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Letter

Characterizing high-dimensional quantum contextuality

Xiao-Dong Yu [1,*] Isadora Veeren,[2,3,†] and Otfried Gühne [2,‡]

[1] *Department of Physics, Shandong University, Jinan 250100, China*

[2] *Naturwissenschaftlich-Technische Fakultät, Universität Siegen, Walter-Flex-Str. 3, D-57068 Siegen, Germany*

[3] *Centro Brasileiro de Pesquisas Físicas (CBPF), Rua Doutor Xavier Sigaud 150, 22290-180 Rio de Janeiro, Brazil*

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As a phenomenon encompassing measurement incompatibility and Bell nonlocality, quantum contextuality is not only central to our understanding of quantum mechanics, but also an essential resource in many quantum information processing tasks. The dimension-dependent feature of quantum contextuality is known ever since its discovery, but there is still a lack of systematic methods for characterizing this fundamental feature. In this work, we propose a systematic and reliable method for certifying the high-dimensional advantages of quantum contextuality. In theory, our work gives a complete characterization of the dimension-constrained quantum contextual behavior, and particularly its nonconvex structure is revealed. In application, our method can be used for dimensionality certification of quantum information processing systems, and also for concentrating the quantum contextual behavior into lower-dimensional systems.

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Introduction. Qubits are the basic building blocks in many quantum information processing protocols. However, treating a real quantum system as a qubit is not only unnecessary, but also merely an approximation in practice. In recent years, experimental progress enabled the control of high-dimensional quantum systems and theoretical works demonstrated potential advantages of information processing in the high-dimensional case [1,2]. Consequently, many efficient methods have been developed to certify the high-dimensional advantages of various quantum resources, such as quantum entanglement [3], quantum coherence [4], and Bell nonlocality [5].

As a phenomenon encompassing measurement incompatibility and Bell nonlocality, quantum contextuality is not only central to our understanding of quantum mechanics [6–8], but also an essential resource in many quantum information processing tasks, such as in quantum computation [9–11], in quantum cryptography [12,13], and in random number generation [14–16]. The study of quantum contextuality originates from the work of Kochen and Specker, which is now referred to as the Kochen-Specker theorem [6]. The modern theory-independent framework for quantum contextuality was proposed by Klyachko *et al.* [17] and further developed to the state-independent scenario by Cabello *et al.* [18–20]. In these works, noncontextuality inequalities are discovered. These inequalities are obeyed by noncontextual hidden variable (NCHV) models, but can be violated by quantum mechanics. This experimentally testable framework greatly promotes both the theoretical and experimental study of quantum contextuality.

Ever since the discovery of quantum contextuality, people have noticed its dimension-dependent feature. For example, both Kochen and Specker [6] and Bell [21] proved that quantum contextuality does not exist in two-dimensional quantum systems. Also, every proof of the Kochen-Specker theorem, or more generally, every state-independent proof of quantum contextuality, is dimension dependent [22,23]. For some noncontextuality inequalities, it was discussed in detail how the largest quantum violation depends on the dimensionality of the quantum system [24]. Recently, Ray *et al.* investigated the problem of calculating finite-dimensional lower bounds of a family of noncontextuality inequalities [25].

Despite all these efforts, there is still a lack of systematic methods for certifying the high-dimensional advantages of quantum contextuality. On one hand, systematic methods to calculate the d-dimensional violation of general noncontextuality inequalities are still missing. On the other hand, it is not known whether using linear inequalities gives a complete characterization of dimension-constrained quantum contextual behavior.

In this work, we solve both of these problems. We first propose an efficient and reliable method for certifying whether or not a quantum contextual behavior can result from a d-dimensional quantum system. This provides a complete characterization of dimension-constrained quantum contextual behaviors. In particular, we prove that not all dimension-constrained quantum contextual behaviors can be characterized by the linear inequality method, which reveals a significant difference between quantum contextual behaviors with and without dimension constraints. Then, we show that the proposed method can also be adapted for calculating d-dimensional violation of general noncontextuality inequalities. Finally, we discuss the implications of our results for certifying the dimensionality of quantum information

*yuxiaodong@sdu.edu.cn
†veeren@cbpf.br
‡otfried.guehne@uni-siegen.de

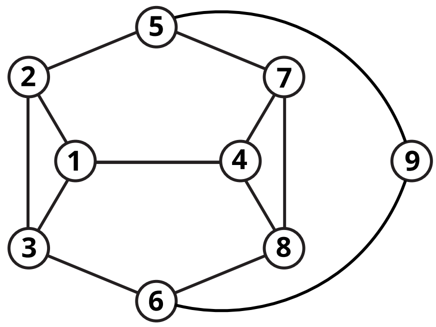

FIG. 1. The nine-vertex graph G_{KK}. In quantum theory, every vertex represents a projector P_i, and two projectors P_i and P_j are connected by an edge when $P_iP_j = 0$, which means that they are exclusive events. The independence number of G_{KK} is $\alpha(G_{\mathrm{KK}}) = 3$, which can be achieved when b_1, b_6, b_7 in Eq. (1) take the value 1. The Lovász number of G_{KK} is $\vartheta(G_{\mathrm{KK}}) = 4.4704$, which can be achieved in a four-dimensional quantum system.

processing systems and concentrating the quantum contextuality into lower-dimensional systems.

Preliminaries. In quantum contextuality theory, a measurement context $\{s_1, s_2, \ldots, s_\alpha\}$ is a set of compatible measurements, which are jointly measurable. An event $e = (o_1, o_2, \ldots, o_\alpha \mid s_1, s_2, \ldots, s_\alpha)$ means in a joint measurement $\{s_1, s_2, \ldots, s_\alpha\}$ the outcome of s_i is o_i for $i = 1, 2, \ldots, \alpha$. Two events $(o_1, o_2, \ldots, o_\alpha \mid s_1, s_2, \ldots, s_\alpha)$ and $(o'_1, o'_2, \ldots, o'_\beta \mid s'_1, s'_2, \ldots, s'_\beta)$ are called exclusive if there exist a, b such that $s_a = s'_b$ but $o_a \neq o'_b$. The events and their exclusive relation can be depicted by a graph, which is called the exclusivity graph. Mathematically, a graph G is denoted by (V, E), where V is the set of vertices and E is the set of edges, i.e., unordered pairs $\{i, j\}$ for some $i, j \in V$ and $i \neq j$. In the exclusivity graph, the vertices represent the set of events $\{e_1, e_2, \ldots, e_n\}$ and edges connect pairs of exclusive events; see Fig. 1 for an example graph G_{KK} and its connection to quantum contextuality. Notably, G_{KK} can be viewed as a variant of the "bug" graph from the original Kochen-Specker argument [6] and has been used for revealing quantum contextuality of almost all qutrit states [26].

In Ref. [27], an important connection between the graph theory and quantum contextuality was discovered. Consider the sum of probabilities $\sum_{i=1}^{n} p(e_i)$, where $p(e_i)$ are the probabilities of the corresponding events. In an NCHV model, determinism and exclusivity imply that this sum is upper bounded by

$$\begin{aligned} \alpha(G) := \max_{b_i} \quad & \sum_{i=1}^{n} b_i, \\ \text{s.t.} \quad & b_i = 0 \text{ or } 1, \\ & b_i b_j = 0 \ \text{ for } \{i, j\} \in E. \end{aligned} \tag{1}$$

Here, $\alpha(G)$ is the so-called independence number of graph G, which corresponds to the maximum number of mutually unconnected vertices in G. In quantum theory, the events e_i are represented by projectors P_i and two events are exclusive if they are orthogonal, i.e., $P_iP_j = 0$. Without loss of generality, we can always assume that the state is pure and P_i are rank one for studying noncontextuality inequalities [8]. Thus, the quantum bound of $\sum_{i=1}^{n} p(e_i) = \sum_{i=1}^{n} \mathrm{Tr}(\rho P_i)$ is given by

$$\begin{aligned} \vartheta(G) := \max_{|\varphi\rangle, |\psi_i\rangle} \quad & \sum_{i=1}^{n} |\langle\varphi|\psi_i\rangle|^2, \\ \text{s.t.} \quad & \langle\psi_i|\psi_j\rangle = 0 \ \text{ for } \{i, j\} \in E. \end{aligned} \tag{2}$$

$\vartheta(G)$ equals to the so-called Lovász number of graph G [28]. Here and in the following, we assume that $|\varphi\rangle$ and $|\psi_i\rangle$ are always normalized unless otherwise stated. We call the vectors $(|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle)$ satisfying the constraints in Eq. (2) a (rank-one) projective representation of G [29]. One can easily see from the definition that $\alpha(G) \leqslant \vartheta(G)$. If $\alpha(G)$ is strictly smaller than $\vartheta(G)$, it implies that there is a gap between the classical (NCHV) bound and the maximally achievable quantum value. Consequently, noncontextuality inequalities can be constructed [30,31]. More generally, the set of all realizable probabilities in quantum theory

$$\begin{aligned} \mathcal{Q}(G) = \{&(p_1, p_2, \ldots, p_n) \mid p_i = |\langle\varphi|\psi_i\rangle|^2, \\ &\langle\psi_i|\psi_j\rangle = 0 \ \text{ for } \{i, j\} \in E\} \end{aligned} \tag{3}$$

corresponds to the so-called theta body of graph G [32]. If $(p_1, p_2, \ldots, p_n) \in \mathcal{Q}(G)$, it is then called a quantum contextual behavior or simply a quantum behavior.

The quantum bound $\vartheta(G)$ and the quantum behaviors $\mathcal{Q}(G)$ reveal a characteristic feature of quantum mechanics, namely, quantum contextuality. However, this feature depends on the dimension of the quantum system. For example, quantum contextuality does not exist in two-dimensional systems, and the maximization in Eq. (2) also depends on the dimension of the quantum system. In this work, we give a systematic study on the dimension-dependent nature of quantum contextuality, and complete methods for characterizing the set of d-dimensional quantum behaviors

$$\begin{aligned} \mathcal{Q}_d(G) = \{&(p_1, p_2, \ldots, p_n) \mid |\varphi\rangle, |\psi_i\rangle \in \mathbb{C}^d, \\ &p_i = |\langle\varphi|\psi_i\rangle|^2, \ \langle\psi_i|\psi_j\rangle = 0 \ \text{ for } \{i, j\} \in E\} \end{aligned} \tag{4}$$

are proposed.

Finite-dimensional quantum contextuality. We start with developing a method for verifying whether a behavior $\boldsymbol{p} = (p_1, p_2, \ldots, p_n)$ can result from a d-dimensional quantum system. Remarkably, there are two different kinds of verification. Verifying that $\boldsymbol{p} \notin \mathcal{Q}_d(G)$ [$\boldsymbol{p} \in \mathcal{Q}_d(G)$] is an outer (inner) approximation problem, which means an affirmative conclusion would imply that $\boldsymbol{p} \notin \mathcal{Q}_d(G)$ [$\boldsymbol{p} \in \mathcal{Q}_d(G)$], otherwise the verification is inconclusive. In this work we will consider both cases. The starting point is the following observation.

Observation 1. The probabilities $(p_1, p_2, \ldots, p_n)$ are a d-dimensional quantum behavior, i.e., $(p_1, p_2, \ldots, p_n) \in \mathcal{Q}_d(G)$, if and only if there exists a Hermitian matrix $[X_{ij}]_{i,j=0}^{n}$ satisfying that

$$X_{0i} = X_{i0} = \sqrt{p_i} \quad \text{for } i = 1, 2, \ldots, n, \tag{5a}$$

$$X_{ii} = 1 \quad \text{for } i = 0, 1, 2, \ldots, n, \tag{5b}$$

$$X_{ij} = 0 \quad \text{for } \{i, j\} \in E, \tag{5c}$$

$$X \geqslant 0, \ \mathrm{rank}(X) \leqslant d. \tag{5d}$$

The main idea for proving Observation 1 is that the dimension of the vector space generated by $\{|v_i\rangle\}_{i=0}^n$ equals to the rank of the corresponding Gram matrix $[\langle v_i|v_j\rangle]_{i,j=0}^n$; for the detailed proof, please see Appendix A in the Supplemental Material (SM) [33].

With Observation 1, we can construct a convex program which is necessary and sufficient for $(p_1, p_2, \dots, p_n)$ being a d-dimensional quantum behavior. Suppose that $X \in \mathbb{C}^{(n+1)\times(n+1)}$ satisfies the constraints (5a)–(5d). As $X \geqslant 0$ and $\mathrm{rank}(X) \leqslant d$, one can construct a purification of X with a d-dimensional auxiliary system, i.e., there exists an unnormalized pure state $|\chi\rangle \in \mathbb{C}^{n+1} \otimes \mathbb{C}^d$, such that

$$\mathrm{Tr}_2(|\chi\rangle\langle\chi|) = X, \tag{6}$$

where $\mathrm{Tr}_2(\cdot)$ is the partial trace operation on the second subsystem $\mathbb{C}^d$. Following the ideas in Refs. [34,35], we consider the two-copy extension

$$\Phi_{AB} = |\chi\rangle\langle\chi|_A \otimes |\chi\rangle\langle\chi|_B, \tag{7}$$

then Φ_{AB} is an unnormalized state in $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^{n+1} \otimes \mathbb{C}^d$. Moreover, Φ_{AB} is in the symmetric subspace

$$V_{AB}\Phi_{AB} = \Phi_{AB}, \tag{8}$$

where the swap operator V_{AB} is defined to satisfy that $V_{AB}|\chi\rangle_A|\xi\rangle_B = |\xi\rangle_A|\chi\rangle_B$ for any pair of states $|\chi\rangle$ and $|\xi\rangle$. By imposing the other constraints in Eqs. (5a)–(5c), one can easily see that if $(p_1, p_2, \dots, p_n) \in \mathcal{Q}_d(G)$, the following convex program is feasible:

$$\begin{aligned} \text{find} \quad & \Phi_{AB} \in \mathrm{SEP} \\ \text{s.t.} \quad & V_{AB}\Phi_{AB} = \Phi_{AB},\ \mathrm{Tr}(\Phi_{AB}) = (n+1)^2, \\ & \mathrm{Tr}_A[(|i\rangle\langle j| \otimes \mathbb{1}_d \otimes \mathbb{1}_B)\Phi_{AB}] = \frac{\mu_{ij}}{n+1}\mathrm{Tr}_A[\Phi_{AB}], \end{aligned} \tag{9}$$

where μ_{ij} denote all the known elements of X_{ij}, i.e., $\mu_{0i} = \mu_{i0} = \sqrt{p_i}$ for $i = 1, 2, \dots, n$, $\mu_{ii} = 1$ for $i = 0, 1, 2, \dots, n$, and $\mu_{ij} = 0$ for $\{i, j\} \in E$, and SEP denotes the set of unnormalized separable states. Moreover, this convex program is also sufficient for $(p_1, p_2, \dots, p_n) \in \mathcal{Q}_d(G)$ [35]. From Eq. (9), a complete hierarchy of semidefinite programs (SDPs) can be constructed for outer approximating $\mathcal{Q}_d(G)$, and the lowest order is replacing $\Phi_{AB} \in \mathrm{SEP}$ with $\Phi_{AB} \in \mathrm{PPT}$. If any of these SDPs is infeasible, it will imply that $(p_1, p_2, \dots, p_n) \notin \mathcal{Q}_d(G)$.

For the inner approximation, i.e., verifying $(p_1, p_2, \dots, p_n) \in \mathcal{Q}_d(G)$, we note that Observation 1 can be viewed as a semidefinite variant of the so-called low-rank matrix recovery, which is a rapidly developing field in computer science [36]. For our problem, the matrix size is relatively small and thus efficient methods can be constructed. The main idea of our method is illustrated in Fig. 2. Let $\mathcal{S}$ and $\mathcal{R}_d^+$ denote the set of Hermitian matrices satisfying Eqs. (5a)–(5c) and satisfying Eq. (5d), respectively, then there exists $(p_1, p_2, \dots, p_n) \in \mathcal{Q}_d(G)$ if and only if the solution of the following optimization problem is zero:

$$\begin{aligned} \min_{X,Y} \quad & \|X - Y\|_F \\ \text{s.t.} \quad & X \in \mathcal{S},\ Y \in \mathcal{R}_d^+, \end{aligned} \tag{10}$$

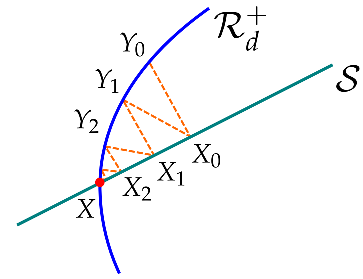

FIG. 2. Illustration of the inner approximation method. The problem is equivalent to finding $X \in \mathcal{S} \cap \mathcal{R}_d^+$, for which we minimize the distance between points in $\mathcal{S}$ and $\mathcal{R}_d^+$. We first randomly choose a point $Y_0 \in \mathcal{R}_d^+$ and find $X_0 \in \mathcal{S}$ that minimizes the distance between Y_0 and $\mathcal{S}$, i.e., $X_0 = \arg\min_{X\in\mathcal{S}} \|X - Y_0\|_F$. Similarly, with X_0 we can then find $Y_1 = \arg\min_{Y\in\mathcal{R}_d^+} \|X_0 - Y\|_F$. Repeating the above procedure, i.e., $X_i = \arg\min_{X\in\mathcal{S}} \|X - Y_i\|_F$ and $Y_{i+1} = \arg\min_{Y\in\mathcal{R}_d^+} \|X_i - Y\|_F$, we get a converging sequence $\|X_i - Y_i\|_F$. If the limit is zero, we obtain the desired $X \in \mathcal{S} \cap \mathcal{R}_d^+$ and Observation 1 implies that the corresponding $(p_1, p_2, \dots, p_n) \in \mathcal{Q}_d(G)$.

where $\|\cdot\|_F$ denotes the Frobenius norm. From Eq. (10) an alternating optimization algorithm for verifying $(p_1, p_2, \dots, p_n) \in \mathcal{Q}_d(G)$ can be constructed. More technical details of the inner and outer approximation algorithms can be found in Appendixes B and C in the (SM) [33].

To illustrate the power of our methods, we consider the nine-vertex graph G_{KK} in Fig. 1 and the behaviors

$$\boldsymbol{p}_1 = \left(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}\right), \tag{11a}$$

$$\boldsymbol{p}_2 = \left(\tfrac{1}{2}, \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, 0, 0, \tfrac{1}{4}, \tfrac{1}{4}, 1\right), \tag{11b}$$

$$\boldsymbol{p}_3 = \left(\tfrac{5}{12}, \tfrac{7}{24}, \tfrac{7}{24}, \tfrac{5}{12}, \tfrac{1}{6}, \tfrac{1}{6}, \tfrac{7}{24}, \tfrac{7}{24}, \tfrac{2}{3}\right). \tag{11c}$$

One can prove that $\boldsymbol{p}_1, \boldsymbol{p}_2 \in \mathcal{Q}_d(G_{\mathrm{KK}})$ with the inner approximation methods, and $\boldsymbol{p}_3 \notin \mathcal{Q}_d(G_{\mathrm{KK}})$ with the outer approximation method. Note also that $\boldsymbol{p}_3$ is a mixture of $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$, i.e., $\boldsymbol{p}_3 = (\boldsymbol{p}_1 + \boldsymbol{p}_2)/2$. This reveals a remarkable difference between the quantum behaviors with and without dimension constraints: the set of general quantum behaviors $\mathcal{Q}(G)$ is convex but the d-dimensional counterpart $\mathcal{Q}_d(G)$ may not be. Similar nonconvexity results also exist for other quantum resources; see Refs. [37–40] for some examples and their applications. Another remarkable property is that although the quantum bound $\vartheta(G_{\mathrm{KK}})$ can already be achieved when $d = 4$, there exist quantum behaviors not in $\mathcal{Q}_4(G_{\mathrm{KK}})$. One such example is

$$\boldsymbol{p}_4 = \left(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, 0, \tfrac{2}{3}, \tfrac{1}{3}, 0, 0, \tfrac{1}{3}\right). \tag{12}$$

Inequality method. The standard method for characterizing quantum contextuality without dimension constraints relies on noncontextuality inequalities. These are linear inequalities closely related to the so-called weighted Lovász number [27]. Similarly, one can also characterize the d-dimensional quantum contextuality with the following quantity, which can be viewed as the d-dimensional weighted Lovász number:

$$\begin{aligned} \vartheta_d(G, \boldsymbol{w}) := \max_{\boldsymbol{p}} \quad & \boldsymbol{w} \cdot \boldsymbol{p} \\ \text{s.t.} \quad & \boldsymbol{p} \in \mathcal{Q}_d(G), \end{aligned} \tag{13}$$

where the weights $\boldsymbol{w} = (w_1, w_2, \dots, w_n) \in \mathbb{R}^n$ and $\boldsymbol{w} \cdot \boldsymbol{p} = \sum_{i=1}^n w_i p_i$. Unlike $\mathcal{Q}(G)$, this inequality method is no longer sufficient for characterizing $\mathcal{Q}_d(G)$ because of the nonconvexity property proved above. Furthermore, contrary to $\mathcal{Q}(G)$ [23], there are no longer reasons to assume that all w_i are nonnegative for characterizing $\mathcal{Q}_d(G)$. What Eq. (13) characterizes is actually the convex hull of $\mathcal{Q}_d(G)$ and thus the inequality method is less general than the direct method given above. Nevertheless, an inequality is sometimes more suitable for experimental tests. In the following, we show that our method can also be adapted for calculating the bound in Eq. (13).

By taking advantage of Observation 1, we get the following equivalent form of $\vartheta_d(G, \boldsymbol{w})$:

$$\begin{aligned} \max_X \quad & \sum_{i=1}^n w_i |X_{0i}|^2 \\ \text{s.t.} \quad & X_{ii} = 1 \quad \text{for } i = 0, 1, 2, \dots, n, \\ & X_{ij} = 0 \quad \text{for } \{i, j\} \in E, \\ & X \geqslant 0,\ \operatorname{rank}(X) \leqslant d. \end{aligned} \tag{14}$$

Similarly, this rank-constrained optimization can be transformed to the convex optimization [35]

$$\begin{aligned} \max_{\Phi_{AB}} \quad & \operatorname{Tr}[W_{AB}\Phi_{AB}] \\ \text{s.t.} \quad & \Phi_{AB} \in \text{SEP},\ V_{AB}\Phi_{AB} = \Phi_{AB},\ \operatorname{Tr}(\Phi_{AB}) = (n+1)^2, \\ & \operatorname{Tr}_A[(|i\rangle\langle j| \otimes \mathbb{1}_d \otimes \mathbb{1}_B)\Phi_{AB}] = 0 \ \text{for } \{i, j\} \in E, \\ & \operatorname{Tr}_A[(|i\rangle\langle i| \otimes \mathbb{1}_d \otimes \mathbb{1}_B)\Phi_{AB}] = \frac{1}{n+1}\operatorname{Tr}_A[\Phi_{AB}] \\ & \text{for } i = 0, 1, \dots, n, \end{aligned} \tag{15}$$

where $W_{AB} = \frac{1}{2}(\sum_{i=1}^n w_i |0\rangle\langle i| \otimes \mathbb{1}_d \otimes |i\rangle\langle 0| \otimes \mathbb{1}_d + \text{H.c.})$, and H.c. denotes the Hermitian conjugate of the previous term.

From Eq. (15) a complete SDP hierarchy can be constructed for upper bounding $\vartheta_d(G, \boldsymbol{w})$, but the low-order relaxations may not give good enough bounds. Thus, we provide another method, which is not always complete but may result in better bounds when low-order relaxations are considered. Consider the Gram matrix of $(|\varphi\rangle, c_1|\psi_1\rangle, c_2|\psi_2\rangle, \dots, c_n|\psi_n\rangle)$, where $c_i = \langle\psi_i|\varphi\rangle$. Similarly to Observation 1, one can prove that $\vartheta_d(G, \boldsymbol{w})$ is upper bounded by the optimization

$$\begin{aligned} \max_X \quad & \sum_{i=1}^n w_i X_{ii} \\ \text{s.t.} \quad & X_{ii} = X_{0i} = X_{i0} \quad \text{for } i = 1, 2, \dots, n, \\ & X_{ij} = 0 \quad \text{for } \{i, j\} \in E, \\ & X_{00} = 1,\ X \geqslant 0,\ \operatorname{rank}(X) \leqslant d, \end{aligned} \tag{16}$$

where the constraints $X_{ii} = X_{0i} = X_{i0}$ result from the conditions that $\langle\varphi|c_i|\psi_i\rangle = \langle\psi_i|c_i^* c_i|\psi_i\rangle = |\langle\psi_i|\varphi\rangle|^2$. Let $\tilde{\vartheta}_d(G, \boldsymbol{w})$ denote the solution of Eq. (16), then one can easily see that $\vartheta_d(G, \boldsymbol{w}) \leqslant \tilde{\vartheta}_d(G, \boldsymbol{w})$. In Ref. [25], it was claimed that $\tilde{\vartheta}_d(G, \boldsymbol{w}) = \vartheta_d(G, \boldsymbol{w})$ when $\mathcal{Q}_d(G)$ is not empty. This is, however, not true. An explicit counterexample is shown below.

From Eqs. (14) and (16), efficient inner and outer approximation methods can be similarly constructed for lower and upper bounding $\vartheta_d(G, \boldsymbol{w})$ and $\tilde{\vartheta}_d(G, \boldsymbol{w})$. As an example, we still consider graph G_{KK} in Fig. 1 and the case that $\boldsymbol{w} = (1, 1, \dots, 1)$, for which $\vartheta_d(G, \boldsymbol{w})$ and $\tilde{\vartheta}_d(G, \boldsymbol{w})$ are denoted by $\vartheta_d(G)$ and $\tilde{\vartheta}_d(G)$, respectively. One can prove that $\vartheta_3(G_{\text{KK}}) = 3.3333$ by showing that 3.3333 is also both a lower bound and an upper bound (up to numerical precision). In addition, graph G_{KK} also provides an explicit example of $\tilde{\vartheta}_d(G) \neq \vartheta_d(G)$. This can be proved by constructing a matrix X satisfying all the constraints in Eq. (16) and $\sum_{i=1}^n X_{ii} = 3.3380$, which then implies that $\tilde{\vartheta}_3(G_{\text{KK}}) \geqslant 3.3380 > \vartheta_3(G_{\text{KK}}) = 3.3333$. See Appendixes D and E for the technical details of the lower and upper bounding algorithms in the (SM) [33].

Discussion and conclusion. Given the extensive theoretical and experimental studies on the high-dimensional advantages of quantum resources in recent years [41–48], our method can be used in various ways. First, our results provide a different approach for constructing so-called dimension witnesses [37,49–54]. These are linear or nonlinear inequalities, which can be used to certify the experimenter's coherent control on a certain amount of levels in quantum information processing. With our outer approximation method, a violation of the inequality $\sum_i w_i p_i \geqslant \vartheta_d(G, \boldsymbol{w})$ can be rigorously proved, which would in turn certify that the amount of controllable levels is larger than d. Second, we consider the so-called contextuality contraction, which aims to achieve the same degree of contextuality with a lower-dimensional system and thus make the utilization of quantum contextuality more experimentally accessible [55]. One can easily see that our inner approximation method can be directly used for reducing the dimension and our outer approximation method can be used for calculating the limit of contextuality contraction. Finally, on a more abstract level, our results may elucidate the role of the quantum dimension in information processing. The original definition of the Lovász number was motivated by notions of communication capacity, and for contextuality, connections to communication tasks have been established [56,57]. Combining these concepts may lead to a deeper understanding of high-dimensional quantum information processing, as well as novel applications.

In conclusion, we have provided powerful methods to characterize quantum contextual behavior under dimension constraints. Our method gives a complete characterization of dimension-constrained quantum contextual behaviors, and particularly we show that not all quantum contextual behaviors can be characterized by the linear inequality method. As applications, our method can be used for dimensionality certification of quantum information processing systems, and also for concentrating the quantum contextuality behavior into lower-dimensional systems.

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