I. INTRODUCTION

Kirkwood-Dirac (KD) distribution is a representation of quantum states. Recently, KD distribution has been found applications in many areas such as in quantum metrology, quantum chaos and foundations of quantum theory. KD distribution is a quasiprobability distribution, and negative or nonreal elements may signify quantum advantages in certain tasks. A quantum state is called KD classical if its KD distribution is a probability distribution. Since most quantum information processes use pure states as ideal resources, therefore it becomes a key problem to determine the general structure of KD classical pure states.

To address this issue, we define the transition matrix $U^{AB}$ and support uncertainty $n_A(\psi) + n_B(\psi)$. The transition matrix $U^{AB}$ of $A$ and $B$ is defined by its entries $U^{AB}_{jk}$ as

$$U^{AB}_{jk} = \langle a_j | b_k \rangle.$$  \hfill (2)

$U^{AB}$ is unitary and $(b_k|a_j) = (U^{AB})^\ast$ appear in Eq. (1), here $(\ldots)^\ast$ stands for the complex conjugate of $(\ldots)$. We also use $(\ldots)^t$ to stand for the transpose of $(\ldots)$, use $\ldots, ||\ldots||$ to denote the standard inner product and standard norm in $\mathbb{C}^d$; and use $(\ldots)$ to denote the absolute value of $(\ldots)$ in the set of complex numbers $\mathbb{C}$ or the numbers of elements in the set $(\ldots)$. The support uncertainty $n_A(\psi) + n_B(\psi)$ is defined by the $A$ support of $|\psi\rangle$, $n_A(\psi)$, and $B$ support of $|\psi\rangle$, $n_B(\psi)$, as

$$n_A(\psi) = |\{ j \in [1, d] | \langle a_j | \psi \rangle \neq 0 \} |,$$ \hfill (3)

$$n_B(\psi) = |\{ k \in [1, d] | \langle b_k | \psi \rangle \neq 0 \} |,$$ \hfill (4)

where $[j_1, j_2]$ represents the set of consecutive integers from $j_1$ to $j_2$. For example, $[2, 5] = \{ 2, 3, 4, 5 \}$.

In Ref. [55], the authors proved that when pure state $|\psi\rangle$ is KD classical and $|\psi\rangle\langle\psi| \notin \{ |a_j\rangle\langle a_j| \}_{j=1}^d$, $|\psi\rangle\langle\psi| \notin \{ \langle b_k|b_k\rangle \}_{k=1}^d$, then

$$n_A(\psi) + n_B(\psi) \leq \frac{3}{2}d.$$  \hfill (5)

De Bièvre showed that [56] when all elements of $U^{AB} = \{ (a_j|b_k) \}_{j,k=1}^d$ are nonzero and $|\psi\rangle$ is KD classical, then

$$n_A(\psi) + n_B(\psi) \leq d + 1.$$  \hfill (6)

De Bièvre also conjectured that [56] when $U^{AB} = \{ (a_j|b_k) \}_{j,k=1}^d$ form a discrete Fourier transformation (DFT) $\{ (a_j|b_k) = \frac{1}{\sqrt{d}} e^{i2\pi jk/d} \}_{j,k=1}^d$ with $i = \sqrt{-1}$, then $|\psi\rangle$ is KD classical iff (if and only if)

$$n_A(\psi)n_B(\psi) = d.$$  \hfill (7)
Some relations between the transition matrix and support uncertainty were discussed in Ref. [57].

In this paper we provide some characterizations for the general structure of KD classical pure states. The rest of this paper is organized as follows. In Sec. II, we establish general structure for KD classical pure states. In Sec. III, we explore the relation between the support uncertainty and the number of zeros in transition matrix. In Sec. IV, we give some examples to demonstrate the applications of our results. Sec. V is a brief summary.

II. GENERAL STRUCTURE OF KD CLASSICAL PURE STATES

In this section, we establish two structure theorems for KD classical pure states. We state Facts 1 to 4, they are immediate consequences of the definition $Q_{jk}(\langle \psi |)$ but useful for subsequent discussions.

Fact 1. All $\{Q_{jk}(\langle \psi |)\}^d_{j,k=1}$ keep invariant if we replace $A = \{|a_j\rangle\}^d_{j=1}$ by $A = \{|e^{i\xi_j}|a_j\rangle\}^d_{j=1}$ and replace $B = \{|b_k\rangle\}^d_{k=1}$ by $B = \{|e^{i\eta_k}|b_k\rangle\}^d_{k=1}$, where $\{\xi_j\}^d_{j=1} \subseteq \mathbb{R}$, $\{\eta_k\}^d_{j=1} \subseteq \mathbb{R}$, $\mathbb{R}$ is the set of all real numbers.

Fact 2. $Q_{jk}(e^{i\theta}|\psi\rangle) = Q_{jk}(\langle \psi |)$ for any $\theta \in \mathbb{R}$. (8)

Fact 3. When $n_A = 1$, the KD classical states are $\{e^{i\alpha_j}|a_j\rangle\}^d_{j=1}$ with $\{\alpha_j\}^d_{j=1} \subseteq \mathbb{R}$. For the KD classical state $e^{i\alpha_j}|a_j\rangle$, we have $n_B = |\{k|\langle b_k|a_j\rangle = 0\}|$. The case of $n_B = 1$ is similar.

Fact 4. Suppose $A = A_1 \cup A_2$, $B = B_1 \cup B_2$, $A_1 \not\subseteq \emptyset$, $A_2 \not\subseteq \emptyset$, $B_1 \not\subseteq \emptyset$, $B_2 \not\subseteq \emptyset$, span$A_1 =$span$B_1$, span$A_2 =$span$B_2$. Then the pure state $|\psi\rangle$ is KD classical with respect to $A$ and $B$, if

$$|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle, \quad (9)$$

with $|\psi_1\rangle \in$span$A_1$ being KD classical with respect to $A_1$ and $B_1$, $|\psi_2\rangle \in$span$A_2$ being KD classical with respect to $A_2$ and $B_2$. Here span$A_1$ denotes the linear span of $A_1$ over the set of complex numbers.

Fact 1 implies that $|\psi\rangle$ is KD classical with respect to $\{|a_j\rangle\}^d_{j=1}$ and $\{|b_k\rangle\}^d_{k=1}$, if $|\psi\rangle$ is KD classical with respect to $\{|e^{i\xi_j}|a_j\rangle\}^d_{j=1}$ and $\{|e^{i\eta_k}|b_k\rangle\}^d_{k=1}$. Fact 2 implies that $|\psi\rangle$ is KD classical if $e^{i\theta}|\psi\rangle$ is KD classical.

Fact 3 determines the structure of the KD classical states with $n_A(\psi) = 1$ (or $n_B(\psi) = 1$), we call such states $\{e^{i\alpha_j}|a_j\rangle\}^d_{j=1}$ the basis states of $A$, the basis states of $B$ are similar. Thus below we mainly consider the case of $\min\{n_A, n_B\} \geq 2$. Fact 3 explicitly shows that for fixed positive integers $\{n_A, n_B\}$, there may not exist a pure state $|\psi\rangle$ such that $n_A(\psi) = n_A$ and $n_B(\psi) = n_B$. For example, for DFT of dimension $d$, there does not exist a pure state $|\psi\rangle$ such that $n_A(\psi) = 1$ and $n_B(\psi) < d$.

Under Fact 4, to determine the KD classical pure states of $A$ and $B$, we first consider whether the transition matrix $U_{AB}$ can be decomposed as the direct sum of $U_{AB} = U_{A_1B_1} \oplus U_{A_2B_2}$. If so, we only need to determine the KD classical pure states of $U_{A_1B_1}$ and $U_{A_2B_2}$, and then use Eq. (9). Below we focus on the case that the transition matrix $U_{AB}$ can not be decomposed into the form of direct sum.

Theorem 1 below shows the general structure of KD classical pure states. To state Theorem 1, we write $\langle a_j|\psi\rangle$, $\langle \psi|b_k\rangle$ and $U_{jk}$ in the polar form as

$$\langle a_j|\psi\rangle = \langle a_j|\psi\rangle e^{i\alpha_j} \text{ if } \langle a_j|\psi\rangle \neq 0, \quad (10)$$

$$\langle \psi|b_k\rangle = \langle \psi|b_k\rangle e^{i\beta_k} \text{ if } \langle \psi|b_k\rangle \neq 0, \quad (11)$$

$$U_{jk} = U_{jk}\text{ if } U_{jk} \neq 0, \quad (12)$$

where $\alpha_j, \beta_k, \theta_{jk} \in \mathbb{R}$.

Theorem 1. A pure state $|\psi\rangle$ is KD classical with respect to $A$ and $B$, if there exist nonempty sets $S_A \subseteq [1, d]$, $S_B \subseteq [1, d]$, $\{\alpha_j\} \subseteq S_A \subseteq \mathbb{R}$, $\{\beta_k\} \subseteq S_B \subseteq \mathbb{R}$, $\{A_j > 0\}_{j \in S_A}$, $\{B_k > 0\}_{k \in S_B}$, such that

$$\theta_{jk} = \alpha_j + \beta_k \mod 2\pi \text{ when } Q_{jk}(\langle \psi |) \neq 0, \quad (13)$$

$$|\psi\rangle = \sum_{j \in S_A} A_j e^{i\alpha_j}|a_j\rangle = \sum_{k \in S_B} B_k e^{-i\beta_k}|b_k\rangle. \quad (14)$$

Proof. Expanding $|\psi\rangle$ in the bases $A$ and $B$, evidently there exist $\emptyset \not\subseteq S_A \subseteq [1, d]$, $\emptyset \not\subseteq S_B \subseteq [1, d]$, $\{A_j > 0\}_{j \in S_A}$, $\{B_k > 0\}_{k \in S_B}$ such that Eq. (13,14) hold.

Obviously $Q_{jk}(\langle \psi |) = \langle a_j|\psi\rangle e^{i\theta_{jk}}|b_k\rangle = 0$ when $j \in [1, d] \setminus S_A$ or $k \in [1, d] \setminus S_B$. For $j \in S_A$ and $k \in S_B$, if $\langle a_j|b_k\rangle = 0$ then $Q_{jk}(\langle \psi |) = 0$; if $\langle a_j|b_k\rangle \neq 0$ and $Q_{jk}(\langle \psi |) > 0$, then $e^{i\alpha_j} e^{i\beta_k} e^{-i\theta_{jk}} = 1$ and $\theta_{jk} = \alpha_j + \beta_k \mod 2\pi$. The claim then follows.

The freedom of global phase for pure KD classical state $|\psi\rangle$ in Fact 1 corresponds to the invariance of Eq. (13) under the transformation: $\alpha_j \rightarrow \alpha_j + \theta$ for all $j \in S_A$, $\beta_k \rightarrow \beta_k - \theta$ for all $k \in S_B$, with $\theta \in \mathbb{R}$. Note that Eq. (14) implies

$$A_j = \sum_{k \in S_B} B_k |\langle a_j|b_k\rangle|, j \in S_A; \quad (15)$$

$$B_k = \sum_{j \in S_A} A_j |\langle a_j|b_k\rangle|, k \in S_B. \quad (16)$$

Further, when $A$ and $B$ are mutually unbiased bases (MUBs), i.e., $\{|\langle a_j|b_k\rangle| = 1/\sqrt{d}\}_{j,k=1}$, Eqs. (15,16) imply Corollary 1 below.

Corollary 1. Suppose $A$ and $B$ are MUBs, then the pure state $|\psi\rangle$ is KD classical with respect to $A$ and $B$ iff

$$n_A(\psi)n_B(\psi) = d. \quad (17)$$

Proof. In [56], De Bièvre showed that when

$$n_A(\psi)n_B(\psi) = \frac{1}{M_{AB}^2}, \quad (18)$$

then $|\psi\rangle$ is KD classical, where $M_{AB} = \max\{|\langle a_j|b_k\rangle|\}_{j,k=1}^d$. For MUBs, Eq. (18) becomes
\[ n_A(\psi)n_B(\psi) = d. \] Conversely, for MUBs, if \(|\psi\rangle\) is KD classical, then Eqs. (15,16) imply Eq. (17).

Note that for MUBs in prime dimension, Fact 3 and Corollary 1 together imply that the only pure KD classical states are the basis states.

We further analyze Eqs. (15,16). Write \( V = (\langle a_j | b_k \rangle)_{j \in S_A, k \in S_B} \) in the form of matrix, \( \begin{bmatrix} A \\ B \end{bmatrix} = (A_1, A_2, ..., A_{n_A})^t, \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} = (B_1, B_2, ..., B_{n_B})^t \), then Eqs. (15,16) imply that
\[
\begin{align*}
\begin{bmatrix} A \\ B \end{bmatrix} &= V \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix}, \\
\begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} &= V^t \begin{bmatrix} A \\ B \end{bmatrix},
\end{align*}
\]
\text{(19) (20) (21) (22)}
\]

Eqs. (19,20,21,22) will be used in the proof of Theorem 2.

Note that Fact 3 is a special case of Theorem 1. In Theorem 1, when \( \min\{n_A, n_B\} \geq 2 \), Eq. (13) implies that
\[
\theta_{j_1 k_1} - \theta_{j_2 k_2} = \alpha_{j_1} - \alpha_{j_2} \mod 2\pi \\
\text{(23)}
\]
when \( \langle a_{j_1} | b_{k_1} \rangle \langle a_{j_2} | b_{k_2} \rangle \neq 0, \forall j_1, j_2 \in S_A, k \in S_B; \)
\[
\theta_{j_1 k_1} - \theta_{j_2 k_2} = \beta_{k_1} - \beta_{k_2} \mod 2\pi \\
\text{(24)}
\]
when \( \langle a_{j_1} | b_{k_1} \rangle \langle a_{j_2} | b_{k_2} \rangle \neq 0, \forall j \in S_A, \forall k_1, k_2 \in S_B. \)

Eq. (23) means that \( \theta_{j_1 k_1} - \theta_{j_2 k_2} \) is independent of \( k \), that is
\[
\theta_{j_1 k_1} - \theta_{j_2 k_2} = \alpha_{j_1} - \alpha_{j_2} \mod 2\pi \\
\text{(25)}
\]
when \( \langle a_{j_1} | b_{k_1} \rangle \langle a_{j_2} | b_{k_2} \rangle \langle a_{j_2} | b_{k_2} \rangle \langle a_{j_2} | b_{k_2} \rangle \neq 0, \forall j_{1}, j_2 \in S_A, \forall k_1, k_2 \in S_B. \) Also, Eq. (24) is obviously equivalent to Eq. (26), then Eq. (23) is equivalent to Eq. (24). Therefore Eq. (25) or Eq. (26) provides a necessary and sufficient condition to check Eq. (13).

Theorem 2 below characterizes the structure of KD classical pure states via the transition matrix. Suppose \(|\psi\rangle\) is a KD classical state, then \(|\psi\rangle\) is of the form in Eq. (14). We relabel \( A = \{<a_j | j = 1 \}^d_{j = 1} \) and \( B = \{b_k \}^d_{k = 1} \) such that \( S_A = \{j \}^n_{j = 1} \) and \( S_B = \{k \}^{n_B}_{k = 1} \). We can further reorder \( S_A = \{j \}^n_{j = 1} \) and \( S_B = \{k \}^{n_B}_{k = 1} \). We can further modify the submatrix \( (1,2,...,n_A)_{1,2,...,n_B} \) to be diagonal and exhibits maximum number of nonzero blocks, here
\[
\begin{bmatrix}
1,2,...,n_A \\
1,2,...,n_B
\end{bmatrix}
\]
denotes the submatrix formed by the \( \{j\}^n_{j = 1} \) rows and \( \{k\}^{n_B}_{k = 1} \) columns of \( U^{AB} \). Then using Fact 1, we can choose \( \bar{A} = \{e^{i\alpha_j} | a_j \}^n_{j = 1} \) and \( \bar{B} = \{e^{-i\beta_k} | b_k \}^{n_B}_{k = 1} \) such that \( \bar{A}|\psi\rangle \geq 0, \langle \bar{a}_j | b_k \rangle \geq 0 \) with \( \langle \bar{a}_j | b_k \rangle = e^{-i\alpha_j} | a_j \rangle \langle b_k | \).

When \( \langle \bar{a}_j | b_k \rangle \geq 0 \) for all \( S_A = \{j\}^n_{j = 1} \) and \( S_B = \{k\}^{n_B}_{k = 1} \), then Eq. (25) means that \( \theta_{j_1 k_1} - \theta_{j_2 k_2} \) is of the form in Eq. (13) implies
\[
\begin{align*}
\text{rank}(C_j) &= \cos(\text{rank}(R_j^{(j)})) - 1, \\
\text{rank}(R_j) &= \cos(\text{rank}(R_j^{(j)})) - 1, \\
n_A(\psi) + n_B(\psi) &\leq d + s, \\
s &\leq \frac{d}{2},
\end{align*}
\]
where \( \cos(\text{rank}(R_j^{(j)})) \) stands for the number of rows (columns) of matrix \( R_j^{(j)} \). When \( \cos(\text{rank}(R_j^{(j)})) = 1 \), then \( R_j = 0 \), when \( \cos(\text{rank}(R_j^{(j)})) = 1 \) then \( C_j = 0 \). When \( \cos(\text{rank}(R_j^{(j)})) \geq 2 \) then \( C_j = 0 \). When \( \cos(\text{rank}(R_j^{(j)})) \geq 2 \), then \( C_j = 0 \) has zero column (row) vector, also the column (row) vectors of \( C_j \) can not be divided into two nonempty sets with orthogonal spanned spaces.

\[
\text{proof.} \quad \text{From Eqs. (19,20,21,22), we have } V = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} A \\ B \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} A \\ B \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}.
\]

Since \( U^{AB} \) is unitary, then
\[
\begin{bmatrix} A \\ B \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} A \\ B \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}, \begin{bmatrix} \bar{A} \\ \bar{B} \end{bmatrix} = (1,2,...,n_A)_{1,2,...,n_B}.
\]
Any two distinct column vectors of $U^{AB}$ are orthogonal, and the inner product of any two distinct column vectors of $R^{(j)}_{\geq 0}$ is in $[0,1)$, then the inner product of any two distinct column vectors of $C_j$ is in $(-1,0]$. When $\text{cols}(R^{(j)}_{\geq 0}) \geq 2$, if $C_j$ has a zero column vector, or the column vectors of $C_j$ can be divided into two nonempty sets with orthogonal spanned spaces, then $R^{(j)}_{\geq 0}$ can be decomposed into the form of direct sum, this contradicts the assumption that $s$ is the maximum number of blocks. Employing Lemma 1, we see that when $\text{cols}(R^{(j)}_{\geq 0}) \geq 2$, the column vectors of $C_j$ (note that all column vectors of $C_j$ are not normalized), after normalization, must have the form of $(A,b)$ or $(A,c)$. From Eq. (33) we get that Eq. (27) holds. Eq. (28) similarly holds.

Eq. (27) yields

$$\sum_{j=1}^{s} \text{rank}(C_j) = \sum_{j=1}^{s} \text{cols}(R^{(j)}_{\geq 0}) - s, \quad (34)$$

$$\text{rank}(C_1, C_2, ..., C_s) = n_B - s, \quad (35)$$

where we compute $\text{rank}(C_j)$ by the column rank (recall that for a matrix, the column rank equals the row rank), and have used the fact that any two column vectors in distinct $\{C_j\}_{j=1}^{s}$ are orthogonal. We compute $\text{rank}(C_1, C_2, ..., C_s)$ on the other hand by the row rank, then we get

$$\text{rank}(C_1, C_2, ..., C_s) \leq d - n_A. \quad (36)$$

Eqs. (35,36) certainly result in Eq. (29).

Lastly, we prove Eq. (30). In Fig. 1, we see that

$$n_A(\psi) + n_B(\psi) = \sum_{j=1}^{s} (\text{rows}(R^{(j)}_{\geq 0}) + \text{cols}(R^{(j)}_{\geq 0})).$$

Since each rows($R^{(j)}_{\geq 0}$)+cols($R^{(j)}_{\geq 0}$) ≥ 3, then

$$n_A(\psi) + n_B(\psi) \geq 3s.$$

Together with Eq. (5), we certainly get Eq. (30). We then finished this proof.

We remark that, Eqs. (29,30) certainly result in Eq. (5) which was obtained in Ref. [55]. We also remark that, when $s \geq 2$, from Fig. 1, there must exist two different columns (rows) in $U^{AB}$, such that the number of total zeros in these two distinct columns (rows) is no less than $n_A$ ($n_B$). Conversely, if $\max\{n_A(\psi), n_B(\psi)\} = \max\{Z_A, Z_B\}$ with $Z_A$ ($Z_B$) denoting the maximum number of zeros in any two different columns (rows) in $U^{AB}$, then $s = 1$ and Eq. (29) yields $n_A(\psi) + n_B(\psi) \leq d + 1$. This returns to the result of Proposition 11 in [58].

III. ZEROS IN TRANSITION MATRIX

We explore the bounds of $n_A(\psi) + n_B(\psi)$ for KD classical pure states in terms of the number of zeros in $U^{AB}$.
To do so, we define \( N_{AB}^{(0)} \) as the number of zeros in \( U^{AB} \),
\[
N_{AB}^{(0)} = \{ |\langle a_j | b_k \rangle | \langle a_j | b_k \rangle = 0, 1 \leq j, k \leq d \}. \tag{37}
\]
The number of zeros in a unitary matrix is an interesting topic, some recent results are reported in Ref. [59]. Obviously, \( N_{AB}^{(0)} \) keeps invariant if we replace \( A = \{ |a_j \rangle \} \) by \( \tilde{A} = \{ e^{i\xi_j |a_j \rangle} \} \) and replace \( B = \{ |b_k \rangle \} \) by \( B = \{ e^{i\eta_k |b_k \rangle} \} \), where \( \xi_j, \eta_k \) are real. Theorem 3 below provides a link between \( N_{AB}^{(0)} \) and \( n_A(\psi) + n_B(\psi) \) for KD nonclassical pure states.

**Theorem 3.** Suppose \( |\psi \rangle \) is a KD classical state, and \( U^{AB} \) is as in Fig. 1. Then it holds that
\[
N_{AB}^{(0)} \geq s(2s - 1) \quad \text{for } s \geq 2. \tag{38}
\]

**Proof.** For given \( s \) with \( s \geq 2 \), when \( \{ R_{ij}^{(s)} \}_{i,j=1} \) are all of the column form \( (r_1^{(s)}, r_2^{(s)}) \) (or when \( \{ R_{ij}^{(s)} \}_{i,j=1} \) are all of the row form \( (r_1^{(s)}, r_2^{(s)}) \) similarly) with \( r_1^{(s)} > 0, r_2^{(s)} > 0, |r_1^{(s)}|^2 + |r_2^{(s)}|^2 = 1 \), as depicted in Fig. 2 and let \( d - n_A = 1 \), then \( N_{AB}^{(0)} \) reaches the minimum. Otherwise, if there exists a \( R_{ij}^{(s)} \) with size larger than \( (r_1^{(s)}, r_2^{(s)}) \) or \( (r_1^{(s)}, r_2^{(s)}) \), then deleting the rows or columns such that \( R_{ij}^{(s)} \) shrinks into the form of \( (r_1^{(s)}, r_2^{(s)}) \) or \( (r_1^{(s)}, r_2^{(s)}) \), \( N_{AB}^{(0)} \) evidently does not increase in such process. If some of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) are all of the column form \( (r_1^{(s)}, r_2^{(s)}) \), but others of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) are all of the row form \( (r_1^{(s)}, r_2^{(s)}) \), we can reorder \( \{ R_{ij}^{(s)} \}_{i,j=1} \) such that \( \{ R_{ij}^{(s)} \}_{i,j=1} \) are all of the column form \( (r_1^{(s)}, r_2^{(s)}) \), but others \( \{ R_{ij}^{(s)} \}_{i,j=1} \) are all of the row form \( (r_1^{(s)}, r_2^{(s)}) \), as depicted in Fig. 3. In Fig. 3, the number of zeros in submatrix formed by the columns of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) and rows of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) is \( s(s - s_1) \); the number of zeros in submatrix formed by the rows of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) and columns of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) is \( 4s_1(s - s_1) \). However, in Fig. 2, the number of zeros in submatrix formed by the columns of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) and rows of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) is \( 2s_1(s - s_1) \); the number of zeros in submatrix formed by the rows of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) and columns of \( \{ R_{ij}^{(s)} \}_{i,j=1} \) is also \( 2s_1(s - s_1) \). Thus \( N_{AB}^{(0)} \) in Fig. 3 is greater than \( N_{AB}^{(0)} \) in Fig. 2, and Fig. 2 reaches the minimum of \( N_{AB}^{(0)} \).

Apparently, in Fig. 2, \( N_{AB}^{(0)} = s(2s - 1) \) when \( s \geq 2 \), this certainly yields Eq. (38). We then finished this proof.

With Theorem 2 and Theorem 3, we now establish Theorem 4 which provides a sufficient condition for pure KD nonclassical states.

**Theorem 4.** For the transition matrix \( U^{AB} \) and pure state \( |\psi \rangle \), if
\[
2 \leq \frac{1 + \sqrt{1 + 8N_{AB}^{(0)}}}{4} < n_A(\psi) + n_B(\psi) - d \tag{39}
\]
or
\[
1 + \sqrt{1 + 8N_{AB}^{(0)}} < 2 \leq n_A(\psi) + n_B(\psi) - d, \tag{40}
\]
then \( |\psi \rangle \) is KD nonclassical.

**Proof.** Theorem 4 is a result of Eqs. (29,38). We prove the contrapositive of Theorem 4. Suppose pure state \( |\psi \rangle \) is KD classical, then we write the transition matrix \( U^{AB} \) as in Fig. 1. If \( s = 1 \), then Eq. (29) yields \( n_A(\psi) + n_B(\psi) - d \leq 1, \) and both Eqs. (39,40) do not hold.

If \( s > 1 \), then both Eqs. (29,38) hold. Eq. (38) implies
\[
1 + \sqrt{1 + 8N_{AB}^{(0)}} \geq s, \tag{41}
\]
and Eq. (29) implies
\[
n_A(\psi) + n_B(\psi) - d \leq s. \tag{42}
\]

Eqs. (41,42) implies
\[
n_A(\psi) + n_B(\psi) - d \leq s \leq 1 + \sqrt{1 + 8N_{AB}^{(0)}} \tag{43}
\]
Eq. (43) obviously contradicts both Eqs. (39,40). ■

For a special case in Theorem 4, we have Corollary 2 below.

**Corollary 2.** For the transition matrix \( U^{AB} \) and pure state \( |\psi \rangle \), if
\[
N_{AB}^{(0)} < 6, \tag{44}
\]
\[
n_A(\psi) + n_B(\psi) > d + 1, \tag{45}
\]
then \( |\psi \rangle \) is KD nonclassical.

**Proof.** We can directly check that Eqs. (44,45) lead to Eq. (40). ■

We remark that Corollary 2 improved the Theorem 4 in Ref. [56] where Eq. (44) is replaced by \( N_{AB}^{(0)} > 0 \).

### IV. EXAMPLES

In this section, we provide some examples to demonstrate the applications of the results in section II and section III.

**Example 1.** The transition matrix is \( U_5 \) expressed in Fig. 4.
In $U_5$, $d = 5$, $\{p_1, q_1, r_1\} \subseteq (0, 1)$, $p_2 = 1 - p_1$, $q_2 = 1 - q_1$, $r_2 = 1 - r_1$, $\alpha \in (0, \frac{\pi}{2})$. $\{\theta_1, \theta_2, \theta_3\} \subseteq \mathbb{R}$. We see that $U_5$ can not be written in the form of direct sum. Consider the pure state expressed in the basis $B = \{|b_k\rangle\}_{k=1}^5$ as

$$|\psi\rangle = \sqrt{T_1}|b_1\rangle + \sqrt{T_2}|b_2\rangle,$$  

(46)

with $t_1 \in (0, 1)$, $t_1 + t_2 = 1$.

Direct computation shows that $|\psi\rangle$ is expressed in the basis $A = \{|a_j\rangle\}_{j=1}^3$ as

$$|\psi\rangle = \sqrt{T_1}p_1|a_1\rangle + \sqrt{T_1}p_2|a_2\rangle + \sqrt{T_2}q_1|a_3\rangle + \sqrt{T_2}q_2|a_4\rangle.$$  

Hence $n_B(\psi) = 2$, $n_A(\psi) = 4$, and $s = 2$ as shown in Fig. 4. From Eq. (1) we can directly get that

$$Q(|\psi\rangle) = \begin{pmatrix} t_1p_1 & 0 & 0 & 0 & 0 \\ t_1p_2 & 0 & 0 & 0 & 0 \\ 0 & t_2q_1 & 0 & 0 & 0 \\ 0 & t_2q_2 & 0 & 0 & 0 \end{pmatrix}.$$  

That is, $|\psi\rangle$ is KD classical. We can check that Eqs. (27,28,29,30) all holds for $U_5$ and $|\psi\rangle$.

Further, in $U_5$, $N_{AB}^{(0)} = 7$. We can check that Theorem 3 holds for $U_5$ and $|\psi\rangle$. Theorem 4 implies that for the pure state $|\varphi\rangle$ if $n_B(\varphi) + n_A(\varphi) > d + 2 = 7$ then $|\varphi\rangle$ is KD nonclassical.

**Example 2.** The transition matrix is discrete Fourier transformation (DFT).

De Bièvre [56] conjectured that for DFT of dimension $d$, a pure state $|\psi\rangle$ is KD classical iff $n_A(|\psi\rangle)n_B(|\psi\rangle) = d$. We see that Corollary 1 answered this conjecture in the affirmative. When $d = 5$ and $d = 6$, these results return to (a) and (b) of Figure 1 in Ref. [56]; when $d = 7$ these results return to the right panel of Figure 1 in Ref. [58].

**Example 3.** The transition matrix is Tao matrix.

The Tao matrix is the following unitary matrix $U_T$ with $d = 6$,

$$U_T = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega & \omega & \omega \\ 1 & \omega & 1 & \omega^2 & \omega & \omega \\ 1 & \omega & \omega & 1 & \omega & \omega \\ 1 & \omega & \omega & \omega & \omega & \omega \\ 1 & \omega^2 & \omega & \omega & \omega & \omega \end{pmatrix},$$  

with $\omega = \exp\left(i\frac{2\pi}{6}\right)$.

Apparently, for Tao matrix, bases $A$ and $B$ are MUBs. From Fact 3 we see that there exist pure KD classical states (basis states in $A$) satisfying $\{n_A = 1, n_B = 6\}$ and there exist pure KD classical states (basis states in $B$) satisfying $\{n_A = 6, n_B = 1\}$. With Corollary 1, the other possible pure KD classical states exist only when $\{n_A, n_B\} = \{2, 3\}$. It is proved that [58] there does not exist pure state satisfying $\{n_A, n_B\} = \{2, 3\}$. As a result, for Tao matrix, the only pure KD classical states are basis states.

**Example 4.** The transition matrix is

$$U_4 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ \cos \alpha & -\cos \alpha & \sin \alpha & -\sin \alpha \\ -\sin \alpha & \sin \alpha & -\cos \alpha & \cos \alpha \end{pmatrix},$$  

with $\alpha \in (0, \frac{\pi}{2})$.

Evidently, $U_4$ can not be written in the form of direct sum. In $U_4$, $d = 4$, $N_{AB}^{(0)} = 4$. Theorem 4 yields that the pure state $|\psi\rangle$ is KD nonclassical if $n_A(|\psi\rangle) + n_B(|\psi\rangle) > d + 1 = 5$. We give an explicit example. Suppose the pure state $|\psi\rangle$ is expressed in the basis $B = \{b_k\}_{k=1}^4$ as

$$|\psi\rangle = \sqrt{T_1}|b_1\rangle + \sqrt{T_2}|b_2\rangle,$$  

(47)

with $t_1 \in (0, 1)$, $t_1 + t_2 = 1$, $\sqrt{T_1} \neq \tan \alpha$. Then direct computation shows that $|\psi\rangle$ is expressed in the basis $A =
\{ (a_j) \}_{j=1}^5 \text{ as}

\[ |\psi\rangle = \frac{1}{\sqrt{2}} [\sqrt{t_1} |a_1\rangle + \sqrt{t_3} |a_2\rangle + (\sqrt{t_1} \cos \alpha + \sqrt{t_3} \sin \alpha) |a_3\rangle + (\sqrt{t_1} \sin \alpha - \sqrt{t_3} \cos \alpha) |a_4\rangle].\]

Hence \( n_B(\psi) = 2 \), \( n_A(\psi) = 4 \). From Eq. (1) we directly get that

\[ Q_{41}(\psi) = \frac{1}{2} \sqrt{t_1} (\sqrt{t_1} \sin \alpha - \sqrt{t_3} \cos \alpha) \sin \alpha, \]

\[ Q_{43}(\psi) = -\frac{1}{2} \sqrt{t_3} (\sqrt{t_1} \sin \alpha - \sqrt{t_3} \cos \alpha) \cos \alpha.\]

Consequently, one of \( \{Q_{51}(\psi), Q_{52}(\psi)\} \) must be negative, and \(|\psi\rangle \) is indeed KD nonclassical.

Remark that, in \( U_4 \), \( Z_r = 4 \), \( Z_c = 2 \), the conditions of Proposition 11 or Theorem 12 in Ref. [58] are not satisfied, thus we can not apply Proposition 11 or Theorem 12 in Ref. [58] to \( U_4 \). Example 4 then shows that for some states Theorem 4 is more advantageous than Proposition 11 or Theorem 12 in Ref. [58].

Example 5. The transition matrix is \( U_6 \) or \( U'_6 \) as

\[ U_6 = \frac{1}{\sqrt{5}} \begin{pmatrix}
  0 & 1 & 1 & 1 & 1 & 1 \\
  1 & 0 & 1 & -1 & 1 & -1 \\
  1 & 1 & 0 & -1 & -1 & 1 \\
  1 & -1 & -1 & 0 & 1 & 1 \\
  1 & 1 & -1 & 1 & 0 & -1 \\
  1 & -1 & 1 & 1 & -1 & 0
\end{pmatrix}, \]

\[ U'_6 = \frac{1}{\sqrt{5}} \begin{pmatrix}
  0 & 1 & 1 & 1 & 1 & 1 \\
  1 & 0 & 1 & -1 & 1 & -1 \\
  1 & 1 & 0 & -1 & -1 & 1 \\
  1 & -1 & -1 & 0 & 1 & 1 \\
  1 & 1 & -1 & 1 & 0 & -1 \\
  1 & -1 & 1 & 1 & -1 & 0
\end{pmatrix}. \]

In \( U_6 \) or \( U'_6 \), \( d = 6 \), \( N_{AB}^{(0)} = 6 \). Eq. (39) in Theorem 4 yields that the pure state \( |\psi\rangle \) is KD nonclassical if \( n_A(\psi) + n_B(\psi) > 8 \). In \( U_6 \) or \( U'_6 \), \( Z_r = Z_c = 2 \). Proposition 11 in Ref. [58] implies that if \( \max\{n_A(\psi), n_B(\psi)\} > 2 \) and \( n_A(\psi) + n_B(\psi) > 7 \), then \(|\psi\rangle \) is KD nonclassical. Theorem 12 in Ref. [58] implies that if \( n_A(\psi) + n_B(\psi) > 7 \), then \(|\psi\rangle \) is KD nonclassical. Example 5 then shows that for some states Proposition 11 or Theorem 12 in Ref. [58] is more advantageous than Theorem 4.

V. SUMMARY

We established general structure for KD classical pure states in Theorem 1 and Theorem 2. We explored the links between KD classical pure states and the number of zeros in transition matrix in Theorem 3 and Theorem 4. Also, we provide some examples to demonstrate the applications of our results.

We emphasize that whether a pure state is KD classical is dependent on the choice of orthonormal bases \( A \) and \( B \). For example, if we choose \( A = B \), then Eq. (1) shows that any pure states are KD classical. Conversely, for any orthonormal bases \( A \) and \( B \), Fact 3 implies that there must exist some KD classical pure states. The choice of orthonormal bases \( A \) and \( B \) would be specific depending on the concrete task in application, for example, the MUBs or DFT discussed in section IV.

There remained many open questions after this paper. First, how to apply the results of this paper to relevant experimental scenarios. Second, how to generalize the results of this paper to mixed states. Third, how to find out the KD classical (pure and mixed) states for some special transition matrices.

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Appendix: a mathematical result

We prove a mathematical result in Lemma 1 below, which is useful in the proof of Theorem 2.

Lemma 1. Let \( \{v_j\}_{j=1}^n \subseteq \mathbb{C}^d \backslash \{0\} \) and \( ||v_j|| = 1 \) for all \( j \). If

\[ -1 \leq \langle v_j | v_k \rangle \leq 0 \] (A1)

for all \( 1 \leq j < k \leq n \), then \( \{v_j\}_{j=1}^n \) has the unique decomposition

\[ \{v_j\}_{j=1}^n = \bigcup_{\alpha=1}^n S_\alpha, \] (A2)

where \( S_\alpha \neq \emptyset \) for any \( \alpha \), \( S_\alpha \cap S_\beta = \emptyset \) for any \( \alpha \neq \beta \), \( \langle v_j | v_k \rangle = 0 \) for any \( v_j \in S_\alpha, v_k \in S_\beta \) and \( \alpha \neq \beta \), any \( S_\alpha \) has one of the structures (A.a), (A.b), or (A.c) below, and any \( S_\alpha \) can not be further decomposed as \( S_\alpha = S_{\alpha_1} \cup S_{\alpha_2} \) with \( \{S_{\alpha_1}, S_{\alpha_2}\} \) having similar properties as \( S_\alpha \).

(A.a) \( S_\alpha = \{v_j\} \). \( S_\alpha \) contains only one element.

(A.b) \( S_\alpha = \{v_j, -v_k\}, \langle v_j | v_k \rangle = -\langle v_k | v_j \rangle \). \( S_\alpha \) contains two elements with opposite directions.

(A.c) \( S_\alpha = \{v_j\}_{j=1}^n \),

\[ -1 < \langle v_j | v_k \rangle \leq 0 \text{ for } \forall v_j, v_k \in S_\alpha, v_j \neq v_k. \] (A3)

\( S_\alpha \) contains more than one element.

For the case of (A.a), \( \dim(\text{span}\{S_\alpha\}) = 1 \); for the case of (A.b), \( \dim(\text{span}\{S_\alpha\}) = 1 \); for the case of (A.c),

\[ |S_\alpha| = \dim(\text{span}\{S_\alpha\}) \text{ or } |S_\alpha| = \dim(\text{span}\{S_\alpha\}) + 1. \] (A4)
Example 6. We first give a concrete example to explain Lemma 1. Suppose \( \{ \vec{v}_j \}_{j=1}^{n} \subseteq \mathbb{C}^{d} \setminus \{0 \} \) and \( \| \vec{v}_j \| = 1 \) for all \( j \), and in a fixed orthonormal basis of \( \mathbb{C}^{4} \), \( \{ \vec{v}_j \}_{j=1}^{6} \) read
\[
\vec{v}_1 = (1, 0, 0, 0), \\
\vec{v}_2 = (0, 1, 0, 0), \\
\vec{v}_3 = (0, 0, 1, 0), \\
\vec{v}_4 = (0, 0, 0, 1), \\
\vec{v}_5 = (0, 0, 0, 0).
\]

We see that \( \{ \vec{v}_j \}_{j=1}^{6} \) satisfies Eq. (A1). Eq. (A2) yields \( \{ \vec{v}_j \}_{j=1}^{6} = S_1 \cup S_2 \cup S_3 \), with \( S_1 = \{ \vec{v}_1, \vec{v}_2, \vec{v}_3 \} \), \( S_2 = \{ \vec{v}_4, \vec{v}_5, \vec{v}_6 \} \). For this case, \( S_1 \) has the form of (A.a), \( S_2 \) has the form of (A.b), \( S_3 \) has the form of (A.c).

Next we consider \( \{ \vec{v}_j \}_{j=1}^{8} \). We see that \( \{ \vec{v}_j \}_{j=1}^{8} \) satisfies Eq. (A1). Eq. (A2) yields \( \{ \vec{v}_j \}_{j=1}^{8} = S_1 \cup S_2 \cup S_3' \), with \( S_3' = \{ \vec{v}_4, \vec{v}_5 \} \). For this case, \( S_3' \) has the form of (A.c).

We depict \( S_1 \), \( S_2 \), \( S_3 \) and \( S_3' \) in Fig. 5. Evidently,
\[
|S_3'| = \dim(\text{span}\{S_3'\}) = 2, \\
|S_3| = \dim(\text{span}\{S_3\}) + 1 = 3.
\]

Applying Eq. (A3) to \( \{ \langle \vec{v}_j | \vec{v}_k \rangle \}_{j=1}^{4} \), we see that \( \{ x_{21}, x_{31}, x_{41} \} \) are all real and are all in \((-1, 0)\). Applying Eq. (A3) to \( \{ \langle \vec{v}_j | \vec{v}_k \rangle \}_{2 \leq j < k \leq 4} \), we see that \( \{ x_{22}x'_{32}, x_{22}x'_{32}x_{32}, x_{32}x'_{42}, x_{22}x_{32}x_{42} \} \) are all real, thus there exist \( \{ \theta, x'_{32}, x'_{32} \} \subseteq \mathbb{R} \) such that \( x_{32} = x'_{32}e^{i\theta}, x_{32} = x'_{32}e^{i\theta}, x_{22} = x_{32}x_{42}e^{i\theta} \). There is at most one zero in \( \{ x_{21}, x_{31}, x_{41} \} \), otherwise, suppose for example \( x_{21} = 0, x_{31} = 0, x_{22} = 1, x_{32} = 1 \), then \( x_{32} = 0 \), contradicting Eq. (A3). Similarly, there is no zero in \( \{ x_{22}, x_{32}, x_{42} \} \). Then Eq. (A3) requires \( x'_{32}x'_{32} \leq 0, x'_{32}x'_{32} \leq 0, x_{22}x_{32}x_{42} \leq 0, x_{22}x_{32}x_{42} \leq 0 \) all hold, these are certainly impossible. Hence, there do not exist four normalized vectors \( \{ \vec{v}_j \}_{j=1}^{4} \) satisfying Eq. (A3), and then Eq. (A4) holds for \( \dim(\text{span}\{S_3\}) = 2 \).

FIG. 5: In Example 6, \( S_1 \) has the form of (A.a), \( S_2 \) has the form of (A.b), \( S_3 \) and \( S_3' \) have the form of (A.c).

Proof of Lemma 1. For \( d = 1 \), since \( \{ \vec{v}_j \}_{j=1}^{n} \subseteq \mathbb{C}^{d} \setminus \{0 \} \) satisfies \( \| \vec{v}_j \| = 1 \) for all \( j \) and Eq. (A1), then it must hold that \( \{ \vec{v}_j \}_{j=1}^{n} = \{ \vec{v}_1 \} \) or \( \{ \vec{v}_j \}_{j=1}^{n} = \{ \vec{v}_1, -\vec{v}_1 \} \), then \( n = 1 \), the claim obviously holds.

For \( d \geq 2 \), we can always divide \( \{ \vec{v}_j \}_{j=1}^{n} \) into a union of nonempty sets \( \bigcup_{a=1}^{n} S_a \), such that any two vectors in distinct \( S_a \) are orthogonal, and any \( S_a \) can not be so decomposed further. If there exists \( \{ \vec{v}_j \}_{j=1}^{n} \subseteq \{ \vec{v}_j \}_{j=1}^{n} \) such that \( \langle \vec{v}_j | \vec{v}_k \rangle = 0 \) for any \( j \geq 2 \), let \( \{ \vec{v}_j \} \) be one element in the decomposition of Eq. (A2). If there exists \( \{ \vec{v}_1, \vec{v}_2 \} \subseteq \{ \vec{v}_j \}_{j=1}^{n} \) such that \( \vec{v}_1 = -\vec{v}_2 \), then Eq. (A1) implies that \( \langle \vec{v}_j | \vec{v}_1 \rangle = -\langle \vec{v}_j | \vec{v}_2 \rangle = 0 \) for any \( j > 2 \), let \( \{ \vec{v}_1, \vec{v}_2 \} \) be one element in the decomposition of Eq. (A2). In this way, we can take out all such elements of structure (A.a) and structure (A.b) in the decomposition of Eq. (A2). The remaining elements in Eq. (A2) must satisfy Eq. (A3), and we only need to prove Eq. (A4).

We prove Eq. (A4) by induction in the dimension \( \dim(\text{span}\{S_c\}) \). When \( \dim(\text{span}\{S_c\}) = 2 \), under any orthonormal basis \( \{ \vec{v}_j \}_{j=1}^{D} \) of span\{S_c\}, let \( \vec{e}_j = \vec{e}_{j}' \) for \( \{ j \}_{j=1}^{D} \). These three normalized vectors \( \{ v_1, v_2, v_3 \} \) certainly satisfy \( -1 < \langle \vec{v}_j | \vec{v}_k \rangle \leq 0 \) for all \( 1 \leq j < k \leq 3 \). Let \( S_c = \{ v_1, v_2 \} \), then \( \dim(\text{span}\{S_c\}) = 1 \). We now show that there do not exist four normalized vectors satisfying \( -1 < \langle \vec{v}_j | \vec{v}_k \rangle \leq 0 \) for all \( 1 \leq j < k \leq 4 \). Otherwise, if there exist such four normalized vectors \( \{ \vec{v}_j \}_{j=1}^{4} \), then we can choose an orthonormal basis \( \{ \vec{e}_j \}_{j=1}^{4} \) of span\{S_c\} with \( \vec{e}_j = \vec{e}_{j}' \), and expand \( \{ \vec{v}_j \}_{j=1}^{4} \) in \( \{ \vec{e}_j \}_{j=1}^{4} \) as
\[
\vec{v}_1 = (1, 0), \\
\vec{v}_2 = (x_{21}, x_{22}), \\
\vec{v}_3 = (x_{31}, x_{32}), \\
\vec{v}_4 = (x_{41}, x_{42}).
\]
this contradicts the hypothesis that $x_{j+1} = 0$ for all $j > 3$ and any vector in $(\langle v_j | v_j \rangle)_{j=1}^{D+2} \setminus \{v_1, v_2, v_3\}$ is orthogonal to any vector in $(\langle v_{j+1} | v_{j+1} \rangle)_{j=1}^{D+2}$, that is, $(\langle v_j | v_j \rangle)_{j=1}^{D+2}$ can be further decomposed as $(\langle v_j | v_j \rangle)_{j=1}^{D+2} = \{v_1, v_2, v_3\} \cup (\langle v_{j+1} | v_{j+1} \rangle)_{j=1}^{D+2} \setminus \{v_1, v_2, v_3\}$, this also contradicts the hypothesis. As a result, $(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2}$ satisfies $-1 < \frac{X_j}{||X_j||} \cdot X_k \leq 0$. Together with Eq. (A5), hence $(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2}$ satisfies

$$-1 < \frac{X_j}{||X_j||} \cdot X_k \leq 0. \quad (A12)$$

We divide $(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2}$ into a union of nonempty sets such that any two vectors in distinct sets are orthogonal,

$$(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2} = \bigcup_{\alpha=1}^{\tilde{m}} T_{\alpha}. \quad (A13)$$

and each $T_{\alpha}$ can not be decomposed further, as we have done for $(\langle v_j | v_j \rangle)_{j=1}^{n}$ in Eq. (A2). In Eq. (A13), each of $(T_{\alpha})_{\alpha=1}^{\tilde{m}}$ has structure (A,a) or (A,c), but not (A,b), since in Eq. (A12), $-1 < \frac{X_j}{||X_j||} \cdot X_k$ but not $-1 < \frac{X_j}{||X_j||} \cdot X_k$. If $\tilde{m} \geq 2$, since $(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2}$ are all real and are all in $[0, 1]$, with Eq. (A3), then there is only one $T_{\alpha}$ (without loss of generality, suppose $T_{\alpha} = T_1$) in $(T_{\alpha})_{\alpha=1}^{\tilde{m}}$ such that $x_{j+1} = 0$ if $\frac{X_j}{||X_j||} \notin T_1$. Consequently, $(\langle v_j | v_j \rangle)_{j=1}^{D+2}$ can be further decomposed by $(\langle v_j | v_j \rangle)_{j=1}^{D+2} \setminus \{v_1, v_2, v_3\}$, this contradicts the hypothesis. Then $\{X_j\}_{2 \leq j \leq D+2}$ is of structure (A,c) and can not be decomposed further. Since each of $(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2}$ has $D - 1$ components by definition, then

$$\dim(\langle x_i | x_i \rangle)_{2 \leq j \leq D+2}) \leq D - 1. \quad (A14)$$

Eq. (A14) contradicts the induction hypothesis that Eq. (A4) is true for all space dimensions $\dim(\langle S_{j+1} \rangle) = 1, 2, 3, ..., D - 1$, with $D \geq 3$. In conclusion, there do not exist $D + 2$ normalized vectors $(\langle v_j | v_j \rangle)_{j=1}^{D+2}$ satisfying Eq. (A3). Then Eq. (A4) holds.

We remark that Lemma 1 can be viewed as a generalization of Lemma 14 in Ref. [58].

Notice that, we can also express Lemma 1 in a slightly different form. When $(\langle v_j | v_j \rangle)_{j=1}^{n} \subseteq C^{d} \setminus \{0\}$ are not necessarily normalized, we can use $(\frac{\langle v_j | v_j \rangle}{||v_j||})_{j=1}^{n} \subseteq C^{d} \setminus \{0\}$ to replace $(\langle v_j | v_j \rangle)_{j=1}^{n} \subseteq C^{d} \setminus \{0\}$.

[1] J. G. Kirkwood, Quantum statistics of almost classical assemblies, Phys. Rev. 44, 31 (1933).
[2] P. A. M. Dirac, On the analogy between classical and quantum mechanics, Rev. Mod. Phys. 17, 195 (1945).
[3] V. Bargmann, Note on wigner’s theorem on symmetry operations, Journal of Mathematical Physics 5, 862
quasiprobability, arXiv preprint arXiv:2309.09162.

[42] J. B. Hartle, Linear positivity and virtual probability, Phys. Rev. A 70, 022104 (2004).

[43] R. B. Griffiths, Consistent histories and the interpretation of quantum mechanics, Journal of Statistical Physics 36, 219 (1984).

[44] S. Goldstein and D. N. Page, Linearly positive histories: Probabilities for a robust family of sequences of quantum events, Phys. Rev. Lett. 74, 3715 (1995).

[45] H. F. Hofmann, M. E. Goggin, M. P. Almeida, and M. Barbieri, Estimation of a quantum interaction parameter using weak measurements: Theory and experiment, Phys. Rev. A 86, 040102 (2012).

[46] H. F. Hofmann, Complex joint probabilities as expressions of reversible transformations in quantum mechanics, New Journal of Physics 14, 043031 (2012).

[47] M. Hofmann and G. Schaller, Probing nonlinear adiabatic paths with a universal integrator, Phys. Rev. A 89, 032308 (2014).

[48] S. Hofmann and M. Schneider, Classical versus quantum completeness, Phys. Rev. D 91, 125028 (2015).

[49] H. F. Hofmann, On the fundamental role of dynamics in quantum physics, The European Physical Journal D 70, 1 (2016).

[50] J. J. Halliwell, Leggett-garg inequalities and no-signaling in time: A quasiprobability approach, Phys. Rev. A 93, 022123 (2016).

[51] B. C. Stacey, Quantum theory as symmetry broken by vitality, arXiv preprint arXiv:1907.02432 (2019).

[52] M. Ban, On sequential measurements with indefinite causal order, Physics Letters A 403, 127383 (2021).

[53] A. Budiyono, B. E. Gunara, B. E. B. Nurhandoko, and H. K. Dipojono, General quantum correlation from non-real values of kirkwood-dirac quasiprobability over orthonormal product bases, Journal of Physics A: Mathematical and Theoretical 56, 435301 (2023).

[54] A. E. Rastegin, On kirkwood-dirac quasiprobabilities and unravelings of quantum channel assigned to a tight frame, arXiv preprint arXiv:2304.14038 (2023).

[55] D. R. M. Arvidsson-Shukur, J. C. Drori, and N. Y. Halpern, Conditions tighter than noncommutation needed for nonclassicality, Journal of Physics A: Mathematical and Theoretical 54, 284001 (2021).

[56] S. De Bièvre, Complete incompatibility, support uncertainty, and kirkwood-dirac nonclassicality, Phys. Rev. Lett. 127, 190404 (2021).

[57] J. Xu, Classification of incompatibility for two orthonormal bases, Phys. Rev. A 106, 022217 (2022).

[58] S. De Bièvre, Relating incompatibility, noncommutativity, uncertainty and kirkwood-dirac nonclassicality, Journal of Mathematical Physics 64, 022202 (2023).

[59] Z. Song and L. Chen, On the zero entries in a unitary matrix, Linear and Multilinear Algebra 70, 1271 (2022).

[60] C. Langrenez, D. R. M. Arvidsson-Shukur, and S. De Bièvre, Characterizing the geometry of the kirkwood-dirac positive states, arXiv preprint arXiv:2306.00086 (2023).