Quantum contextuality of a qutrit state

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Quantum contextuality of a qutrit state

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We present a study of quantum contextuality of three-dimensional mixed states for the Klyachko-Can-Binicioğlu-Shumovsky (KCBS) and the Kurzyński-Kaszlikowski (KK) noncontextuality inequalities. For any class of states whose eigenvalues are arranged in decreasing order, a universal set of measurements always exists for the KK inequality, whereas none does for the KCBS inequality. This difference can be reflected from the spectral distribution of the overall measurement matrix. Our results would facilitate the error analysis for experimental setups, and our spectral method in the paper combined with graph theory could be useful in future studies on quantum contextuality.

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I. INTRODUCTION

Noncontextual hidden variable (NCHV) theory assumes that the value of an observable revealed by a measurement is predetermined by hidden variables no matter which compatible observable is measured alongside. Quantum contextuality, which was independently discovered by Kochen and Specker (KS) [1], and Bell [2], is a fundemental property of quantum correlations that cannot be explained by any NCHV theories. It can be revealed by the KS sets in a logic manner, or by violation of statistical noncontextuality inequalities which are satisfied in NCHV theories. So far, many theoretical and experimental works have been accomplished in order to find the optimal noncontextuality inequalities [3–6] or KS sets [7–11], which in turn contribute to the use of speeding up quantum algorithms [12].

New theoretical tools [13, 14] have been invented to study contextuality. Graph theory is a such representative that finds its wide applications and effectiveness in discussing the contextual behavior [13]. A special kind of noncontextuality inequality $\sum_i \langle P_i\rangle \leq \alpha$ which assumes exclusivity relation between measurements P_i's can be studied with graph theory efficiently, where P_i's are rank-1 projective measurements and P_1 is said to be exclusive with P_2 if $P_1P_2 = 0$. (In this paper, we only consider this kind noncontextuality inequality. Actually, in the most general NCHV theories without restriction of exclusivity relation such bounds do not hold and different inequalities should be used [16].) The exclusivity relation of P_i's can be effectively represented in an exclusivity graph G consisting of vertices and edges, where a pair of vertices i, j are connected if and only if the corresponding measurements P_i, P_j are mutually exclusive. For each exclusivity graph, the classical bound α of the noncontextuality inequality equals to the independence $\alpha(G)$, and the maximal quantum prediction is just the Lovász number $\vartheta(G)$ [15] which can be achieved by pure states.

Nevertheless, there is no perfectly "pure" state in actual experiment. It is quite necessary to consider mixed states and analyze their influence upon contextuality. Although there are state-independent noncontextuality (SIC) inequalities, whose quantum violation is independent of which state is to be measured, yet in general the maximal violation C_q of a noncontextuality inequality for a given state may depend on its mixedness. There have been proposed various measures of the mixedness of a state, linear entropy [17] among them is an efficient one easy to compute: For a d-dimensional mixed state ρ, the linear entropy is defined as $S_l(\rho) = \frac{d}{d-1}(1 - \mathrm{Tr}[\rho^2])$. On the other hand, $\vartheta(G)$ is just the maximal eigenvalue of all possible overall measurement matrix M defined by $\sum_i P_i$. Thus, the spectral distribution of M is promising to uncover more details of contextuality.

The KCBS inequality [3] is the simplest noncontextuality inequality, in the sense that it requires the minimal number of projective measurements, while the KK inequality [6] is a first one that can be violated by almost all states except the maximally mixed state. In this paper, we focus on these two inequalities. In Section II, the maximal contextuality of mixed states (MCMS) for a fixed linear entropy is presented for each inequality. Section III then aims to give a spectral analysis on the overall measurement matrix, endeavoring to explore the question of how the existence of a universal set of measurements depends on the spectral distribution. At last, we give some conclusion and discussions.

II. THE MAXIMALLY CONTEXTUAL MIXED STATES FOR THE KCBS AND KK NONCONTEXTUALITY INEQUALITIES

To start with, the KCBS and the KK inequalities are two of the simple and well-known noncontextuality inequalities for three-dimensional systems, usually written as respectively

$$I_{KCBS} = \sum_{i=1}^{5} \langle P_i\rangle \overset{\text{NCHV}}{\leq} 2 \overset{\text{QM}}{\leq} \sqrt{5},$$

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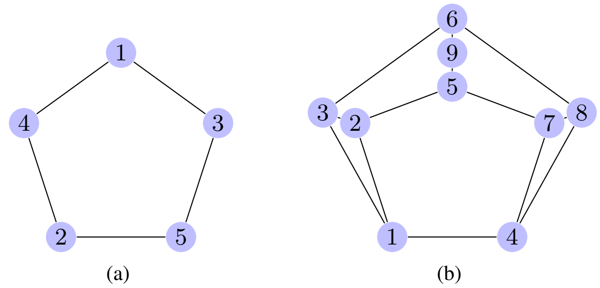


FIG. 1: The exclusivity graph of KCBS (a) and KK (b).

and

$$I_{KK}=\sum_{i=1}^{9}\langle P_i\rangle \overset{\text{NCHV}}{\leq} 3 \overset{\text{QM}}{\leq} \frac{10}{3},$$

where $\langle P_i\rangle \equiv \mathrm{Tr}[\rho P_i]$, ρ is the general mixed state, and P_i's are rank-1 projective measurements with exclusivity relations shown in Figs. 1(a) and 1(b). Note that the former is the simplest inequality that requires the minimal number of measurements, while the latter is a first one that is quantum mechanically violated by all but the maximally mixed state.

Without loss of generality and for the sake of convenience, we consider the diagonal quantum state, that is,

$$\rho=\begin{bmatrix}\lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3\end{bmatrix}, \tag{1}$$

with λ_i in decreasing order, and $\vec{\lambda}\equiv(\lambda_1,\lambda_2,\lambda_3)$. This makes sense since for a fixed general state and its optimal measurement set, one can always be able to diagonalize the state and change accordingly its overall measurement set by a global rotation. For a general state, one should rotate it into form (1) and then applies the following results.

For a given mixed state ρ which is determined by $\vec{\lambda}$, its maximally contextuality C_q and linear entropy S_l are all functions of $\vec{\lambda}$. In what follows we shall investigate the region of C_q with respect to a fixed linear entropy S_l, for each inequality mentioned above. For a fixed linear entropy S_l, we numerate over all possible states and measurements to find the upper and the lower bounds of C_q.

We plot the upper and lower bounds of C_q when S_l varies in Fig. 2, together with the optimal measuring directions shown in Table I or II. While, the specific states and the analytic expressions for each curve (except Arc(AC), whose expression is missing) are listed as follows (for convenient, denote the linear entropy S_l as s):

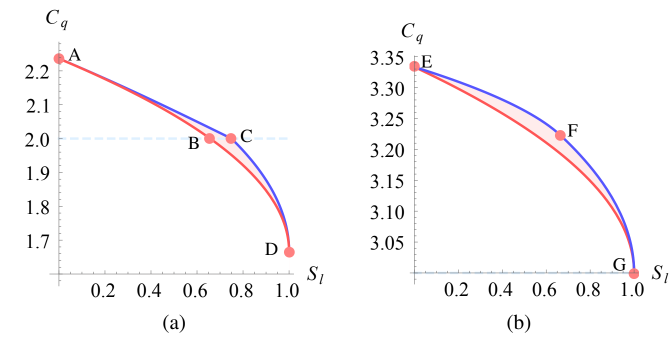


FIG. 2: (Color online) The upper (blue) and lower (red) bounds of C_q of mixed states for KCBS (a) and KK (b), where $A\ (0,\sqrt{5})$, $B\ (\frac{3}{40}(11-\sqrt{5}),2)$, $C\ (\frac{3}{4},2)$, $D\ (1,\frac{5}{3})$, $E\ (0,10/3)$, $F\ (2/3,29/9)$, $G\ (1,3)$.

$\vert i\rangle$	i_1	i_2	i_3
$\vert 1\rangle$	1	0	0
$\vert 2\rangle$	1	0	0
$\vert 3\rangle$	0	1	0
$\vert 4\rangle$	0	1	0
$\vert 5\rangle$	0	0	1

(a)

$\tau\vert i\rangle$	i_1	i_2	i_3
$\tau\vert 1\rangle$	$\sqrt{\cos(\beta)}$	1	0
$\tau\vert 2\rangle$	$\sqrt{\cos(\beta)}$	$\cos(2\beta)$	$\sin(2\beta)$
$\tau\vert 3\rangle$	$\sqrt{\cos(\beta)}$	$\cos(4\beta)$	$\sin(4\beta)$
$\tau\vert 4\rangle$	$\sqrt{\cos(\beta)}$	$\cos(6\beta)$	$\sin(6\beta)$
$\tau\vert 5\rangle$	$\sqrt{\cos(\beta)}$	$\cos(8\beta)$	$\sin(8\beta)$

(b)

TABLE I: The set of measurements for KCBS where the state ρ is in form (1), (a) for Arc(CD) while (b) for Arc(AD), where $\tau=\frac{1}{\sqrt{1+\cos(\beta)}}$, $\beta=\pi/5$.

$$\mathrm{Arc}(AC):\quad \vec{\lambda} = \left(\frac{1+\sqrt{1-4s/3}}{2},\frac{1-\sqrt{1-4s/3}}{2},0\right), \tag{2}$$

$$\begin{aligned}\mathrm{Arc}(CD):\quad \vec{\lambda} &= \left(\frac{1+\sqrt{1-s}}{3},\frac{1+\sqrt{1-s}}{3},\frac{1-2\sqrt{1-s}}{3}\right),\\ C_q &= \frac{2\sqrt{1-s}+5}{3},\end{aligned} \tag{3}$$

$$\begin{aligned}\mathrm{Arc}(AD):\quad \vec{\lambda} &= \left(\frac{1+2\sqrt{1-s}}{3},\frac{1-\sqrt{1-s}}{3},\frac{1-\sqrt{1-s}}{3}\right),\\ C_q &= \frac{(3\sqrt{5}-5)\sqrt{1-s}+5}{3},\end{aligned} \tag{4}$$

$$\begin{aligned}\mathrm{Arc}(EF):\quad \vec{\lambda} &= \frac{(3+\sqrt{9-12s},3-\sqrt{9-12s},0)}{6},\\ C_q &= \frac{\sqrt{9-12s}+57}{18},\end{aligned} \tag{5}$$

$$\begin{aligned}\mathrm{Arc}(FG):\quad \vec{\lambda} &= \frac{(1+\sqrt{4-3s},1,1-\sqrt{4-3s})}{3},\\ C_q &= \frac{2\sqrt{1-s}}{3\sqrt{3}}+3,\end{aligned} \tag{6}$$

$$\begin{aligned}\mathrm{Arc}(EG):\quad \vec{\lambda} &= \frac{(1+2\sqrt{1-s},1-\sqrt{1-s},1-\sqrt{1-s})}{3},\\ C_q &= \frac{\sqrt{1-s}+9}{3}.\end{aligned} \tag{7}$$

Here we take the curve Arc(AC) in Fig. 2(a) for example to explain the figures, tables and equations. Given a linear

$\|i\rangle$	i_1	i_2	i_3
$\|1\rangle$	$-1/\sqrt{2}$	$1/\sqrt{2}$	0
$\|2\rangle$	$-1/2$	$-1/2$	$1/\sqrt{2}$
$\|3\rangle$	$1/2$	$1/2$	$1/\sqrt{2}$
$\|4\rangle$	$-1/\sqrt{2}$	$-1/\sqrt{2}$	0
$\|5\rangle$	$-\sqrt{2}/\sqrt{3}$	0	$-1/\sqrt{3}$
$\|6\rangle$	$-\sqrt{2}/\sqrt{3}$	0	$1/\sqrt{3}$
$\|7\rangle$	$-1/2$	$1/2$	$1/\sqrt{2}$
$\|8\rangle$	$-1/2$	$1/2$	$-1/\sqrt{2}$
$\|9\rangle$	0	1	0

TABLE II: The set of measurements for KK where the state ρ is in form (1).

entropy $s \in [0, \frac{3}{4}]$, the maximal C_q is located on the curve Arc(AC), while the corresponding mixed state ρ is determined by $\vec{\lambda}$ in Eq. (2) and the set of measurements which can obtain this C_q is shown in Table I (b).

III. A SPECTRAL ANALYSIS

With the above results, we note that there exist a universal set of measuring directions up to a global rotation for the KK inequality to obtain the upper and lower bound of C_q with respect to the linear entropy s; however, this is not true for the KCBS inequality. To proceed, we shall do a spectral analysis on the measuring sets relative to these inequalities.

Define

$$M = \sum_i P_i, \tag{8}$$

which is precisely the expression of inequalities before taking average with a specific state. The quantum prediction can be denoted as $\langle M \rangle = \text{Tr}[M\rho]$. Note that the maximal quantum violation $\vartheta(G)$ is just the maximal eigenvalue of all possible M.

To make it clear, the spectral analysis can be divided into three steps:

1. Prove that we can only consider M's which are diagonal if ρ is in form (1);
2. Show that the spectral distributions of KCBS and KK are both restrained to a curve;
3. Present the reason why there exist a universal set of measuring directions for the KK inequality, and why this is not true for the KCBS inequality.

Step 1: First, we introduce a lemma on Hermitian matrices:
Lemma 1 *Assume that*

$$A = \begin{bmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{bmatrix}, B = U \begin{bmatrix} b_1 & & & \\ & b_2 & & \\ & & \ddots & \\ & & & b_n \end{bmatrix} U^\dagger,$$

where $a_1 \geq a_2 \geq \cdots \geq a_n$, $b_1 \geq b_2 \geq \cdots \geq b_n$, $U = (u_{ij})$ is a unitary matrix. Then

$$Tr[AB] \leq \vec{a}.\vec{b},$$

where $\vec{a} = (a_1, a_2, \cdots, a_n)$, $\vec{b} = (b_1, b_2, \cdots, b_n)$.
PROOF Directly computation shows that

$$\text{Tr}[AB] = \vec{a}W\vec{b},$$

where $W = (w_{ij})$ with $w_{ij} = |u_{ij}|^2$.

Then W is a doubly stochastic matrix by the definition of doubly stochastic matrices. The Birkhoff-von Neumann theorem says that the set of $n \times n$ doubly stochastic matrices forms a convex polytope whose vertices are the $n \times n$ permutation matrices. If we consider the linear functional $f(W) = \vec{a}W\vec{b}$ on that convex polytope, then its optimal can be achieved at the vertices, i.e., the permutation matrices. Since $\vec{a}, \vec{b}$ are already in decreasing order, the maximal of $f(W) = \vec{a}.\vec{b}$ can be achieved when $W = I_n$, which implies $U = I_n$. ■

Given a state

$$\rho = \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{bmatrix},$$

where, $\lambda_1 \geq \lambda_2 \geq \lambda_3$. And the set of measurements $\{|i\rangle\}$ is optimal for ρ. Assume U is such a unitary matrix that $U^\dagger \left(\sum_i |i\rangle\langle i|\right) U$ is diagonal and the diagonal is in decreasing order, Lemma 1 tells us that the set of measurements $\{|\tilde{i}\rangle = U^\dagger |i\rangle\}$ is also optimal while $M = \sum_i |\tilde{i}\rangle\langle\tilde{i}|$ is diagonal. Thus, for our purpose, we can only consider the diagonal M:

$$M = \begin{bmatrix} m_1 & & \\ & m_2 & \\ & & m_3 \end{bmatrix},$$

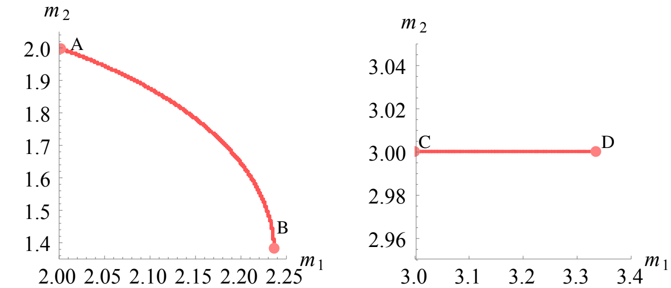
with m_i in decreasing order, $m_1 + m_2 + m_3 = n$, and n being the total number of settings (i.e., 5 for KCBS and 9 for KK).
Step 2: Denote $\vec{m} = (m_1, m_2, m_3)$. The condition $m_1 + m_2 + m_3 = n$ restrains $\vec{m}$ within an, e.g., m_1m_2-plane. In general, $C_q = \vec{\lambda} \cdot \vec{m} \leq n\lambda_1$. In particular, $C_q = n\lambda_1$, which holds only to an edgeless exclusivity graph G, that is, there is no exclusive relation between any pair of events of probability. In fact, the exclusivity relation will further limit the distribution of $\vec{m}$. As the numerical computation shows, the exclusivity relations for the KCBS and KK inequalities are so strong that $\vec{m}$ will be dramatically restrained to a curve, rather than a region in the plane.

The curves of (m_1, m_2) for KCBS and KK inequalities are plotted in Fig. 3(a) and Fig. 3(b), respectively. Obviously, m_2 must be a function of m_1. Then the maximal contextuality C_q is a function of m_1,

$$\begin{aligned} C_q(m_1) &= \vec{\lambda} \cdot \vec{m} \\ &= n\lambda_3 + (\lambda_1 - \lambda_3)m_1 + (\lambda_2 - \lambda_3)m_2(m_1). \end{aligned}$$

By differentiating the expression with respect to m_1,

$$\frac{dC_q(m_1)}{dm_1} = (\lambda_1 - \lambda_3) + (\lambda_2 - \lambda_3)\frac{dm_2(m_1)}{dm_1},$$



(a) (b)

FIG. 3: The curve of (m_1, m_2) for KCBS (a) and KK (b), where $A(2,2)$, $B(\sqrt{5}, \frac{5-\sqrt{5}}{2})$, $C(3,3)$, $D(\frac{10}{3}, 3)$.

and check the extremum we will obtain the optimal m_1. By use of the spectral distribution Fig. 3(a) and 3(b), one can determine the optimal overall measurement matrix M for a given state ρ.

Step 3: In eq. (2) and etc. we already know the form of the optimal states for each curves, then we can try to find the corresponding optimal overall measurement matrix M.

For the KCBS inequality, we have $dm_2/dm_1 \leq -1$ and $dm_2/dm_1 = -1$ only at the point $(m_1, m_2) = (2, 2)$ which is easy to see from the symmetry of m_1, m_2, and

(i):

$$\mathrm{Arc}(AC): \quad \frac{dC_q}{dm_1} = \frac{1+\sqrt{1-\frac{4s}{3}}}{2} + \frac{1-\sqrt{1-\frac{4s}{3}}}{2}\frac{dm_2}{dm_1}.$$

Then $\frac{dC_q}{dm_1} = 0$ implies that

$$\frac{dm_2}{dm_1} = -\frac{1+\sqrt{1-\frac{4s}{3}}}{1-\sqrt{1-\frac{4s}{3}}}.$$

Hence, the optimal m_1 varies with s, meaning that there is no universal set of measurements for this curve.

(ii):

$$\mathrm{Arc}(CD): \quad \frac{dC_q}{dm_1} = \sqrt{1-s}\left(1 + \frac{dm_2}{dm_1}\right) < 0.$$

This shows that the optimal m_1 is 2, then, using the spectral distribution Fig. 3(a), we have $m_2 = 2$ and $m_3 = n - m_1 - m_2 = 1$. This implies that the set of measurements in Table I (a) is optimal whose overall measurement matrix M corresponds to $(m_1, m_2, m_3) = (2, 2, 1)$.

(iii):

$$\mathrm{Arc}(AD): \quad \frac{dC_q}{dm_1} = \sqrt{1-s} > 0.$$

Again, this shows that the optimal m_1 is $\sqrt{5}$, which implies that the set of measurements in Table I (b) is optimal whose overall measurement matrix M corresponds to $(m_1, m_2, m_3) = (\sqrt{5}, \frac{5-\sqrt{5}}{2}, \frac{5-\sqrt{5}}{2})$.

With the help of spectral analysis Fig. 3(a), the quantum violation of the KCBS inequality by all diagonal states which are convex mixtures of $|1\rangle$, $|3\rangle$, $|5\rangle$ in Table I is shown in Fig. 4.

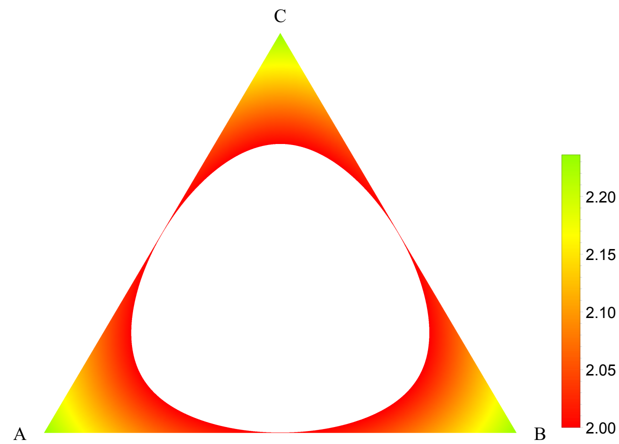


FIG. 4: The violation C_q of diagonal states for KCBS, where A, B, C stands for pure states $|1\rangle, |3\rangle, |5\rangle$ respectively and each point in the triangle stands for a mixed state which is a convex mixture of $|1\rangle, |3\rangle, |5\rangle$. The inner white region is the set of states which do not violate the classical bound 2.

For the KK inequality, we find that $dm_2/dm_1 = 0$ (i.e., $dc_q/dm_1 \geq 0$) always holds. So the optimal m_1 is always $\frac{10}{3}$, which implies that all the states that violate the inequality possess the same set of measurements shown in Table II whose overall measurement matrix M corresponds to $(m_1, m_2, m_3) = (10/3, 3, 8/3)$.

Moreover, the condition $m_1 + m_2 + m_3 = n$ yields

$$\frac{dm_3}{dm_1} = -\left(1 + \frac{dm_2}{dm_1}\right).$$

For KCBS, this yields $\frac{dm_3}{dm_1} > 0$, a monotonically increasing relation between m_1 and m_3, implying that they take their maxima simultaneously, while for KK this yields $\frac{dm_3}{dm_1} < 0$, a monotonically decreasing relation, implying that the maximal m_3 is obtained when m_1 reaches its minimum, and vice versa.

Consequently, the spectral distribution of a noncontextuality inequality can reveal more details of contextuality and here reflects the nature as to whether there exist a universal set of measurements up to a global rotation, so that possible experimental setups could be greatly facilitated.

IV. CONCLUSION AND DISCUSSIONS

In this paper, we have investigated the quantum contextuality of mixed states for the KCBS and the KK noncontextuality inequalities, and explored the question of why there exists a universal set of measurements for the latter, whereas none does for the former inequality. We have shown that a spectral analysis on the set of measurements may provide insightful clues toward the ultimate answer to this question. We believe that further works on combining graph theory and spectral theory in studying quantum contextuality may shed new light on these problems.

Acknowledgments

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