Resource theory of superposition: State transformations

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A combination of a finite number of linear independent states forms superposition in a way that cannot be conceived classically. Here, using the tools of resource theory of superposition, we give the conditions for a class of superposition state transformations. These conditions strictly depend on the scalar products of the basis states and reduce to the well-known majorization condition for quantum coherence in the limit of orthonormal basis. To further superposition-free transformations of d-dimensional systems, we provide superposition-free operators for a deterministic transformation of superposition states. The linear independence of a finite number of basis states requires a relation between the scalar products of these states. With this information in hand, we determine the maximal superposition states which are valid over a certain range of scalar products. Notably, we show that, for d ≥ 3, scalar products of the pure superposition-free states have a greater place in seeking maximally resourceful states. Various explicit examples illustrate our findings.

I. INTRODUCTION

Research and understanding of the principles of quantum mechanics offer tremendous potential for developing new (quantum) technologies. Quantum superposition [1] is one of the most pivotal nonclassical features that can be dealt with in this context. The existence of superposition as a resource delivers significant performance gains on many information processing tasks that cannot be classically achievable. Two particular examples are communication complexity [2, 3], and channel discrimination task [4]. While the role of superposition in such scenarios is invaluable, it is essential to acquire a thorough understanding of superposition as a resource.

What we know about any study of quantum resource theories (QRTs) [5, 6] is to start with defining two main elements: the free states and the free operations. The key point is that the free operations must transform free states into free states and allow for the resource to be manipulated but not freely created. From the perspective of QRTs, a leading guide is quantum entanglement [7]. In the case of entanglement theory, the free states and the free operations are the separable states and local operations and classical communication, respectively. All states which are not free contain resource and are considered costly, and free operations are physical transformations which do not create any resources (for reviews, see Refs. [5, 6]). Recently, researchers [8] have extended the tools of QRTs to scenarios in which multiple resources are present and derived conditions for the interconversion of these resources. In Ref. [8], their construction of multi-resource theories is based on the definition of their class of allowed operations. Over the past decade a considerable amount of literature has been published on various resource theories [9–23].

The existing body of research on quantum superposition aims to characterize it in all its parts. To this end, quantitative understandings of coherent superposition of quantum states have been achieved [4, 24, 25]. By relaxing the orthogonality of the basis states to linear independence, superposition theory can be formed as a generalization of the coherence theory [26]. In this sense, Theurer et al. [4] introduced a resource theory of superposition. There, using the tools of QRTs, superposition-free states and operations were defined, and several quantitative superposition measures were proposed. Åberg [24] introduced the concept of superposition measures with respect to given orthogonal decompositions of the Hilbert space of a quantum system. The notion of quantum coherence for superpositions over states which are not necessarily mutually orthogonal was presented in Ref. [25]. Beyond states, coherent superpositions are also possible among quantum evolutions [27]. The author of Ref. [27] developed a resource theoretic framework to quantify superposition present in a quantum evolution.

Given a particular set of resources, a fundamental aspect of any QRTs is the manipulation of these resources. This task deals with whether it is possible to transform one resource into another under free operations. In this paper, inspired by Ref. [28], we study the transformations of single copies of the pure superposition states. We here provide superposition-free operators for a deterministic transformation and give the conditions for a class of superposition state transformations whereby the tools of resource theory of superposition [4] are utilized. These conditions strictly depend on the scalar products of the basis states and reduce to the well-known majorization condition in the limit of coherence theory [29], i.e., in the limit of orthonormal basis. Moreover, we determine the maximal superposition states—the state with the greatest resource value—which are valid over a certain range of scalar products. We show that states with the symmetric superposition of the basis states is the maximally resourceful one for a given set of pure superposition states. Such contributions are important for our understanding of resource theory of superposition. To reinforce our findings, we give various examples.

The structure of the paper is as follows. Section II reviews the basics of the resource theory of superposition. In Sec. III we discuss the superposition-free transformations. The linear independence of basis states is truly at the core of the superposition state transformations. We discuss this crucial point in Sec. III A. We then present a clear explanation for the deterministic transformation of superposition states in Sec. III B.

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We focus on the maximal resourceful states in Sec. IV: qubit systems in Sec. IV A and d-dimensional systems in Sec. IV B. We conclude our work in Sec. V.

II. OVERVIEW OF THEORY

Before scrutinizing the superposition-free transformations, it is useful to review some of the basics of the resource theory of superposition. For a rigorous resource theory framework for the quantification of superposition we refer to [4, 24].

Let \( \{|c_i\}_i \) be a normalized, linear independent and not necessarily orthogonal basis of the Hilbert space represented by \( \mathbb{C}^d \), \( d \in \mathbb{N} \). Any density operator written as

\[
\rho = \sum_{i=1}^d \rho_i |c_i\rangle \langle c_i|,
\]

where the \( \rho_i \) form a probability distribution, is called superposition-free. The set of superposition-free density operators is denoted by \( \mathcal{F} \) and forms the set of free states. All density operators which are not superposition-free are called superposition states and form the set of resource states [4]. Then the pure superposition states are in the form \( |\psi\rangle = \sum_{i=1}^d \psi_i |c_i\rangle \).

A Kraus operator \( K_i \) is called superposition-free if \( K_i \rho K_i^\dagger \in \mathcal{F} \) for all \( \rho \in \mathcal{F} \). More precisely, a Kraus operator \( K_n \) is superposition-free if and only if it is of the form

\[
K_n = \sum_k c_{k,n} |c_{k,n}(k)\rangle \langle c_{k,n}^\dagger|,
\]

where \( c_{k,n} \in \mathbb{C} \), \( f_n(k) \) are arbitrary index functions [4], and \( \langle c_{k,n}^\dagger|c_{j}\rangle = \zeta_i \delta_{ij} \) for \( \zeta_i \in \mathbb{C} \) where the vectors \( |c_{k,n}^\dagger\rangle \) are normalized. Moreover, quantum operations \( \Phi(\rho) \) are called superposition-free if they are trace preserving and can be written such that \( \Phi(\rho) = \sum_i K_i \rho K_i^\dagger \), where all \( K_i \) are free. The set of superposition-free operations forms the free operations and is denoted by \( \mathcal{F}O \).

One of the most common procedures for defining an order relation between the resource states is related to the concept of free operations. If a state \( \rho \) can be transformed into another state \( \sigma \) by some free operation, then \( \rho \) cannot be less resourceful than \( \sigma \) since any task achievable by \( \sigma \) is also achievable by \( \rho \). However, the converse is not necessarily true. Furthermore, one can introduce resource quantifiers as functionals that preserves this order. To this goal, the \( l_1 \) norm of superposition [4] was introduced, and is given by

\[
l_1(\rho) = \sum_{i \neq j} |\rho_{ij}|,
\]

for \( \rho = \sum_{i,j} \rho_{ij} |c_i\rangle \langle c_j| \). We will use the \( l_1 \) norm of superposition when comparing the resource value of two states. With these definitions at hand, we are ready to present our protocol and results for the superposition-free transformations.

III. SUPERPOSITION-FREE TRANSFORMATIONS

A. Gram Matrix and Linear Independence of Basis States

Two particularly important points are worth highlighting. First, scalar products of the basis states determine the whole structure of the superposition state transformations. In Sec. (III B) we will give the conditions for a deterministic transformation that clearly depend on the scalar products. Second, for the linear independence of the basis states \( \{|c_i\}_i \), scalar products must obey a certain inequality.

**Gram matrix** is a useful tool to compute whether a given set of vectors are linearly independent [30, 31]. A set of vectors are linearly independent if and only if the determinant of the Gram matrix is positive definite [32]. Given a finite set of vectors \( \{v_1, v_2, \ldots, v_m\} \) in an inner products space, the **Gram matrix** of the vectors \( \{v_1, v_2, \ldots, v_m\} \) with respect to the inner product \( \langle \cdot | \cdot \rangle \) is \( G = [\langle v_i | v_j \rangle]_{i=1,\ldots,m} \in M_{m \times m} \) where \( M_{m \times m} \) is a \( m \times m \) square matrix [32]. The Gram matrix is positive definite if and only if the vectors \( \{v_1, v_2, \ldots, v_m\} \) are linearly independent. Otherwise, it is positive semi-definite. For instance, if one transforms an orthonormal basis to a linear independent basis with a transformation matrix \( V \) in a way that \( V|i\rangle = |c_i\rangle \) then the Gram matrix equals to \( V^\dagger V \). Moreover, for given two vectors \( |\psi\rangle = \sum_i \psi_i |c_i\rangle \) and \( |\phi\rangle = \sum_m \phi_m |c_m\rangle \), the inner product can be expressed as \( \langle \psi | \phi \rangle = \sum_i G_{ij} \psi_i \phi_j \) (i.e., Gram matrix is a metric tensor [33]) where \( G_{ij} \) is complex conjugate of \( G_{ij} \).

We show that majorization conditions obtained for the superposition and the coherence theories are related by the Gram matrix (see Appendix (A)).

To obtain the inequality between scalar products, one can construct the corresponding Gram matrix for a given set of basis vectors \( \{|c_1\rangle, |c_2\rangle, \ldots, |c_d\rangle \} \). Defining \( \langle c_i|c_j\rangle := \mu_{ij} \), then the Gram matrix can be written in the following way:

\[
G = \begin{pmatrix}
1 & \mu_{12} & \cdots & \mu_{1d} \\
\mu_{21} & 1 & \cdots & \mu_{2d} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{d1} & \mu_{d2} & \cdots & 1
\end{pmatrix}.
\]

Consider the case \( d = 2 \); \( \det(G) = 1 - |\mu_{12}|^2 > 0 \). If we take \( \mu_{12} \in \mathbb{R} \) it is obvious that \( \mu_{12} \in (-1,1) \). However, for \( d \geq 3 \) the scalar products are constrained with a certain inequality. Consider the case \( d = 3 \) and \( \mu_{ij} \in \mathbb{R} \), we have,

\[
\det(G) = 1 - \mu_{12}^2 - \mu_{13}^2 - \mu_{23}^2 + 2 \mu_{12} \mu_{13} \mu_{23} > 0.
\]

Therefore, linear independence of the basis states requires a relation between the scalar products of basis states for \( d \geq 3 \), e.g., Eq. (5) for \( d = 3 \).

Importantly, since the difficulty of the superposition state transformations is mainly caused by nonorthogonality, we take all the scalar products real and equal throughout the rest of the paper for simplicity and convenience: \( \langle c_i|c_j\rangle = \mu \) for \( i \neq j \). Taking the scalar products such that, one can immediately obtain \( -1/2 < \mu < 1 \) for \( d = 3 \) from Eq. (5). By considering a linear independent set \( \{|c_i\}_i \), one can then obtain \( 1/(1-d) < \mu < 1 \) for \( d \geq 2 \). This is one of our starting points to explore superposition-free transformations. We remark that
the conditions for a deterministic transformation presented below also hold in nonequal scalar products settings, i.e., when \( \langle c_i | c_j \rangle = \mu_{ij} \) for \( i \neq j \).

### B. Deterministic Transformations of Superposition States

In this subsection, we present a clear explanation for the deterministic transformation of superposition states. We consider the transformations between single copies of pure states. The problem is to transform an initial state \( |\psi\rangle \) into a final state \( |\phi\rangle \) under superposition-free operators:

\[
|\psi\rangle = \sum_{i=1}^d \psi_i |c_i\rangle \xrightarrow{\mathcal{E}_0} |\phi\rangle = \sum_{i=1}^d \phi_i |c_i\rangle. \tag{6}
\]

Here the superposition states under consideration have nonzero real coefficients \( \psi_i \) and \( \phi_i \). The initial and final states have thus same superposition rank [4], i.e., the number of nonzero coefficients of \( |\psi\rangle \) and \( |\phi\rangle \) are equal, \( r_S(|\psi\rangle) = r_S(|\phi\rangle) = d \). Since we take all the scalar products equal, the coefficients \( \psi_i \) and \( \phi_i \) can be ordered with superposition-free map operators in a way that \( |\psi_l\rangle \geq |\psi_{l+1}\rangle \) and \( |\phi_l\rangle \geq |\phi_{l+1}\rangle \) for any \( l \in [1,d-1] \). We also note that the states \( |\psi\rangle \) and \( |\phi\rangle \) given in Eq. (6) are normalized, that is \( \sum_i \psi_i (\psi_i + \mu \psi_j) = 1 \) and \( \sum_i \phi_i (\mu \phi_i + \phi_j) = 1 \) where \( i \neq j \).

Now we construct superposition-free operators for the transformation given by Eq. (6). There are \( d! \) different ordering index functions \( f_n(k) \). Thus, the number of Kraus operators which leaves the superposition rank of a \( d \)-dimensional initial state invariant is equal to \( d! \) in general [4]. However, in our framework of superposition-free operators are sufficient, and they are given by

\[
K_n = \sum_{k=1}^d c_{k,n} |c_{f_n(k)}\rangle \langle c_{f_n(k)}|, \tag{7}
\]

for \( n = 1,2,\ldots,d \) where \( c_{k,n} = \sqrt{p_n} (\phi_{f_n(k)}/\psi_k) \). The Kraus operators \( \{K_n\}_{n=1}^d \) given by Eq. (7) are the most general superposition-free operators which give the desired state with probabilities \( \{p_n\}_{n=1}^d \), respectively, i.e.,

\[
K_n |\psi\rangle = \sqrt{p_n} \sum_{k=1}^d \phi_{f_n(k)} |c_{f_n(k)}\rangle = \sqrt{p_n} |\phi\rangle. \tag{8}
\]

where \( p_n \geq 0 \) and \( \sum_{n=1}^d p_n = 1 \). To satisfy the completeness relation, we introduce another set of superposition-free Kraus operators which are given by [4]

\[
F_m = \sum_{k=1}^d c_{k,m} \frac{|c_{f_m(k)}\rangle \langle c_{f_m(k)}|}{|c_k\rangle \langle c_k|}, \tag{9}
\]

for \( m = (d+1), (d+2), \ldots, 2d \) where \( c_{k,m} \in \mathbb{C} \). Then the completeness relation is written as

\[
\sum_{n=1}^d K_n^\dagger K_n + \sum_{m=d+1}^{2d} F_m^\dagger F_m = I. \tag{10}
\]

### TABLE I. The table shows us the order of the index functions \( f_n(k) \). From (8) we have outputs \( \sum_{k=1}^d \phi_{f_n(k)} |c_{f_n(k)}\rangle \), and here we give the values of \( \{f_n(k)\}_{k=1}^d \) for \( d = 2, 3, 4 \) and \( n = 1, 2, \ldots, d \). The first row of the table shows the index functions for the Kraus operators \( K_1 \) and \( K_2 \), respectively; The second and third row of the table corresponds to a particular case of \( d = 3 \), \( \psi_2 \geq \psi_3 \) for the former and \( \psi_2 \leq \psi_3 \) for the latter; and the rest are for 4-dimensional systems where each one corresponds to a particular case, e.g., the fourth row of the table (first case of \( d = 4 \)) corresponds to the case \( \psi_2 \geq \psi_3 \) and \( \psi_1 \geq \psi_4 \).

| \( f_n(k) \) |
|-----------------|
| \( f_1(k) \) |
| \( f_2(k) \) |
| \( f_3(k) \) |
| \( f_4(k) \) |

| \( d=2 \) |
| \( \{1,2\} \) |
| \( \{2,1\} \) |

| \( d=3 \) |
| \( \{1,2,3\} \) |
| \( \{3,2,1\} \) |
| \( \{2,1,3\} \) |
| \( \{2,3,1\} \) |
| \( \{1,4,3,2\} \) |
| \( \{1,3,2,4\} \) |
| \( \{1,2,3,4\} \) |

| \( d=4 \) |
| \( \{1,2,3,4\} \) |
| \( \{4,2,3,1\} \) |
| \( \{2,1,3,4\} \) |
| \( \{3,2,1,4\} \) |
| \( \{2,1,3,4\} \) |
| \( \{4,2,3,1\} \) |
| \( \{1,4,3,2\} \) |
| \( \{1,3,2,4\} \) |
| \( \{1,2,3,4\} \) |

While the Kraus operators defined by Eq. (7) give the target state (as seen from Eq. (8)), the Kraus operators \( \{F_m\}_{m=(d+1)}^{2d} \) give nothing, i.e., \( F_m |\psi\rangle = 0 \).

Next step is to determine the index functions \( f_n(k) \). To this goal, we benefit from the results of deterministic transformations of coherent states under incoherent operations presented in Ref. [28]. There, incoherent Kraus operators were constructed for \( d \)-dimensional systems by explicitly presenting permutations. These permutations provide us the index functions \( f_n(k) \). We then define

\[
|c_{f_n(k)}\rangle := |c_k\rangle, \tag{11}
\]

\[
|c_{f_n(k)}\rangle := |c_{m-d}\rangle, \tag{12}
\]

and for each \( n \in [2,d] \) there is a pair \( (\alpha, \beta) \in [1,d] \) such that

\[
|c_{f_n(\alpha)}\rangle := |c_\beta\rangle, \quad |c_{f_n(\beta)}\rangle := |c_\alpha\rangle. \tag{13}
\]

This corresponds to the permutation \(|\alpha\rangle \leftrightarrow |\beta\rangle| \) for coherence transformations [28]. Then we have

\[
|c_{f_n(\gamma)}\rangle := |c_\gamma\rangle, \tag{14}
\]

for \( n \in [2,d] \) and \( \gamma = 1,2,\ldots,d \) but \( \gamma \neq \alpha \) and \( \gamma \neq \beta \). To clarify above definitions which are related with the results [28] we give the terms \( \{f_n(k)\}_{k=1}^d \) for \( d = 2, 3, 4 \) (see Table (I)).

So far, we have introduced the superposition-free Kraus operators to be used. Now we investigate the condition(s) for superposition-free transformations. The authors of Ref. [29] built the counterpart of the celebrated Nielsen theorem [34] for coherence manipulations and showed that majorization is the necessary and sufficient condition for a deterministic transformation. In this respect, in principle, a similar approach is highly expected for superposition manipulation. In the following we give the condition(s) for the superposition-free transformations given by Eq. (6).
The completeness relation given by (10) is essential for us to investigate condition(s) for deterministic transformations. We start by defining

$$\tilde{\psi}_i := \psi_i(\Psi_i + \mu \sum_{j=1 \atop (j \neq i)}^d \psi_j), \quad \tilde{\phi}_i := \phi_i(\Phi_i + \mu \sum_{j=1 \atop (j \neq i)}^d \phi_j),$$

(15)

for $i = 1, 2, \ldots, d$ where the coefficients $\tilde{\psi}_i$ and $\tilde{\phi}_i$ are in an order such that $\tilde{\psi}_i \geq \tilde{\psi}_{i+1}$ and $\tilde{\phi}_i \geq \tilde{\phi}_{i+1}$ for any $l \in [1, d - 1]$. Using superposition-free operators given by (7) and (9) it may be possible to transform $|\psi\rangle$ into another state $|\phi\rangle$ deterministically if the majorization (for superposition) is satisfied:

**Majorization:** $\sum_{i=1}^k \tilde{\psi}_i \leq \sum_{i=1}^k \tilde{\phi}_i$, \hspace{1cm} (16)

for any $k \in [1,d]$ where equality holds for $k = d$. Contrary to coherence manipulation [29], majorization alone is not the necessary and sufficient condition for superposition-free transformations. The completeness equation given by (10) also dictates one more condition to be satisfied, which we call as condition on completeness (CoC). It is given such that

**CoC:** $\sum_{i=1}^d p_i \omega_{ij} \leq \psi_j^2$, \hspace{1cm} (17)

for $j = 2, 3, \ldots, d$. Here $\omega_{ij}$ is the $(ij)$th element of a $d \times d$ matrix $\omega$. There exists a permutation matrix $P_i$ such that

$$\begin{pmatrix} \omega_{11} \\ \omega_{22} \\ \vdots \\ \omega_{dd} \end{pmatrix} = P_i \begin{pmatrix} \phi_1^2 \\ \phi_2^2 \\ \vdots \\ \phi_d^2 \end{pmatrix}. \hspace{1cm} (18)$$

This $P_i$ corresponds with the permutation $|\alpha\rangle \leftrightarrow |\beta\rangle$ given in Eq. (13). Also, first row of the matrix $\omega$ is equal to $(\phi_1^2, \phi_2^2, \ldots, \phi_d^2)$, i.e., $P_1$ is identity. To obtain the probabilities $\{p_n\}_{n=1}^d$ in Eq. (8) (and in Eq. (17)) one needs to solve the following equations

$$\sum_{n=1}^d p_n \tilde{\phi}_{nk}(k) = \psi_k, \hspace{1cm} k = 1, 2, \ldots, d. \hspace{1cm} (19)$$

When (16) and (17) are both satisfied for a transformation $|\psi\rangle \xrightarrow{\text{CoC}} |\phi\rangle$, then $l_1(|\psi\rangle \langle \psi|) \geq l_1(|\phi\rangle \langle \phi|)$ (see Fig. (1)), i.e., neither is sufficient alone for a deterministic transformation. In addition, the theory of superposition contains coherence theory as a special case. In this respect, when the basis states are orthogonal, i.e., for $\mu = 0$, Eq. (16) turns into the well known majorization condition for coherence [29] and the equality holds in Eq. (17) as well. Obtaining (16) and (17) requires some algebra which we do in Appendix (B).

1. Qubit systems

To establish a useful and efficient protocol for the superposition-free transformation, first the problem should be solved in all its details for the simplest case, $d = 2$. In this direction, let us consider the transformation

$$|\psi_1 e^{i\alpha_1} |c_1\rangle + |\psi_2 e^{i\alpha_2} |c_2\rangle \xrightarrow{\text{CoC}} |\phi_1 e^{i\beta_1} |c_1\rangle + |\phi_2 e^{i\beta_2} |c_2\rangle, \hspace{1cm} (20)$$

where $\alpha_i \in [0, 2\pi], \beta_i \in [0, 2\pi]$, and $\langle c_1 | c_2 \rangle = \mu$. This is the most general transformation for qubit systems. The states are normalized as usual and we can choose, without loss of generality, $\alpha_1 = \beta_1 = 0$. In what follows we show that different choices of local phases $\alpha_2$ and $\beta_2$ produce different results.

We start with the case $\alpha_2 = \beta_2 = 0$. There is no local phase for both the initial and the final states. By using the superposition-free operators

$$K_1 = \sqrt{p_1} \left( \begin{array}{c} \phi_1 \\ \psi_1 \end{array} \right) \left( \begin{array}{c} |c_1\rangle \\ (c_1^\dagger |c_1\rangle) \end{array} \right) + \sqrt{p_2} \left( \begin{array}{c} \phi_2 \\ \psi_2 \end{array} \right) \left( \begin{array}{c} |c_2\rangle \\ (c_2^\dagger |c_2\rangle) \end{array} \right), \hspace{1cm} (21)$$

$$K_2 = \sqrt{p_3} \left( \begin{array}{c} \phi_2 \\ \psi_2 \end{array} \right) \left( \begin{array}{c} |c_2\rangle \\ (c_2^\dagger |c_2\rangle) \end{array} \right) + \sqrt{p_4} \left( \begin{array}{c} \phi_1 \\ \psi_1 \end{array} \right) \left( \begin{array}{c} |c_1\rangle \\ (c_1^\dagger |c_1\rangle) \end{array} \right), \hspace{1cm} (22)$$

$F_3,$ and $F_4$ defined by (9), one can achieve the transformation $|\psi\rangle \xrightarrow{\text{CoC}} |\phi\rangle$ deterministically where $K_1 |\psi\rangle = \sqrt{p_1} |\phi\rangle$, $K_2 |\psi\rangle = \sqrt{p_2} |\phi\rangle$, $F_3 |\psi\rangle = 0$, and $F_4 |\psi\rangle = 0$. The completeness condition defined by Eq. (10) gives us three equations. By using (15), the first two can be written as

$$p_1 \phi_1 + p_2 \phi_2 = \psi_1, \hspace{1cm} p_1 \phi_2 + p_2 \phi_1 = \psi_2, \hspace{1cm} (23)$$

where $p_1 + p_2 = 1$. Then the probabilities are found to be

$$p_1 = \frac{\phi_1 - \psi_2}{\phi_1 - \phi_2}, \hspace{1cm} p_2 = \frac{\psi_2 - \phi_1}{\phi_1 - \phi_2}. \hspace{1cm} (24)$$
The positivity of the probabilities given by Eq. (24) leads to the condition (16). Another constraint on the Kraus operators comes from the third equation of the completeness condition (10) which implies

$$c_{2,3}^2 + c_{2,4}^2 = \left(\frac{\mu}{\sqrt{\mu^2}}\right) (\psi_1 \psi_2 - \psi_1 \psi_2).$$

(25)

The left-hand side of the above is non-negative, yielding

$$\mu(\psi_1 \psi_2 - \psi_1 \psi_2) \geq 0.$$  

This inequality can be written such that

$$p_1 \psi_2^2 + p_2 \psi_2^2 \leq \psi_2^2,$$  

(26)

which gives us the condition (17) for qubit systems. Thus, a single condition, (16), is not sufficient and one more condition, (17), is necessary. Also, equality holds in Eq. (26) and the results become same with Ref. [28] in the limit of orthonormal basis.

Note that the explicit construction of $F_3$ and $F_4$ is not necessary [4]. Here, different choices of $c_{2,3}$ and $c_{2,4}$ given in Eq. (25) give us different sets of $\{F_3, F_4\}$, provided that Eq. (25) is satisfied. For instance, if we choose $c_{2,4} = 0$ and $c_{2,3} = 0$ then we have only three superposition-free Kraus operators, $\{K_1, K_2, F_1\}$ (or $\{K_1, K_2, F_2\}$). On the other hand, for $c_{2,3} \neq 0$ and $c_{2,4} \neq 0$, we need four superposition-free Kraus operators to make the entire operation trace preserving.

To better understand what we aim to depict by the Fig. (1), let us consider the following examples. We have an initial state $|\psi\rangle$ and a target state $\varphi$, i.e., we have a pair of superposition states such that $\{|\psi\rangle, |\varphi\rangle\}$, for each region $R_i, i = 1, \ldots, 5$:

$$R_1 : \left\{\frac{3|c_1| - |c_2|}{\sqrt{7}}, \frac{4|c_1| - |c_2|}{\sqrt{13}}\right\},$$

(27)

$$R_2 : \left\{\frac{3|c_1| + |c_2|}{\sqrt{13}}, \frac{4|c_1| - |c_2|}{\sqrt{13}}\right\},$$

(28)

$$R_3 : \left\{\frac{4|c_1| + |c_2|}{\sqrt{21}}, \frac{3|c_1| + |c_2|}{\sqrt{13}}\right\},$$

(29)

$$R_4 : \left\{\frac{3|c_1| + |c_2|}{\sqrt{13}}, \frac{4|c_1| + |c_2|}{\sqrt{21}}\right\},$$

(30)

$$R_5 : \left\{\frac{4|c_1| - |c_2|}{\sqrt{13}}, \frac{3|c_1| + |c_2|}{\sqrt{13}}\right\},$$

(31)

and $\mu = 1/2$. The majorization condition given by (16) and CoC given by (17) are only satisfied for the pair of states given in (27). Then it is easy to show that the transformation $|\psi\rangle \xrightarrow{FC} |\varphi\rangle$ given in Eq. (27) can be achieved deterministically: $K_1 |\psi\rangle = \frac{300}{2000} |\varphi\rangle$, $K_2 |\psi\rangle = \frac{1000}{2000} |\varphi\rangle$, $F_1 |\psi\rangle = 0$, and $F_2 |\psi\rangle = 0$. However, for the pairs of states given in (28), (29), (30), and (31) a deterministic transformation is not possible under superposition-free operations while the conditions (16) and (17) are not satisfied at the same time. As it is seen from the given examples, the $l_1$ norm of superposition of the initial state is greater than the final state both for given examples (30) and (31). Furthermore, the transformations given in Eqs. (28) and (31) and Eqs. (29) and (30) are obviously the opposite of each other, i.e., neither $|\psi\rangle \xrightarrow{FC} |\varphi\rangle$ nor $|\varphi\rangle \xrightarrow{FC} |\psi\rangle$ is a deterministic transformation. Overall, for a given initial state $|\psi\rangle$ and final state $|\varphi\rangle$, $l_1(|\psi\rangle) \geq l_1(|\varphi\rangle)$ does not necessarily mean that the state $|\psi\rangle$ can be transformed into the state $|\varphi\rangle$ with unit probability under the superposition-free operators.

Defining $\psi_1/\psi_2 := \alpha$ and $\varphi_1/\varphi_2 := \beta$ and after some algebra, it is possible to reduce the conditions for a deterministic transformation, for qubit systems, into the following forms:

$$\lambda < 0 \Rightarrow 0 \leq \mu < -\frac{\kappa + \lambda}{1 + \kappa \lambda}.$$  

(32)

or

$$\lambda > 0 \Rightarrow -\frac{\kappa + \lambda}{1 + \kappa \lambda} < \mu \leq 0,$$  

(33)

where $|\kappa| \geq |\lambda|$ for both cases. The inferences about (32) and (33) are fairly straightforward. A deterministic transformation can be achieved only for certain values of scalar product of basis states depending on whether the $\lambda$ is negative or positive. Furthermore, Eq. (32) and Eq. (33) exhibit a clear observation about maximal superposition states for qubit systems. If $\lambda = -1$ then $0 \leq \mu < 1$ and if $\lambda = 1$ then $-1 < \mu \leq 0$. Thus, there are two maximal superposition states for qubit systems: one is $\psi_1 = -\psi_2$ with $\mu \in [0, 1)$ and the other is $\psi_1 = \psi_2$ with $\mu \in (-1, 0]$. We will discuss the maximal superposition states in Sec. (IV). However, seeking maximal superposition states becomes dramatically harder for $d > 2$.

We conclude by briefly considering two other possible cases: only the final state has a local phase, i.e., $\alpha_2 = 0 \& \beta_2 \neq 0$, or only the initial state has a local phase, i.e., $\alpha_2 \neq 0 \& \beta_2 = 0$. While a deterministic transformation is possible for the former only when $\psi_1 = +\psi_2$, a deterministic transformation is not possible for the latter. By constructing Kraus operators for the case $\alpha_2 \neq 0 \& \beta_2 = 0$, one obtains an equation such that $\kappa \lambda \mu \sin \alpha_2 = 0$. However, this equation is satisfied only for the orthogonal limit, i.e., for $\mu = 0$. Therefore, in the case of superposition, a deterministic transformation is not possible when only the initial state has a local phase.

### 2. Three-dimensional systems

Once the deterministic transformation of superposition states have been presented for qubit systems, we can now systematically examine the same problem for $d = 3$. The transformation under investigation is as follows:

$$\sum_{i=1}^{3} \psi_i |c_i\rangle \xrightarrow{FC} \sum_{i=1}^{3} \varphi_i |c_i\rangle,$$  

(34)

where there is no local phase for both initial and final states. We take advantage of the results presented in Ref. [28]. To this goal, using the Eqs. (7) and (9), we explicitly give the terms $c_{k,n} = \sqrt{p_{n}(k)} |\psi_{n}(k)\rangle$ and $|\varphi_{n}(k)\rangle$ for $k = 1, 2, 3$ and $n = 1, 2, 3$, and construct the Kraus operators step by step. To enhance the understanding of high-dimensional solutions, it is
When we perform Kraus operator $K_1$ to the initial state, we obtain $\varphi_1$ with probability $p_1$. As seen from Table (I), we have $c_{1,1} = \sqrt{p_1} (\varphi_1/\psi_1)$, $c_{1,2} = \sqrt{p_2} (\varphi_2/\psi_1)$, $c_{1,3} = \sqrt{p_3} (\varphi_3/\psi_1)$. Then, the Kraus operators $K_2$ and $K_3$ are given by

\[
K_2 = \sqrt{p_2} \left( \frac{4}{3} \left| c_1 \right| \left| c_1 \right> \left< c_1 \right| \sqrt{\frac{c_2}{\zeta_2}} + \left| c_2 \right| \left| c_2 \right> \left< c_2 \right| \sqrt{\frac{c_3}{\zeta_3}} \right),
\]

\[
K_3 = \sqrt{p_3} \left( \frac{2}{3} \left| c_2 \right| \left| c_2 \right> \left< c_2 \right| \sqrt{\frac{c_1}{\zeta_1}} + \left| c_1 \right| \left| c_1 \right> \left< c_1 \right| \sqrt{\frac{c_3}{\zeta_3}} \right).
\]

We stress that both the majorization condition (16) and CoC (17) need to be satisfied, and the corresponding $\omega$ matrix is given by

\[
\omega = \left( \begin{array}{ccc} \varphi_1^2 & \varphi_2^2 & \varphi_3^2 \\ \varphi_1^2 & \varphi_2^2 & \varphi_3^2 \\ \varphi_1^2 & \varphi_2^2 & \varphi_3^2 \end{array} \right).
\]

Let us consider the following two examples. We have an initial superposition state

\[
|\psi\rangle = \sqrt{\frac{2}{17}} \left( \left| c_1 \right| + 2 \left| c_2 \right| + \left| c_3 \right| \right),
\]

with $\mu = -1/4$. Then, for a given target state

\[
|\phi_1\rangle = \frac{1}{\sqrt{14}} \left( 4 \left| c_1 \right| + 2 \left| c_2 \right| + \left| c_3 \right| \right),
\]

the transformation $|\psi\rangle \xrightarrow{\mathcal{FO}} |\phi_1\rangle$ can be achieved deterministically by using the Kraus operators defined above, i.e., superposition-free Kraus operators are given by

\[
K_1 = \sqrt{p_1} \left( \frac{2}{3} \left| c_1 \right| \left| c_1 \right> \left< c_1 \right| \sqrt{\frac{c_2}{\zeta_2}} + \left| c_2 \right| \left| c_2 \right> \left< c_2 \right| \sqrt{\frac{c_3}{\zeta_3}} \right),
\]

\[
K_2 = \sqrt{p_2} \left( \frac{2}{3} \left| c_2 \right| \left| c_2 \right> \left< c_2 \right| \sqrt{\frac{c_1}{\zeta_1}} + \left| c_1 \right| \left| c_1 \right> \left< c_1 \right| \sqrt{\frac{c_3}{\zeta_3}} \right),
\]

\[
K_3 = \sqrt{p_3} \left( \frac{2}{3} \left| c_3 \right| \left| c_3 \right> \left< c_3 \right| \sqrt{\frac{c_1}{\zeta_1}} + \left| c_1 \right| \left| c_1 \right> \left< c_1 \right| \sqrt{\frac{c_2}{\zeta_2}} \right).
\]

This means our $(\alpha, \beta) \in [1, d]$ pair given in Eq. (13) is (1, 2). When we perform Kraus operator $K_3$ to the initial state, we obtain $\varphi_3$ with probability $p_3$. The Kraus operators $F_4$, $F_5$, and $F_6$ are given by (9) in a way that yield $\sum_{n=1}^{d} K_n^* K_n + \sum_{n=1}^{d} F_n^* F_n = I$. For this case, the probabilities, in Eqs. (36), (37), and (38), are found to be

\[
p_1 = 1 - p_2 - p_3, \quad p_2 = \frac{\psi_2 - \varphi_2}{\varphi_1 - \varphi_3}, \quad p_3 = \frac{\psi_3 - \varphi_3}{\varphi_1 - \varphi_2}.
\]
yields $\sum_{n=1}^{3} K_n^\dagger K_n + \sum_{m=4}^{6} F_m^\dagger F_m = I$. For this case, the probabilities, in Eqs. (36), (37), and (47), are found to be

$$p_1 = 1 - p_2 - p_3, \quad p_2 = \frac{\phi_1 - \psi_1}{\phi_1 - \phi_3}, \quad p_3 = \frac{\phi_2 - \psi_2}{\phi_2 - \phi_3}. \quad (48)$$

Here again we stress that both the majorization condition (16) and CoC (17) need to be satisfied, and the corresponding $\phi$ matrix is given by

$$\omega = \begin{pmatrix} \phi_1^2 & \phi_1 \phi_2 & \phi_1 \phi_3 \\ \phi_1 \phi_2 & \phi_2^2 & \phi_2 \phi_3 \\ \phi_1 \phi_3 & \phi_2 \phi_3 & \phi_3^2 \end{pmatrix}. \quad (49)$$

It is easy to find examples for the regions $\{R_i\}_{i=1,\ldots,5}$ where only the transformations in the region $R_1$ are deterministic.

To recap, for $d = 3$, we obtain the complete solution of superposition-free transformations by discussing the problem under two cases, $\bar{\psi}_3 \geq \phi_3$ and $\bar{\psi}_2 \leq \phi_2$. One can use the solutions presented here for the desired transformations by taking notice of (16) and (17).

3. $d$-dimensional systems

Inspired by [28], we follow a similar route to discuss the problem for $d$-dimensional systems. In the following, since the problem is too complicated for $d \geq 4$, we will limit ourselves to discussing how to construct superposition-free Kraus operators. The key point is to determine a true set of index functions $\{f_n(k)\}_{k=1}^d$ for $n = 1, \ldots, d$. Then, constructing the superposition-free Kraus operators $\{K_n\}_{n=1}^d$ given by Eq. (7) is straightforward.

As mentioned before, for $d = 3$, the relations $\bar{\psi}_1 \leq \phi_1$ and $\bar{\psi}_3 \geq \phi_3$ follow from the majorization conditions given by Eq. (16); but, there are two possible relations between $\bar{\psi}_2$ and $\phi_2$. Similarly, for $d$-dimensional systems, the relations $\bar{\psi}_1 \leq \phi_1$ and $\bar{\psi}_d \geq \phi_d$ follow from the majorization conditions given by Eq. (16). However, for the remaining coefficients we have either $\bar{\psi}_k \geq \phi_k$ or $\bar{\psi}_k \leq \phi_k$ for $k = 2, \ldots, (d-1)$, i.e., there are $2^{d-2}$ possible cases for $d \geq 3$. By adapting the protocol presented in Ref. [28], all set of index functions $\{f_n(k)\}_{k=1}^d$ for $n = 1, \ldots, d$ can be easily obtained for any possible cases between the coefficient $\bar{\psi}_k$ and $\phi_k$ for $k = 2, \ldots, (d-1)$.

In general, for coherence theory, constructing a general form of Kraus operators (i.e., constructing a general form of probabilities) is a highly nontrivial problem, and also the problem becomes exponentially difficult as dimension gets greater [28]. The situation is clearly similar for superposition-free transformations. However, we are able to extrapolate a complete solution for some special cases of $d$-dimensional systems. Here, we give two examples. First, let us consider the case $\bar{\psi}_k \geq \phi_k$ for any $k = 2, \ldots, (d-1)$. One can obtain all $(\alpha, \beta) \in [1,d]$ pairs given in Eq. (13) for index functions $\{f_n(k)\}_{k=1}^d$. We then have $\{(1,k)\}_{k=2}^d$, i.e., the order of index functions are given by

$$\{f_2(k)\}_{k=1}^d = \{2,1,3,4,5,\ldots,(d-1),d\}, \quad \text{(for } K_2\text{)},$$
$$\{f_3(k)\}_{k=1}^d = \{3,2,1,4,5,\ldots,(d-1),d\}, \quad \text{(for } K_3\text{)},$$
$$\{f_4(k)\}_{k=1}^d = \{4,2,3,1,5,\ldots,(d-1),d\}, \quad \text{(for } K_4\text{)},$$
$$\cdots$$
$$\{f_d(k)\}_{k=1}^d = \{d,2,3,4,5,\ldots,(d-1),1\}, \quad \text{(for } K_d\text{)}, (50)$$

where, for the superposition-free Kraus operator $K_1$, $\{f_1(k)\}_{k=1}^d = \{1,2,3,\ldots,d\}$. Here, the probabilities are found to be

$$p_1 = 1 - \sum_{k=2}^d p_k, \quad p_k = \frac{\bar{\psi}_k - \phi_k}{\phi_1 - \phi_k}, \quad (51)$$

where $\sum_{n=1}^d p_n = 1 (p_n \geq 0)$. Second, let us consider the case $\bar{\psi}_k \leq \phi_k$ for any $k = 2, \ldots, (d-1)$. One can obtain all $(\alpha, \beta) \in [1,d]$ pairs given in Eq. (13) for index functions $\{f_n(k)\}_{k=1}^d$. We then have $\{(k,d)\}_{k=1}^d$, i.e., the order of index functions are given by

$$\{f_2(k)\}_{k=1}^d = \{d,2,3,4,5,\ldots,(d-1),1\}, \quad \text{(for } K_2\text{)},$$
$$\{f_3(k)\}_{k=1}^d = \{1,d,3,4,5,\ldots,(d-1),2\}, \quad \text{(for } K_3\text{)},$$
$$\{f_4(k)\}_{k=1}^d = \{1,2,d,4,5,\ldots,(d-1),3\}, \quad \text{(for } K_4\text{)},$$
$$\cdots$$
$$\{f_d(k)\}_{k=1}^d = \{1,2,3,4,5,\ldots,d,(d-1)\}, \quad \text{(for } K_d\text{)}, (52)$$

where, for the superposition-free Kraus operator $K_1$, $\{f_1(k)\}_{k=1}^d = \{1,2,3,\ldots,d\}$. Here, the probabilities are found to be

$$p_1 = 1 - \sum_{k=2}^d p_k, \quad p_k = \frac{\bar{\psi}_k - \psi_k}{\phi_1 - \phi_k}, \quad (53)$$

where $\sum_{n=1}^d p_n = 1 (p_n \geq 0)$. These are just two examples of some of the generalizable cases. As a result, a transformation can be achieved for any given initial and final states (of course, conditions given by Eq. (16) and Eq. (17) must be satisfied) by adapting the protocol presented in Ref. [28] to superposition.

As we mentioned before, the conditions given by Eqs (16) and (17) presented above for a deterministic transformation also hold when the scalar products of the basis states are nonequal, $\langle \epsilon_i | \epsilon_j \rangle = \mu_{ij}$ for $i \neq j$. Just a small change in Eq. (15) is sufficient:

$$\bar{\psi}_i := \psi_i (\psi_i + \mu_{ij} \sum_{j \neq i} \psi_j), \quad \phi_i := \phi_i (\phi_i + \mu_{ij} \sum_{j \neq i} \phi_j), \quad (54)$$

for $i = 1, 2, \ldots, d$ where the coefficients $\bar{\psi}_i$ and $\phi_i$ are in an order such that $\bar{\psi}_i \geq \psi_{i+1}$ and $\phi_i \geq \phi_{i+1}$ for any $l \in [1,d-1]$. Thus, everything regarding the protocol we have introduced is same, only Eq (15) is replaced by Eq. (54).
IV. MAXIMAL SUPERPOSITION STATES

In any resource theory, a vital issue is to identify the levels of resourcefulness. In this section, we focus on the maximal resourceful state—the state with the greatest resource value, i.e., the state at the top of the hierarchy of resourcefulness. By the definition, a $d$-dimensional superposition state is said to have maximal superposition if it can be used to generate all other $d$-dimensional states deterministically using $\mathcal{FO}$.

The existence of maximally resourceful states is well defined for the resource theory of coherence [26], a maximally coherent state is given by $|\Psi_d\rangle := (1/\sqrt{d}) \sum_{i=1}^{d} |i\rangle$. In analogy to the theory of coherence, one may try to formulate maximal superposition states; but it is not trivial in general. It has been shown that such golden units exist only for qubits in superposition theory [4]. However, thorough seeking can give us more interesting results.

In superposition theory, nonorthogonality of the basis states determines every aspect of the theory including the existence of the maximally resourceful states. Even in the simplest case ($d = 2$) there are two maximally resourceful states depending on whether the scalar product is positive or negative. It turns out that the maximal state is a symmetric superposition of basis states for a negative scalar product. To gain more insight into the maximally superposition states, it would be a more correct step to delve into the resourcefulness for negative scalar products. Keeping in mind that a state with maximal superposition has to maximize the $l_1$ norm of superposition, we study the maximal resourceful states for negative values of scalar products. The following subsections aim to explore these kinds of states for $d \geq 2$ with various examples.

A. Qubit Systems

Here we present maximally resourceful state(s) for $d = 2$. As mentioned before, one first needs to observe whether the scalar product of basis states is positive or negative. In this sense, there are two maximal superposition states for qubit systems:

$|\Psi_-\rangle = \frac{1}{\sqrt{2(1-\mu)}} \left( |c_1\rangle - |c_2\rangle \right)$, \hspace{1cm} (55)

for $0 \leq \mu < 1$ [4] and

$|\Psi_+\rangle = \frac{1}{\sqrt{2(1+\mu)}} \left( |c_1\rangle + |c_2\rangle \right)$, \hspace{1cm} (56)

for $-1 < \mu \leq 0$ where $\mu = \langle c_1, c_2 \rangle$. The state given in Eq. (55) (where $\lambda < 0$) and the state given in Eq. (56) (where $\lambda > 0$) can be transformed to any other state $|\phi\rangle = \phi_1|c_1\rangle + \phi_2|c_2\rangle$ ($|\phi_1| \geq |\phi_2|$) when $\mu \in [0,1)$ and $\mu \in (-1,0)$, respectively, by using the Kraus operators presented above for $d = 2$.

Once again, the role of the scalar product is central in considering the maximally resourceful states. For instance, the state given in Eq. (55) cannot be transformed into another state (with unit probability) when $\mu$ is negative. This clearly shows that scalar product has a major impact on superposition-free transformations. As a result, we have two sets of superposition states: $\{ |\Psi_-\rangle, \phi_1|c_1\rangle + \phi_2|c_2\rangle \}$ where $\mu \in [0,1)$ and $\{ |\Psi_+\rangle, \chi_1|c_1\rangle + \chi_2|c_2\rangle \}$ where $\mu \in (-1,0)$. The state $|\Psi_-\rangle$ is the maximal one for the former and the state $|\Psi_+\rangle$ is the maximal one for the latter.

B. $d$-dimensional Systems

At first sight, the results obtained for qubit systems give an idea for higher dimensions, however, the problem in dimensions greater than two is more complicated. The results show us that the maximal superposition states are

$|\Psi_+\rangle := \frac{1}{\sqrt{d(1+(d-1)\mu)}} \sum_{i=1}^{d} |c_i\rangle$, \hspace{1cm} (57)

where the scalar product can be $1/(1-d) < \mu \leq 0$ for $d \geq 3$ and $\mu = \langle c_i, c_j \rangle$ for $i = 1, \ldots, d, \mu \neq j)$. The state given in Eq. (57) may be transformed to any other state $|\phi\rangle = \sum_{i=1}^{d} \phi_i |c_i\rangle$ where the coefficients are organized such that $|\phi_i| \geq |\phi_{i+1}|$ for any $l \in [1,d-1]$. Here our findings regarding the state given by Eq. (57) is as follows: The state given in Eq. (57) can be treated as ‘maximal resourceful’ for target states $|\phi\rangle = \sum_{i=1}^{d} \phi_i |c_i\rangle$ where $\phi_i > 0$. Therefore, we have a set of states

$\{ |\Psi_+\rangle, \sum_{i=1}^{d} \phi_i |c_i\rangle \}$, \hspace{1cm} (58)

where $\phi_i > 0$ (a symmetric superposition of basis states). Then the state $|\Psi_+\rangle$, given by Eq. (57), is the ‘maximally resourceful’ state of this set. Such an approach is reasonable for the investigation of maximal superposition states.

To elucidate the above discussion, we now give explicit examples for $d = 3, 4$. First, let us consider the case $d = 3$ where the maximal resourceful state is given by

$|\Psi_+\rangle = \frac{1}{\sqrt{3(1+2\mu)}} \sum_{i=1}^{3} c_i \mu \in (-\frac{1}{2}, 0)]$. \hspace{1cm} (59)

For $d = 3$, one can find examples where only either the solutions of the case $\Psi_0 \geq \Psi_2$ or $\Psi_2 \leq \Psi_2$ can be used; also, there are examples where these two cases work for a specific range of scalar product separately. Consider, for instance, the given final state

$|\phi\rangle = \frac{1}{\sqrt{45+76\mu}} \left( 5|c_1\rangle + 4|c_2\rangle + 2|c_3\rangle \right)$. \hspace{1cm} (60)

The basic outline of the path to be followed is simple. First, find $\Psi_2$ and $\Psi_2$ for the given (initial and final) states; $\Psi_2 = 1/3$ and $\Psi_2 = (16+28\mu)/(45+76\mu)$. Second, find the range of $\mu$ for each case $\Psi_0 \geq \Psi_2$ and $\Psi_0 \leq \Psi_2$: $-1/2 \leq \mu \leq -0.375$ works for the former and $-0.375 \leq \mu \leq 0$ works for the latter. Next, check the majorization condition (16) and CoC (17) to be satisfied. Then, the transformation $|\Psi_+\rangle \xrightarrow{\mathcal{FO}} |\phi\rangle$ can be
achieved for an arbitrary $\mu \in (-\frac{1}{3}, 0]$ by using the solutions of three-dimensional systems.

Second, consider the case $d = 4$ where the maximal resourceful state is given by

$$|\Psi_+\rangle = \frac{1}{\sqrt{4(1 + 3\mu)}} \sum_{i=1}^{4} c_i, \quad (\mu \in (-\frac{1}{3}, 0]). \quad (61)$$

There are five possible cases for $d = 4$ as seen from Table (I) (or from Ref. [28] for coherence). Consider, for instance, the given final state

$$|\chi\rangle = \frac{1}{\sqrt{110 + 214\mu}} (9|c_1\rangle + |c_2\rangle + 3|c_3\rangle + 2|c_4\rangle). \quad (62)$$

For $-1/3 < \mu \leq 0$ the transformation $|\Psi_+\rangle \xrightarrow{E(\mathbb{C})} |\chi\rangle$ can be achieved deterministically by constructing Kraus operators with the help of Table (I). The case $\psi_2 \geq \chi_2$ & $\psi_3 \geq \chi_3$ (corresponds to the fourth row of the Table (I)) works for $\mu \in (-\frac{1}{3}, 0]$.

In summary, a hierarchy can be defined among pure superposition states by classifying the states according to the range of scalar product, i.e., whether $\mu$ is negative or positive. This classification leads to a set of states given by Eq. (58) where the state given by Eq. (57) is the 'maximal resourceful' state. This way of thinking about resourcefulness allows us to partially explore the existence of maximal superposition states.

V. CONCLUSION

In this work, inspired by [28], we have developed an explicit framework for the manipulation of superposition states as being one of the central problems of the resource theory of superposition [4]. For this purpose, we first have provided superposition-free operators for a deterministic transformation. Moreover, we have presented the conditions for a class of superposition state transformations. These conditions strictly depend on the scalar products of the basis states and reduce to the well-known majorization condition for quantum coherence [29] in the limit of orthonormal basis. Along the way, we have completely solved the problem for $d = 2, 3$ and discussed for $d \geq 4$ how to construct superposition-free Kraus operators for the desired transformations by adapting the protocol introduced in Ref. [28].

We further have expanded our study by examining the maximally resourceful states. We have determined the maximal superposition states which are valid over a certain range of scalar products. Importantly, we have observed that the state with the symmetric superposition of the basis states, where the scalar product is negative, can be treated as maximal for a given particular set of states. We have explicitly discussed this problem for the cases $d = 2, 3, 4$ with various examples. More broadly, research is also needed to determine the resourceful states for high-dimensional systems especially in the case of positive scalar products.

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APPENDIX A: MAJORIZATION AND GRAM MATRIX

It is known that a vector $x$ is majorized by another vector $y$ (equivalently $y$ majorizes $x$), written $x \preceq y$, if and only if $x = Dy$ where $D$ is a doubly stochastic matrix [35, 36]. In the resource theory coherence, the majorization condition for a deterministic transformation of coherent states under incoherent operations [29], is given as $(\psi_1^2, \psi_2^2) \prec (\phi_1^2, \phi_2^2)$ (in dimension two) or in terms of doubly stochastic matrix

$$\begin{pmatrix} \psi_1^2 + \mu \psi_1 \psi_2 & \psi_2^2 + \mu \psi_1 \psi_2 \\ \psi_2^2 + \mu \psi_1 \psi_2 & \psi_1^2 + \mu \psi_1 \psi_2 \end{pmatrix} = D \begin{pmatrix} \phi_1^2 + \mu \phi_1 \phi_2 & \phi_2^2 + \mu \phi_1 \phi_2 \\ \phi_2^2 + \mu \phi_1 \phi_2 & \phi_1^2 + \mu \phi_1 \phi_2 \end{pmatrix}. \quad (A1)$$

Additionally, in Ref. [4] it was shown that the superposition-free operators can be written as $\mathcal{K}_n = V \mathcal{K}_n V^{-1}$ where $\mathcal{K}_n$ is an incoherent operator and $V$ is a basis transformation matrix. The condition to be a trace preserving operation is given by $\sum_n (V^\dagger)^{-1} \mathcal{K}_n^2 V V^\dagger \mathcal{K}_n V^{-1} = I$. By multiplying this condition with $V^\dagger$ and $V$ from left and right, respectively, it becomes $\sum_n \mathcal{K}_n^2 \mathcal{G} \mathcal{K}_n = G$. Since off-diagonal terms of the Gram matrix $G_{ij} = \mu_{ij}$, in the limit of orthonormal basis $G \rightarrow I$, this suggests a continuity in majorization condition due to the scalar product $\mu$ as we obtained in Eq. (16). Then, in the resource theory of superposition, the majorization condition given by Eq. (16) can be written as $(\psi_1^2 + \mu \psi_1 \psi_2, \psi_2^2 + \mu \psi_1 \psi_2) \prec (\phi_1^2 + \mu \phi_1 \phi_2, \phi_2^2 + \mu \phi_1 \phi_2)$ for $d = 2$ or in terms of doubly stochastic matrix

$$\begin{pmatrix} \psi_1^2 + \mu \psi_1 \psi_2 & \psi_2^2 + \mu \psi_1 \psi_2 \\ \psi_2^2 + \mu \psi_1 \psi_2 & \psi_1^2 + \mu \psi_1 \psi_2 \end{pmatrix} = D \begin{pmatrix} \phi_1^2 + \mu \phi_1 \phi_2 & \phi_2^2 + \mu \phi_1 \phi_2 \\ \phi_2^2 + \mu \phi_1 \phi_2 & \phi_1^2 + \mu \phi_1 \phi_2 \end{pmatrix}. \quad (A2)$$

Furthermore, the above equation can be decomposed into

$$\begin{pmatrix} \psi_1 & 0 \\ 0 & \psi_2 \end{pmatrix} G \begin{pmatrix} \psi_1 & \psi_2 \\ \psi_2 & \psi_1 \end{pmatrix} = D \begin{pmatrix} \phi_1 & 0 \\ 0 & \phi_2 \end{pmatrix} G \begin{pmatrix} \phi_1 & \phi_2 \\ \phi_2 & \phi_1 \end{pmatrix}, \quad (A3)$$

where $G$ is the Gram matrix given in Eq. (4). It is now obvious that the majorization condition given by Eq. (16) or Eq. (A3) is the generalized version of the majorization obtained in the coherence theory, i.e., in the limit of orthonormal basis, the Gram matrix $G \rightarrow I$, above expression reduces to $(\psi_1^2, \psi_2^2) \prec (\phi_1^2, \phi_2^2)$. Even though we have shown it for a qubit systems explicitly, it is straightforward to show that this relation holds for an arbitrary dimension of Hilbert space.

APPENDIX B: DERIVATION OF THE CONDITIONS FOR DETERMINISTIC TRANSFORMATIONS

In this Appendix, we show how to obtain the majorization conditions for superposition given by Eq. (16) and CoC given by Eq. (17). All the details are hidden in the completeness.
relation given by Eq. (10), and can be derived by a careful calculation.

As stated in Ref. [4], assume one has an (incomplete) set of Kraus operators \( \{ K_n \} \) such that \( \sum K_n^\dagger K_n \leq I \). Then, it was proven [4] that there always exist superposition-free Kraus operators \( \{ F_m \} \) with \( \sum_n K_n^\dagger F_m + \sum_m F_m^\dagger F_m = I \). Here, the identity operator can be represented in the following way:

\[
I = \sum_{i,j} \frac{|c_i^+|^2 |c_j^+|^2}{(c_i^+ c_j^+)^\dagger c_i^\dagger c_j^\dagger} (c_i^\dagger c_j^\dagger).
\]  

(B1)

Additionally, it is not necessary to obtain the Kraus operators \( \{ F_m \} \) explicitly; however, the completeness relation provides constraints on superposition-free Kraus operators \( \{ F_m \} \), i.e., on the terms of Kraus operators given by Eq. (9). The CoC given by Eq. (17) is obtained as a result of these constraints.

Using the same notation used in Sec. III B for the Kraus operators given by Eq. (9), we first define

\[
\sum_{m=d+1}^{2d} c_{j,m}^2 \equiv \mathcal{X}_j,
\]  

(B2)

for \( j = 2, 3, \ldots, d \), and

\[
\sum_{m=d+1}^{2d} c_{j,m} c_{j,m} \equiv \mathcal{Y}_j,
\]  

(B3)

for \( j = 2, 3, \ldots, d \), \( l = 3, 4, \ldots, d \), and \( j < l \). The completeness relation given by Eq. (10) gives us \( d \) \((d+1)/2\) equations. We divide these equations into three separate groups by combining them with Eqs. (B2) and (B3).

The first group consists of \( (d-2)(d-1)/2 \) equations which give us the terms \( \mathcal{Y}_j \) defined by Eq (B3) in terms of \( \{ \psi_i \}_{i=1}^d \), \( \{ \phi_i \}_{i=1}^d \), \( \mu \), and \( \{ p_n \}_{n=1}^d \). In addition, the terms \( \mathcal{Y}_j \) can be either positive or negative. Therefore, the terms \( \mathcal{Y}_j \) defined by Eq. (B3) do not indicate any condition (or constraint).

The second group consists of \( (d-1) \) equations which give us the terms \( \{ \mathcal{X}_j \}_{j=2}^d \) defined by Eq. (B2). Equations in this group also contain the terms \( \mathcal{Y}_j \) defined by Eq. (B3). By combining the equations in the first group and second group together in a way that we obtain the terms \( \{ \psi_i \}_{i=1}^d \) in terms of \( \{ \psi_i \}_{i=1}^d \), \( \{ \phi_i \}_{i=1}^d \), \( \mu \), and \( \{ p_n \}_{n=1}^d \). It is obvious that the terms \( \{ \mathcal{X}_j \}_{j=2}^d \) defined by Eq. (B2) must be non-negative. Therefore, the positivity of these terms implies the CoC.

The third group consists of \( d \) equations where the unknowns are probabilities \( \{ p_n \}_{n=1}^d \). Equations in this group also contain the terms \( \mathcal{Y}_j \) and \( \mathcal{X}_j \). These \( d \) equations can be reduced into the form given by Eq. (19) by using the definitions given by Eqs. (15), (B2), and (B3). By solving these, one obtains the probabilities in terms of just \( \{ \psi_i \}_{i=1}^d \) and \( \{ \phi_i \}_{i=1}^d \). We show that Eq. (19) can be written in a way that contains a doubly stochastic matrix which provides us majorization condition for superposition.

In what follows, we obtain the majorization condition given by Eq. (16) and the CoC given by Eq. (17) for \( d = 2, 3 \) and give the procedure to be applied for arbitrary dimension. Now, first consider the simplest case, qubit systems. The index functions for the Kraus operators \( K_1, K_2, F_3, \) and \( F_4 \) are given such that \( \{ f_1(1), f_1(2) \} = \{ 1, 2 \}, \{ f_2(1), f_2(2) \} = \{ 2, 1 \}, \{ f_3(1), f_3(2) \} = \{ 1, 1 \}, \) and \( \{ f_4(1), f_4(2) \} = \{ 2, 2 \}, \) respectively. After constructing the Kraus operators given by Eqs. (7) and (9), the completeness relation given by Eq. (10) gives us the following three equations:

\[
c_1^2 + c_2^2 + c_3^2 + c_4^2 = 1,
\]  

(B4)

\[
c_1^2 + c_2^2 + c_3^2 + c_4^2 = 1,
\]  

(B5)

\[
(c_1 c_{2,1} + c_1 c_{2,2}) \mu + c_{1,3} c_{2,3} + c_{1,4} c_{2,4} = \mu.
\]  

(B6)

As we mentioned above, we divide these equations into three groups. Here, there is no equation in the first group. In the second group we have only one equation, Eq. (B6), and in the third group we have two equations, Eqs. (B4) and (B5). Also, from \( K_n |\psi\rangle = \sqrt{\mu} |\phi\rangle \) we have

\[
c_{1,1} = \sqrt{\mu} |\psi_1 \rangle |\psi_1 \rangle, \quad c_{2,1} = \sqrt{\mu} |\psi_2 \rangle |\psi_2 \rangle,
\]  

(B7)

\[
c_{1,2} = \sqrt{\mu} |\psi_2 \rangle |\psi_1 \rangle, \quad c_{2,2} = \sqrt{\mu} |\psi_1 \rangle |\psi_2 \rangle.
\]  

(B8)

Combining Eqs. (B7), (B8), and (B2) with Eq. (B6), we obtain

\[
X_2 = \frac{1}{\sqrt{\mu}} \left( |\psi_1 \rangle |\psi_2 \rangle - |\psi_1 \rangle |\psi_2 \rangle \right).
\]  

(B9)

Here, the term \( X_2 \) is non-negative, then the right hand side of Eq. (B9) must be non-negative, yielding \( \mu |\psi_1 \rangle |\psi_2 \rangle - |\psi_1 \rangle |\psi_2 \rangle \geq 0 \). This inequality can also be written such that

\[
p_1 |\phi_1 \rangle |\phi_2 \rangle + p_2 |\phi_2 \rangle |\phi_1 \rangle \leq |\psi_2 \rangle |\psi_2 \rangle,
\]  

(B10)

which gives us the CoC (for qubit systems) defined by Eq. (17). As mentioned before, the explicit construction of \( F_3 \) and \( F_4 \) is not necessary [4]. Furthermore, while \( X_2 \) given in Eq. (B9) is equal to \( c_{2,3}^2 + c_{2,4}^2 \), different choices of \( c_{2,3} \) and \( c_{2,4} \) give us different sets of \( \{ F_3, F_4 \} \), provided that Eq. (B9) is satisfied. For instance, if we choose \( c_{2,4} = 0 \) (or \( c_{2,3} = 0 \)) then we have only three superposition-free Kraus operators, \( \{ K_1, K_2, F_3 \} \) (or \( \{ K_1, K_2, F_3 \} \)). On the other hand, for \( c_{2,3} \neq 0 \) and \( c_{2,4} \neq 0 \), we need four superposition-free Kraus operators to make the entire operation trace preserving. We now proceed with equations in the third group. Combining Eqs. (B7), (B8), (B9), (B2), and (15) with Eqs. (B4) and (B5), we get

\[
p_1 |\phi_1 \rangle + p_2 |\phi_2 \rangle = |\psi_1 \rangle,
\]  

(B11)

\[
p_1 |\phi_2 \rangle + p_2 |\phi_1 \rangle = |\psi_2 \rangle.
\]  

(B12)

The above equations can be written in the compact form

\[
\begin{pmatrix} p_1 \ & p_2 \\ p_2 & p_1 \end{pmatrix} \begin{pmatrix} |\phi_1 \rangle \\ |\phi_2 \rangle \end{pmatrix} = \begin{pmatrix} |\psi_1 \rangle \\ |\psi_2 \rangle \end{pmatrix},
\]  

(B13)

where \( p_1, p_2 \geq 0 \) and \( p_1 + p_2 = 1 \). The transformation matrix given in Eq. (B13) is a doubly stochastic matrix:

\[
D(|\phi_1 \rangle |\phi_2 \rangle) = (|\psi_1 \rangle |\psi_2 \rangle)^T.
\]  

Hence, the vector \((|\psi_1 \rangle |\psi_2 \rangle)^T\) is majorized by the vector \((|\phi_1 \rangle |\phi_2 \rangle)^T\) written \((|\psi_1 \rangle |\psi_2 \rangle)^T < (|\phi_1 \rangle |\phi_2 \rangle)^T\), where \( |\psi_1 \rangle \leq |\psi_2 \rangle \) and \( |\phi_1 \rangle \geq |\phi_2 \rangle \). Furthermore, in the limit
of orthonormal basis, equality holds in Eq. (B10), and also Eqs. (B10) and (B12) become same, i.e., majorization is the only condition, which is necessary and sufficient, for the deterministic coherence transformations.

Second, consider the case \( \bar{\psi}_2 \geq \bar{\phi}_2 \) of \( d = 3 \). After constructing the Kraus operators (by using the given index functions given in Table (I)), the completeness relation given by Eq. (10) gives us the following six equations:

\[
\sum_{j=1}^{6} c_{j,j}^2 = 1, \quad (B14)
\]

for \( j = 1, 2, 3 \),

\[
\mu \sum_{i=1}^{3} c_{1,i} c_{2,j} + \sum_{i=4}^{6} c_{1,i} c_{2,i} = \mu, \quad (B15)
\]

\[
\mu \sum_{i=1}^{3} c_{1,i} c_{3,j} + \sum_{i=4}^{6} c_{1,i} c_{3,i} = \mu, \quad (B16)
\]

Here, we again divide these equations into three groups. There is one equation in the first group, Eq. (B17); in the second group we have two equations, Eqs. (B15) and (B16); and in the third group we have three equations given in Eq. (B14). Also, from \( F_m \left| \psi \right> = 0 \) we have

\[
c_{1,i} = - (c_{2,i} \psi_2 + c_{3,i} \psi_3) / \psi_1, \quad (B18)
\]

for \( i = 4, 5, 6 \). We start with the equation in the first group. Combining Eqs. (36), (37), (38), and (B3) with Eq. (B17) we obtain

\[
Y_{23} = \left( \frac{\mu}{\psi_2^2} \right) \left( \psi_2 \psi_3 - p_1 \psi_2 \varphi_3 - p_2 \varphi_1 \psi_2 - p_3 \varphi_1 \varphi_3 \right). \quad (B19)
\]

The term \( Y_{23} \) given above can be either positive or negative, and therefore, provides no condition. We now proceed with equations in the second group. By suitably combining Eqs. (36), (37), (38), (B18), and (B2) with Eqs. (B15) and (B16), we obtain

\[
X_2 = \left( \frac{\mu}{\psi_2^3} \right) \left( p_1 [\psi_1 \varphi_2 + \varphi_1 \psi_2] + p_2 [\psi_1 \varphi_2 + \varphi_2 \varphi_1] + p_3 [\psi_1 \varphi_2 + \varphi_1 \varphi_3] - [\psi_1 \psi_2 + \psi_2 \psi_1] \right), \quad (B20)
\]

\[
X_3 = \left( \frac{\mu}{\psi_3^3} \right) \left( p_1 [\psi_1 \varphi_3 + \varphi_1 \psi_3] + p_2 [\psi_1 \varphi_2 + \varphi_2 \varphi_1] + p_3 [\psi_1 \varphi_3 + \varphi_3 \varphi_1 - [\psi_1 \psi_3 + \psi_3 \psi_1] \right). \quad (B21)
\]

Here, the terms \( X_2 \) and \( X_3 \) are non-negative, then the right hand side of Eqs. (B20) and (B21) must be non-negative. Then, from the positivity of Eq. (B20) and Eq. (B21), we get

\[
p_1 \psi_1^2 + p_2 \psi_2^2 + p_3 \varphi_1^2 \leq \psi_2^2, \quad (B22)
\]

\[
p_1 \psi_1^2 + p_2 \varphi_1^2 + p_3 \varphi_3^2 \leq \psi_2^2, \quad (B23)
\]

which gives us the CoC (for three-dimensional systems) defined by Eq. (17). Last, we look at equations in the third group. Combining Eqs. (36), (37), (38), (B18), (B2), and (B3) with three equations given in Eq. (B14), we get

\[
p_1 \bar{\phi}_1 + p_2 \bar{\phi}_3 + p_3 \bar{\varphi}_2 = \psi_1, \quad (B24)
\]

\[
p_1 \bar{\varphi}_1 + p_2 \bar{\varphi}_2 + p_3 \bar{\phi}_1 = \psi_2, \quad (B25)
\]

\[
p_1 \bar{\varphi}_3 + p_2 \bar{\psi}_1 + p_3 \bar{\varphi}_3 = \psi_3. \quad (B26)
\]

The above equations can be written in the compact form

\[
\begin{pmatrix}
p_1 & p_3 & p_2 \\
p_3 & p_1 + p_2 & 0 \\
p_2 & 0 & p_1 + p_3
\end{pmatrix}
\begin{pmatrix}
\bar{\phi}_1 \\
\bar{\phi}_3 \\
\bar{\varphi}_1
\end{pmatrix}
= \begin{pmatrix}
\psi_1 \\
\psi_2 \\
\psi_3
\end{pmatrix}. \quad (B27)
\]

where \( p_i \geq 0 \) and \( \sum_{i=1}^{3} p_i = 1 \). The transformation matrix given in Eq. (B27) is a doubly stochastic matrix: \( D(\phi_1, \phi_2, \phi_3) = (\psi_1, \psi_2, \psi_3) \). Hence, the vector \( (\psi_1, \psi_2, \psi_3) \) is majorized by the vector \( (\phi_1, \phi_2, \phi_3) \) written \( \psi_1 \geq \psi_2 \geq \psi_3 \) and \( \phi_1 \geq \phi_2 \geq \phi_3 \). Furthermore, in the limit of orthonormal basis, equality holds in Eqs. (B22) and (B23), and also Eqs. (B22) and (B23) become same with Eqs. (B25) and (B26), respectively.

This procedure can be easily generalized to the case of high-dimensional systems by following a similar path. Using the Kraus operators defined by Eqs. (7) and (9), the completeness relation given by Eq. (10) gives us the following \( d(d+1)/2 \) equations: \( d \) equations in the form

\[
\sum_{i=1}^{2d} c_{j,i}^2 = 1, \quad (B28)
\]

for \( j = 1, 2, \ldots, d; \) and \( (d-1)d/2 \) equations in the form

\[
\mu \sum_{i=1}^{d} c_{j,i} c_{i,j} + \sum_{i=d+1}^{d} c_{j,i} c_{i,j} = \mu, \quad (B29)
\]

for \( j = 1, 2, \ldots, (d-1), l = 2, 3, \ldots, d, \) and \( j < l \). The unitary transformations—permutations—presented in Ref. [28] give
us the index functions. Also, from $F_m|\psi\rangle = 0$ we have
\[ c_{1,i} = -(c_2,i\psi_2 + c_3,i\psi_3 + \cdots + c_{d,i}\psi_d)/\psi_1, \]  \hspace{1cm} (B30)
for $i = (d+1), \ldots, 2d$. Then, we divide above $d(d+1)/2$ equations (Eqs. (B28) and (B29)) into three separate groups and examine each one step by step. These are final steps for obtaining the CoC given by Eq. (17) and majorization condition for superposition given by Eq. (16). With this formulation above, conditions for a class of superposition transformations and the transformation itself can be achieved effectively.

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