensional system, then the NC inequality corresponding to G can also be violated by the system.

IV. EXAMPLES

A. Exclusive graphs with higher-order cliques

A critical feature of high-dimensional system is the existence of multiple mutually orthogonal states, which implies the existence of high-order sets of mutually exclusive events. The exclusive graph for a set of mutually exclusive events is a complete graph. Here, we consider dimension-dependent NC inequalities with exclusive graphs have subgraphs as high-order complete graphs, i.e., high-order cliques.

Let us consider a special set of graphs $\mathcal{G}_n^{c,s}$ of which each graph has n vertices, and each vertex is included by s maximum cliques of order c. For example, $C_5 \in \mathcal{G}_5^{2,2}$. It is easy to see that a graph $G \in \mathcal{G}_n^{c,s}$ has ns/c maximum cliques in total.

Theorem 2. Given a graph $G \in \mathcal{G}_n^{c,s}$, (i) $\alpha(G) \leqslant \lfloor n/c \rfloor$; (ii) $\alpha^*(G) = n/c$.

Proof. (i) Given an independent vertex set $I_v(G) \subseteq V(G)$ with elements that are mutually nonadjacent vertices, one can construct a corresponding maximum clique set $I_c(G) \subseteq C(G)$ with the elements are all the maximum cliques that include a vertex in $I_v(G)$. Since each vertex is shared by s maximum cliques, a vertex in $I_v(G)$ corresponds to s elements in $I_c(G)$. Moreover, two nonadjacent vertices cannot share any clique, so a set $I_v(G)$ of order $|I_v(G)|$ implies that the set $I_c(G)$ is on the order of $|I_c(G)| = s|I_v(G)|$. Since there are ns/c maximum cliques in total, the order of the independent set satisfies $|I_v(G)| = |I_c(G)|/s \leqslant (ns/c)/s = n/c$. Since $|I_v(G)|$ is an integer, the independence number $\alpha(G) = \max |I_v(G)| \leqslant \lfloor n/c \rfloor$.

(ii) Assuming sums of probabilities of events in all maximum cliques are 1. The sum of these probabilities of all maximum cliques is ns/c where the probabilities of each vertex is counted for s times. Hence, the fractional packing number is $\alpha^*(G) = n/c$. ■

Theorem 2 does not predict any QCG since the lack of the Lovász theta, which is usually calculated through semidefinite programming (SDP). Whereas, the fractional packing number provides an upper bound of the Lovász theta, $\vartheta(G) \leqslant \alpha^*(G)$. Thus, this excludes those graphs with $\alpha(G) = \alpha^*(G)$ as a QCG.

For concrete examples, let us consider a kind of circulant graphs Ci_n^c with $c \leqslant \lfloor n/2 \rfloor - 1$, which have n vertices in $[0 \cdots n-1]$ and each vertex i is adjacent to vertices $j = (i \pm l)$ for all $l \in [1 \cdots c-1]$. For the sake of simplicity, we omit the subscript of the module in the following.

It is easy to verify that $Ci_n^c \in \mathcal{G}_n^{c,c}$. Moreover, the independence number is $\lfloor n/c \rfloor$ since one can choose an independent set with vertices lc for $l \in [0 \cdots \lfloor n/c \rfloor - 1]$ and the upper bound in Theorem 2. According to Theorem 2, we have $\alpha^*(Ci_n^c) = n/c$. We have numerically calculated the Lovász theta of some of these graphs for $c \in [2 \cdots 6]$ except those with $(n/c) \notin \mathbb{Z}$. The numerical results are shown in Table I. Interestingly, all these graphs are QCGs.

We now discuss two typical classes of these graphs and analyze the relation between the violation of corresponding NC inequalities and the dimension of quantum systems.

B. Typical example 1: Ci_{2c+1}^c.

These graphs Ci_{2c+1}^c as shown in Fig. 2 have been well studied as QCGs [24]. The independence number is $\alpha(Ci_{2c+1}^c) = 2$. The Lovász theta is $\vartheta(Ci_{2c+1}^c) = \frac{1+\cos[\pi/(2c+1)]}{\cos[\pi/(2c+1)]}$, which can be obtained through the well-known Lovász theta of cyclic graphs C_{2c+1}, which are complementary graphs of Ci_{2c+1}^c [29], and a theorem of Lovász theta [23,24].

Let us consider the rank-constrained Lovász theta of graphs Ci_{2c+1}^c. A coarse result is that $\vartheta^{c-1}(Ci_{2c+1}^c) = 2$ according to Theorem 1. We are not going to prove this result because a tighter one was proved in Ref. [24] that is $\vartheta^{\lfloor (4c+2)/3 \rfloor - 1}(Ci_{2c+1}^c) = 2$. Here, we improve the result through a constructive manner.

Lemma 2. $\vartheta^{2c-2}(Ci_{2c+1}^c) = 2$.

Proof. Let d-dimensional quantum states $|\phi\rangle$ and $|\psi_i\rangle$ for $i \in [0 \cdots 2c]$ being a d-DQR of graph Ci_{2c+1}^c, so states $|\psi_{(i+l)}\rangle$ for $l \in [0 \cdots c-1]$ are mutually orthogonal.

TABLE I. The Lovász theta ϑ for graphs Ci_n^c. Here, the independence number is $\lfloor \vartheta \rfloor$.

$c=2$	n	5	7	9	11	13	15	17
	ϑ	2.2361	3.3177	4.3601	5.3863	6.4042	7.4171	8.4270
$c=3$	n	7	8	10	11	13	14	16
	ϑ	2.1099	2.3431	3.1672	3.4518	4.2011	4.5055	5.2235
$c=4$	n	9	10	11	13	14	15	17
	ϑ	2.0642	2.2361	2.4082	3.1060	3.3177	3.5294	4.1329
$c=5$	n	11	12	13	14	16	17	18
	ϑ	2.0422	2.1436	2.2877	2.4535	3.0744	3.2134	3.3867
$c=6$	n	13	14	15	16	17	19	20
	ϑ	2.0299	2.1099	2.2361	2.3431	2.4875	3.0556	3.1672

Let us first show the statement: (S1) if $S_Q > 2$, then $\langle \psi_i \mid \psi_{(i+c)} \rangle \neq 0$.

Suppose that $\langle \psi_i \mid \psi_{(i+c)} \rangle = 0$, we have $S_Q < \vartheta(G_o)$ with G_o a graph $V(G_o) = V(G)$ and $E(G_o) = E(G) \cup \{i, i+c\}$. The graph G_o can be separated into two cliques with vertices $\{(i+l) \colon l \in [0 \cdots c]\}$ and $\{(i+c+l') \colon l' \in [0 \cdots c-1]\}$, so $\vartheta(G_o) = 2$, which contradicts with that $S_Q > 2$. Hence, statement (S1) is true.

Statement (S1) can be rephrased as following: (S1$'$) If $S_Q > 2$, then $\langle \psi_i \mid \psi_{c+j} \rangle = 0$ if $j \neq i, i+1$, and $\langle \psi_i \mid \psi_{c+j} \rangle \neq 0$ if $j = i, i+1$, where $i, j \in [0 \cdots c-1]$. In the following, we show another statement: (S2) Given states ψ_i that satisfy the inner products as (S1$'$), one can always construct $(2c-1)$ mutually orthogonal states from linear combination of those states. When the statement (S2) is true, these state must have dimension no less then $(2c-1)$, which proves the lemma.

Since $\langle \psi_0 \mid \psi_c \rangle \neq 0$, we can denote state $|\psi_c\rangle$ as $|\psi_c\rangle = \beta_0 |\psi_0\rangle + \eta_0 |s_0\rangle$ with nonzero state $|s_0\rangle$ that satisfies $\langle \psi_0 \mid s_0 \rangle = 0$, where $\beta_0 \neq 0$. As the inner product $\langle \psi_{c+1} \mid \psi_c \rangle = \beta_0 \langle \psi_{c+1} \mid \psi_0 \rangle + \eta_0 \langle \psi_{c+1} \mid s_0 \rangle = 0$ and $\beta_0 \langle \psi_{c+1} \mid \psi_0 \rangle \neq 0$, we have $\eta_0 \neq 0$ and $\langle \psi_{c+1} \mid s_0 \rangle \neq 0$. Moreover, for $i \in [1 \cdots c-1]$, we have $\langle \psi_i \mid \psi_c \rangle = \eta_0 \langle \psi_i \mid s_0 \rangle = 0$. Noting that $\langle \psi_0 \mid s_0 \rangle = 0$, so $\langle \psi_i \mid s_0 \rangle = 0$ for $i \in [0 \cdots c-1]$.

The result that $\eta_0 \neq 0$ implies that we can obtain state $|s_0\rangle$ from linear combination (Gram-Schmidt orthonormalization) of $|\psi_0\rangle$ and $|\psi_c\rangle$. As $\langle \psi_i \mid s_0 \rangle = 0$ for $i \in [0 \cdots c-1]$, we obtain $(c+1)$ mutually orthogonal states that are $|\psi_i\rangle$ for $i \in [0 \cdots c-1]$ and $|s_0\rangle$. Therefore, statement (S2) is true for $c = 2$.

For $c \geqslant 3$, we have $\langle \psi_{c+k} \mid \psi_c \rangle = \eta_0 \langle \psi_{c+k} \mid s_0 \rangle = 0$ for $k \in [2 \cdots c-1]$. Since $\eta_0 \neq 0$, we have $\langle \psi_{c+k} \mid s_0 \rangle = 0$ for $k \in [2 \cdots c-1]$.

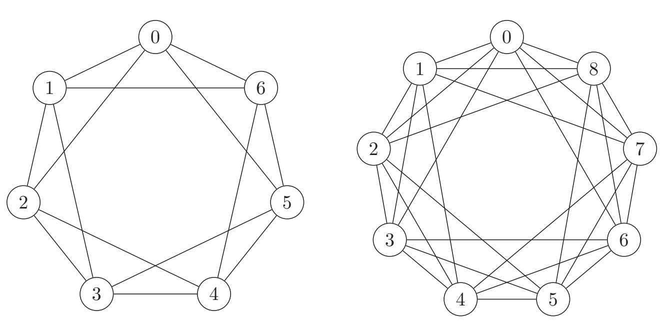

FIG. 2. Graphs Ci_{2c+1}^c with $c = 3$ (left) and $c = 4$ (right).

Since $\langle \psi_0 \mid \psi_{c+1} \rangle \neq 0$, $\langle \psi_1 \mid \psi_{c+1} \rangle \neq 0$, and $\langle s_0 | \psi_{c+1} \rangle \neq 0$, we can denote state $|\psi_{c+1}\rangle$ as $|\psi_{c+1}\rangle = \alpha_1 |\psi_0\rangle + \beta_1 |\psi_1\rangle + \gamma_1 |s_0\rangle + \eta_1 |s_1\rangle$ with a nonzero state $|s_1\rangle$ that satisfies $\langle \psi_0 \mid s_1 \rangle = \langle \psi_1 \mid s_1 \rangle = \langle s_0 \mid s_1 \rangle = 0$, where $\alpha_1, \beta_1, \gamma_1 \neq 0$. As $\langle \psi_{c+2} \mid \psi_{c+1} \rangle = \beta_1 \langle \psi_{c+2} \mid \psi_1 \rangle + \eta_1 \langle \psi_{c+2} \mid s_1 \rangle = 0$ and $\beta_1 \langle \psi_{c+2} \mid \psi_1 \rangle \neq 0$, we have $\eta_1 \neq 0$ and $\langle \psi_{c+2} \mid s_1 \rangle \neq 0$. For $i \in [2 \cdots c-1]$, we have $\langle \psi_i \mid \psi_{c+1} \rangle = \eta_1 \langle \psi_i \mid s_1 \rangle = 0$. Considering that $\langle \psi_0 \mid s_1 \rangle = \langle \psi_1 \mid s_1 \rangle = 0$, we have $\langle \psi_i \mid s_1 \rangle = 0$ for $i \in [0 \cdots c-1]$.

Since the results that $\langle s_0 \mid s_1 \rangle = 0$, $\eta_1 \neq 0$, and $\langle \psi_i | s_1 \rangle = 0$ for $i \in [0 \cdots c-1]$, we can obtain $(c+2)$ mutually orthogonal states that are $|\psi_i\rangle$ for $i \in [0 \cdots c-1]$, $|s_0\rangle$, and $|s_1\rangle$. Therefore, statement (S2) is true for $c = 3$.

For $c \geqslant 4$, we have $\langle \psi_{c+k} \mid \psi_{c+1} \rangle = \eta_1 \langle \psi_{c+k} \mid s_1 \rangle$ for $k \in [3 \cdots c-1]$. Since $\eta_1 \neq 0$, we have $\langle \psi_{c+k} \mid s_1 \rangle = 0$ for $k \in [3 \cdots c-1]$.

In the following, we show this statement: (S3) For all $j \in [1 \cdots c-2]$, states $|\psi_{c+j}\rangle$ can be denoted as $|\psi_{c+j}\rangle = \alpha_j |\psi_{j-1}\rangle + \beta_j |\psi_j\rangle + \gamma_j |s_{j-1}\rangle + \eta_j |s_j\rangle$ with $\alpha_j, \beta_j, \gamma_j, \eta_j \neq 0$, $\langle \psi_{j+1} \mid s_j \rangle \neq 0$, and $\langle \psi_i \mid s_j \rangle = \langle s_{j'} \mid s_j \rangle = 0$ for $i \in [0 \cdots c-1]$ and $j' \in [0 \cdots j-1]$; moreover, if $j \leqslant c-3$, then $\langle \psi_{c+k} \mid s_j \rangle = 0$, $k \in [j+2 \cdots c-1]$.

It has been shown that statement (S3) is true for $j = 1$. Assuming that (S3) is true for $m \in [0 \cdots c-3]$, we have $\langle \psi_c \mid \psi_{c+m+1} \rangle \neq 0$, $\langle \psi_{c+1} \mid \psi_{c+m+1} \rangle \neq 0$, and $\langle s_m \mid \psi_{c+m+1} \rangle \neq 0$. Therefore, we can denote state $|\psi_{c+m+1}\rangle$ as $|\psi_{c+m+1}\rangle = \alpha_{m+1} |\psi_m\rangle + \beta_{m+1} |\psi_{m+1}\rangle + \gamma_{m+1} |s_m\rangle + \eta_{m+1} |s_{m+1}\rangle$ with a nonzero state $|s_{m+1}\rangle$ that satisfies $\langle \psi_m \mid s_{m+1} \rangle = \langle \psi_{m+1} \mid s_{m+1} \rangle = \langle s_m \mid s_{m+1} \rangle = 0$, where $\alpha_{m+1}, \beta_{m+1}, \gamma_{m+1} \neq 0$. Due to $\langle \psi_{c+m+2} \mid \psi_{c+m+1} \rangle = \beta_{m+1} \langle \psi_{c+m+2} \mid \psi_{m+1} \rangle + \eta_{m+1} \langle \psi_{c+m+2} \mid s_{m+1} \rangle = 0$ and $\beta_{m+1} \langle \psi_{c+m+2} \mid \psi_{m+1} \rangle \neq 0$, we have $\eta_{m+1} \neq 0$ and $\langle \psi_{c+m+2} \mid s_{m+1} \rangle \neq 0$. For $i \in [0 \cdots c-1]$ and $i \neq m, m+1$, we have $\langle \psi_i \mid \psi_{c+m+1} \rangle = \eta_{m+1} \langle \psi_i \mid s_{m+1} \rangle = 0$. Considering that $\langle \psi_m \mid s_{m+1} \rangle = \langle \psi_{m+1} \mid s_{m+1} \rangle = 0$, we have $\langle \psi_i \mid s_{m+1} \rangle = 0$ for $i \in [0 \cdots c-1]$. For $j' \in [0, m-1]$, we have $\langle s_{j'} \mid \psi_{m+1} \rangle = \eta_{m+1} \langle s_{j'} \mid s_{m+1} \rangle = 0$. Considering that $\langle s_m \mid s_{m+1} \rangle = 0$, we have $\langle \psi_{j'} \mid s_{m+1} \rangle = 0$ for $j' \in [0 \cdots m]$. Moreover, if $m+1 \leqslant c-3$ since $\langle \psi_{c+k} \mid \psi_{c+m+1} \rangle = \eta_{m+1} \langle \psi_{c+k} \mid s_{m+1} \rangle$ for $k \in [m+2 \cdots c-1]$ and $\eta_{m+1} \neq 0$, we have $\langle \psi_{c+k} \mid s_{m+1} \rangle = 0$ for $k \in [m+2 \cdots c-1]$. Therefore, statement (S3) is true.

Since statement (S3) is true, one can obtain $(2c-1)$ mutually orthogonal states that are $|\psi_i\rangle$ for $i \in [0 \cdots c-1]$ and $|s_j\rangle$

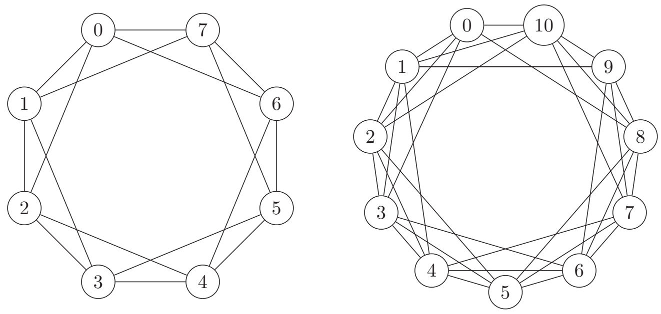

FIG. 3. Graphs Ci^c_{3c-1} with $c = 3$ (left) and $c = 4$ (right).

for $j \in [0 \cdots c-2]$. Therefore, statement (S2) is true, which proves the Lemma. ■

We have numerically calculated the rank-constrained Lovász theta $\vartheta^{2c-1}(Ci^c_{2c+1})$ for $c \in [2 \cdots 11]$. To calculate rank-constrained Lovász theta requires rank-constrained SDP, which is NP-hard problems. We adopt the heuristic approach proposed by Ray *et al.*, which iteratively solve two SDPs with one to satisfy all the Lovász theta SDP condition and the other restricts the rank of the solution [18]. The calculation shows that $\vartheta^{2c-1}(Ci^c_{2c+1}) = \vartheta(Ci^c_{2c+1})$ for $c \in [2 \cdots 11]$. The numerical results and Lemma 5 suggest the following result.

Result 1. For graphs Ci^c_{2c+1}, (i) Ci^c_{2c+1} is not a d-QCG for $d \leqslant 2c-2$; (ii) at least, for $c \in [2 \cdot\cdot 11]$, Ci^c_{2c+1} is a d-QCG if and only if $d = 2c-1$.

It remains an open question whether the statement (ii) of Result 1 is true for arbitrary large c. Numerically, when calculate $\vartheta^{21}(Ci^{11}_{23})$, the heuristic method successfully gives the valid result 12 times during 1000 iterations.

C. Special example 2: Ci^c_{3c-1}.

These graphs Ci^c_{3c-1} as shown in Fig. 3 have the same independence number 2 as that of graphs Ci^c_{2c+1}, but a larger fractional packing number $\alpha^*(Ci^c_{3c-1}) = 2 + (c-1)/c$ for $c \geqslant 3$, which, in principle, allows larger violations.

These graphs Ci^c_{3c-1} for $c \geqslant 2$ are QCG. This is because for $c \geqslant 2$, the graph $Ci^{(c-1)}_{3(c-1)-1}$ is an induced subgraph of Ci^c_{3c-1} by removing the vertices v_{c-1}, v_{2c-1}, and v_{3c-2}. Therefore, for $c < c'$, graph Ci^c_{3c-1} is an induced subgraph of $Ci^{c'}_{3c'-1}$. According to Lemma 1, graphs Ci^c_{3c-1} are QCG with maximum quantum values as $\vartheta(Ci^c_{2c+1}) \geqslant \vartheta(Ci^{c-1}_{2(c-1)+1})$ and $\vartheta(Ci^2_5) = \sqrt{5}$. Moreover, for arbitrary c and $c' \geqslant c$ if Ci^c_{3c-1} is violated with the d-dimensional system, $Ci^{c'}_{3c'-1}$ can also be violated by the d-dimensional system with an amount of violation no less than that of Ci^c_{3c-1}.

Let us consider the rank-constrained Lovász theta of graph Ci^3_8.

Lemma 3. For graph Ci^3_8, $\vartheta^3(Ci^3_8) = \vartheta^3(C_5)$, $\vartheta^4(Ci^3_8) \leqslant \vartheta^4(Ci^3_8 - v_j) \leqslant \vartheta(Ci^3_8 - v_j)$, where graph $Ci^3_8 - v_j$ is the induced subgraph of Ci^3_8 by removing a vertex v_j.

Proof. Given states $|\psi_i\rangle$ that are the d-DQR of graph Ci^3_8, let us consider the orthogonal graph G_o of these states in three cases.

(C1) Graph G_o has no induced subgraph as C_5. According to the necessary condition of QCG in Ref. [24], that if $\vartheta(G_o) > 2$ the graph G_o must have an induced subgraph cyclic graph with odd vertices, we have $\vartheta^2(Ci^3_8) = 2$. Therefore, according to Theorem 1, $\vartheta^d(G) = 2$ if these d-DQRs only allow the orthogonal graph as (C1).

(C2) G_o has an induced subgraph as C_5. In this case, it is well known that the dimension of state is, at least, 3. Considering the result of (C1), we have $\vartheta^2(G) = 2$.

(C3) G_o has an induced subgraph as C_5, and one of the states that corresponds to vertices not in the C_5 is nonzero. In the following, without loss of generality, let us denote the induced subgraph C_5 as the one that includes vertices $\{0, 1, 3, 4, 6\}$. If $|\psi_2\rangle$ is nonzero, states $|\psi_0\rangle$–$|\psi_2\rangle$ are mutually orthogonal. Therefore, state $|\psi_3\rangle = \alpha_3|\psi_0\rangle + \beta_3|x_3\rangle$ with $\langle\psi_0 \mid x_3\rangle = \langle\psi_1 \mid x_3\rangle = \langle\psi_2 \mid x_3\rangle = 0$ and $\beta_3 \neq 0$. Hence, the dimension of states is, at least, 4. For other cases $|\psi_5\rangle$ or $|\psi_7\rangle$ is nonzeros, the result is also true. Therefore, according to Theorem 1, we have $\vartheta^3(Ci^3_8) \leqslant \vartheta^3(C_5)$. Considering Lemma 1, which is $\vartheta^3(Ci^3_8) \geqslant \vartheta^3(C_5)$, we have $\vartheta^3(Ci^3_8) = \vartheta^3(C_5)$.

(C4) G_o has an induced subgraph as C_5 and all states are nonzero. Let us assume that the dimension of states is 4. One can denote state $|\psi_3\rangle = \alpha_3|\psi_0\rangle + \beta_3|x_3\rangle$ with nonzero α_3 and β_3. For $i \in [4 \cdots 7]$, we can denote $|x_i\rangle = \beta^*_{i-1}|\psi_{i-4}\rangle - \alpha^*_{i-1}|x_{i-1}\rangle$ and $|\psi_i\rangle = \alpha_i|\psi_{i-3}\rangle + \beta_i|x_i\rangle$. In this case, we have $\langle\psi_{i-j} \mid x_i\rangle = 0$ for $i \in [3 \cdots 7]$ and $j \in [1 \cdots 3]$. With this notation, let us consider three inner products $\langle\psi_0 \mid \psi_6\rangle = \alpha_6\langle 0 \mid \psi_3\rangle + \beta_6\langle 0 \mid x_5\rangle = 0$, $\langle\psi_1 \mid \psi_7\rangle = \alpha_7\langle 1 \mid \psi_4\rangle + \beta_7\langle 1 \mid x_6\rangle = 0$, and $\langle\psi_0 \mid \psi_7\rangle = \alpha_7\langle 0 \mid \psi_4\rangle + \beta_7\langle 0 \mid x_6\rangle = 0$. From the first two equalities, we got $\beta_6 = -\alpha_6\langle 0 \mid \psi_3\rangle/\langle 0 \mid x_5\rangle$ and $\beta_7 = -\alpha_7\langle 1 \mid \psi_4\rangle/\langle 1 \mid x_6\rangle$. Substituting those two into the third equality and evaluates the inner products finally gives $|\alpha_5|^2|\beta_3|^2 + |\alpha_3|^2 = 0$, which contradicts with that α_3 is nonzero. Therefore, such states must have dimension, at least, 5. In other words, a 4-DQR of graph Ci^3_8 must include, at least, one zero state. According to Theorem 1, we have $\vartheta^4(Ci^3_8) \leqslant \vartheta^4(Ci^3_8 - v_j) \leqslant \vartheta(Ci^3_8 - v_j)$. ■

Through numerical calculation, we have $\vartheta(Ci^3_8 - v_j) = 2.2361 \approx \sqrt{5}$ and $\vartheta^5(Ci^3_8) = 2.3431 = \vartheta(Ci^3_8)$. Therefore, according to Theorem 3, we have the following result.

Result 2. For $c = 3$, graph Ci^c_{3c-1} is d-QCG if and only if $d = 3, 5$.

For large c, it is interesting to investigate whether Result 2 can be generalized as that graph Ci^c_{3c-1} is d-QCG if and only if $d = 2e-1$ with $e \in [2 \cdots c]$. We have numerically calculated the rank-constrained Lovász theta for $c = [2 \cdots 11]$. The numerical results show $\vartheta^{2c}(Ci^{c'}_{3c'-1}) = \vartheta^{2c-1}(Ci^{c'}_{3c'-1}) = \vartheta(Ci^c_{3c-1})$ for $c' \geqslant c$, which support this conjecture.

V. CONCLUSION AND DISCUSSION

To summarize, we study the relation between the violation of the noncontextuality inequality and the dimension of quantum systems. We evaluate the upper bound of rank-constrained Lovász theta ϑ^d of a graph through the Lovász theta of graphs corresponding to d-DQR of that graph. As examples, we consider two typical kinds of NC inequalities, for one of which, the violation provides a witness of a dimension, for the other one, different amounts of violations provide witnesses of different dimensions. Our paper fulfills the knowledge about quantum contextuality, and the method might inspire further investigations of the dimension dependence of NC inequalities.

In order to produce better witness of dimension d, graphs that are d-QCG should have the properties with larger ratio $\vartheta^d/\vartheta^{d-1}$. A limitation of our examples is that such ratio is small, especially for large d. This limitation also exists for the graphs in Ref. [18]. We expect that better graphs might be singled out within future NC inequalities with larger violations [18,26,30].

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