Anomalies of the weight-based coherence measure and mixed maximally coherent states

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As an analogy of best separable approximation (BSA) in the framework of entanglement theory, here we concentrate on the notion of best incoherent approximation, with application to characterizing and quantifying quantum coherence. From both analytical and numerical perspectives, we have demonstrated that the weight-based coherence measure displays some unusual properties, in sharp contrast to other popular coherence quantifiers. First, by deriving a closed formula for single-qubit states, we have shown the exact value of weight-based coherence measure does not depend solely on the off-diagonal element but relies on the geometry of a given qubit state, thus exhibiting a rich structure even in this simplest case. Second, albeit the fact that almost all popular coherence measures only assign a maximal value to pure maximally coherent states, we have demonstrated the existence of mixed maximally coherent states (MMCS) with respect to this coherence measure and discussed the characteristic feature of MMCS in high-dimensional Hilbert spaces. Especially, we present several important families of MMCS by gaining insights from the numerical simulations. Moreover, it is pointed out that some considerations in this work can be generalized to general convex resource theories and a numerical method of improving the computational efficiency for finding the BSA is also discussed.

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I. INTRODUCTION

Recently, the characterization and quantification of quantum coherence remains to be one of the attractive subjects in the field of quantum information theory, not only for its fundamental implications, but also for practical applications [1,2]. It is worth noting that quantum resource theory (QRT) *per se* has also attracted great attention due to its successful application in this topic [3,4]. Within the framework of QRT, a plethora of coherence monotones and measures has been proposed, such as the relative entropy of coherence [3], the l_1 norm of coherence [3], the coherence of formation [5–7], the geometric measure of coherence [8], and the robustness of coherence (ROC) [9,10].

However, we also notice that the majority of these popular coherence measures are not originally operational defined with the exception of ROC, which quantifies the minimal noise or mixing required to destroy all the coherence contained in a quantum state [9,10]. In fact, there exists another coherence measure also manifesting itself as an inherently operational definition, i.e., the weight-based coherence measure, which quantifies the minimal coherence resource needed to prepare or construct a given state [11].

In a specific convex resource theory, the idea of weight-based measure originates from a simple fact that for any given state ρ there always exist convex decompositions such as

$$\rho = \lambda\rho_f + (1-\lambda)\rho_r. \tag{1}$$

Here the resource under investigation can be some physical property of quantum states or phenomenon that emerges from the principles of quantum mechanics. ρ_f belongs to the (convex) set of free states, while ρ_r denotes a more resourceful state. When optimizing over all allowed free states, we will find the maximal weight $\lambda^\star$ according to the decomposition (1) and naturally the weight-based resource measure can be defined as $1-\lambda^\star$.

Actually, the essence of weight-based measure can date back to the Elitzur-Popescu-Rohrlich (EPR2) approach for quantifying nonlocality of joint probability distributions [12–14]. Meanwhile, the word "weight" is also dubbed as "part," "content," "cost," or "fraction" in different scenarios and such a line of thought has also been employed to measure quantum entanglement [15–27], steering [28–30], contextuality [31–34], measurement informativeness [35], or even arbitrary resources [36,37].

Within the context of convex QRT, although the weight-based resource measure satisfies desirable properties, such as faithfulness, monotonicity, and convexity, it exhibits unusual features, in sharp contrast to other popular quantifiers. In this work, we concentrate on the weight-based coherence measure, namely coherence weight [11]. Specifically, we focus on the following three points. First, the coherence weight is a coarse-grained measure for all pure coherent states, which means that the coherence weight of any pure coherent state is the same, that is, the maximum value 1 [11]. Indeed, this phenomenon has also been mentioned for entanglement weight [38] and steering weight [28]. Here we mainly explore another two aspects of coherence weight: (i) by presenting a closed-form formula of coherence weight for single-qubit

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states, we illustrate that the evaluation of coherence weight does not depend solely on the off-diagonal element but relies on the relationship between the absolute values of diagonal and off-diagonal entries (in the incoherent basis). This intriguing fact is quite remarkable comparing with single-letter formulas of other popular coherence measures [3,7–9]; (ii) under the framework of QRT, almost all popular coherence measures only assign the maximal value to pure maximally coherent states [39], which excludes the existence of mixed maximally coherent states for these measures. However, we propose the notion of mixed maximally coherent states and demonstrate its existence with respect to the weight-based coherence measure. It is worthy noting that such a similar phenomenon, i.e., the existence of mixed maximally entangled states or mixed maximally steerable states, was verified in quantifying quantum entanglement [38] and steering [28].

The rest of this paper is organized as follows. In Sec. II, we review the definition of the weight-based resource measure and discuss its special properties, especially from the geometric viewpoint. In Sec. III, we offer a closed formula of coherence weight for single-qubit states, and consequently, an exhaustive investigation of single-qubit case is put forward by gaining insights from numerical simulations. In Sec. IV, we propose a definition of mixed maximally coherent states according to the weight-based coherence measure. Moreover, we provide a detailed numerical analysis of coherence weight for high-dimensional Hilbert spaces and several important families of MMCS are confirmed. Discussions and final remarks are given in Sec. V and several open questions are raised for future research.

II. BEST FREE APPROXIMATION AND WEIGHT-BASED COHERENCE MEASURE

Before focusing on the resource theory of quantum coherence, we begin with the notion of best free approximation (BFA) in a general convex resource theory, generalizing the concept of best separable approximation (BSA) [40]. In a d-dimensional Hilbert space, let $\mathcal{D}$ and $\mathcal{F}$, respectively, denote the set of density matrices and the convex set of free states. Hence the BFA of a given state ρ can be defined through an optimization over convex decompositions

$$\mathrm{BFA}(\rho) = \min_{\rho_r \in \mathcal{D}} \{1-\lambda \mid \rho = \lambda\rho_f + (1-\lambda)\rho_r,\ \rho_f \in \mathcal{F}\}, \tag{2}$$

$$= \min_{\rho_r \in \mathcal{D}} \{1-\lambda \mid \rho \succeq \lambda\rho_f,\ \rho_f \in \mathcal{F}\}, \tag{3}$$

where the matrix inequality $A \succeq B$ means that $A - B$ is positive semidefinite. To discuss the properties of BFA, we would like to mention another prominent resource quantifier, that is, the generalized robustness measure, which is a dual quantity to the BFA in some sense [41]

$$\mathcal{R}(\rho) = \min_{\tau \in \mathcal{D}} \left\{ s \geqslant 0 \;\middle|\; \frac{\rho + s\,\tau}{1+s} =: \rho_f \in \mathcal{F} \right\}, \tag{4}$$

$$= \min_{\tau \in \mathcal{D}} \{ s \mid \rho \preceq (1+s)\rho_f,\ \rho_f \in \mathcal{F}\}. \tag{5}$$

Within the framework of QRT, it is generally known that the generalized robustness is a valid resource monotone satisfying the following axiomatic criteria [4,40].

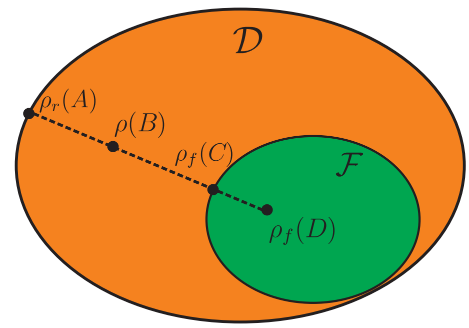

FIG. 1. The geometric interpretation of BFA. The optimal states $\rho_f^\star$ and $\rho_r^\star$ achieving the minimum in Eq. (2) are on the boundaries of $\mathcal{F}$ and $\mathcal{D}$, respectively. See Appendix B for more details.

(C1) Faithfulness: $\mathcal{R}(\rho) = 0$ if and only if $\rho \in \mathcal{F}$.

(C2) Convexity: $\mathcal{R}(\sum_i p_i\rho_i) \leqslant \sum_i p_i \mathcal{R}(\rho_i)$ for $\rho_i \in \mathcal{D}$, $p_i \geqslant 0$, $\sum_i p_i = 1$.

(C3) Strong monotonicity: $\mathcal{R}(\rho) \geqslant \sum_i \mathrm{Tr}[\Theta_i(\rho)]\mathcal{R}[\frac{\Theta_i(\rho)}{\mathrm{Tr}[\Theta_i(\rho)]}]$, where the instrument $\{\Theta_i\}$ is a collection of resource nongenerating subchannels, i.e., $\Theta_i(\sigma)/\mathrm{Tr}[\Theta_i(\rho)] \in \mathcal{F}$ for any $\sigma \in \mathcal{F}$ and $\sum_i \Theta_i$ constitutes a completely positive trace-preserving map.

In fact, the weight-based resource measure is also a sound quantifier fulfilling properties (C1)–(C3).

Lemma 1. The BFA(ρ) is a faithful, convex, and strong monotonic measure in any convex resource theory.

Proof. If we denote by $\tau^\star$ and $\rho_f^\star$ the optimal states achieving the minimum in Eq. (4), then ρ can be written as a pseudomixture [42]

$$\rho = [1 + \mathcal{R}(\rho)]\rho_f^\star - \mathcal{R}(\rho)\tau^\star. \tag{6}$$

Comparing with the convex mixture in the definition of Eq. (2), we are aware of a crucial fact that any procedure or technic used in proving $\mathcal{R}(\rho)$ to satisfy (C1)–(C3) can be applied to the BFA in the same manner, owing to the linearity of quantum (sub)channels and the convexity of the set of free states (see Ref. [9] or Appendix A for a complete proof). ■

On the other hand, similar to the arguments for the robustness of entanglement [43], we can give an explicit geometric interpretation of the BFA (see Fig. 1).

Lemma 2. For any convex resource theory and any (mixed) resourceful state ρ, the optimal states $\rho_f^\star$ and $\rho_r^\star$ achieving the minimum in Eq. (2) are on the boundaries of $\mathcal{F}$ and $\mathcal{D}$, respectively.

Proof. See Appendix B.

Moreover, note that the BFA is not extensive, i.e., does not scale with the dimension of the state space. Therefore, when we compare it with other popular resource measures, a proper normalization is necessary.

Lemma 3. For any convex resource theory and any other convex resource monotone $\mathcal{X}(\rho)$, the normalized version of $\mathcal{X}(\rho)$ is upper bounded by BFA(ρ), i.e., $\overline{\mathcal{X}}(\rho) \leqslant \mathrm{BFA}(\rho)$, where $\overline{\mathcal{X}}(\rho) = \mathcal{X}(\rho)/\mathcal{X}_d$ and $\mathcal{X}_d$ is the maximal value associated with d-dimensional Hilbert space.

Proof. If we denote by $\rho_f^\star$ and $\rho_r^\star$ the optimal states achieving the minimum in Eq. (2), that is, $\rho = [1 - \mathrm{BFA}(\rho)]\rho_f^\star +$

$\text{BFA}(\rho)\rho_r^\star$, then from the convexity of $\mathcal{X}(\rho)$ we have

$$\begin{aligned}\mathcal{X}(\rho) &\leqslant [1-\text{BFA}(\rho)]\mathcal{X}(\rho_f^\star)+\text{BFA}(\rho)\mathcal{X}(\rho_r^\star)\\ &=\text{BFA}(\rho)\mathcal{X}(\rho_r^\star)\leqslant \text{BFA}(\rho)\mathcal{X}_d.\end{aligned} \tag{7}$$

After the normalization, the proof is complete. ■

Apart form the above general results, we should take a closer look at the resource theory of quantum coherence [3]. In this framework, the free states are those diagonal in a prefixed orthogonal basis, i.e., the incoherent basis $\{|i\rangle\}_{i=0}^{d-1}$. The free operations are usually chosen to the so-called incoherent operations, which admit a Kraus decomposition $\Theta(\rho)=\sum_i K_i\rho K_i^\dagger$ such that every Kraus operator is required to fulfill $K_i\rho K_i^\dagger/\text{Tr}(K_i\rho K_i^\dagger)\in\mathcal{F}$ for all $\rho\in\mathcal{F}$ [3,44]. However, from Lemma 1, it is evident that the coherent weight (i.e., best incoherent approximation) is a MIO monotone, where the abbreviation MIO stands for maximal incoherent operations, which is recognized as the largest class of incoherent operations and is equivalent to the definition of resource nongenerating channels in Lemma 1 [5,45].

Moreover, the coherence weight can be recast into a simple semidefinite program (SDP) [11]

$$C_w(\rho)=\max\{\text{Tr}(\rho\omega)\mid \Delta\omega\preceq 0,\omega\preceq \mathbb{1}\}. \tag{8}$$

Nevertheless, from the Eq. (3) and the definition of incoherent states, $C_w(\rho)$ can be directly expressed as

$$C_w(\rho)=\min\left\{1-\sum_i\lambda_i\;\middle|\;\rho-\sum_i\lambda_i|i\rangle\langle i|\succeq 0\right\}. \tag{9}$$

Such an alternative SDP has an advantage over Eq. (8) in that it can indicate the closest incoherent with respect to ρ. More precisely, we can make use of the CVX package to evaluate the coherence weight and simultaneously obtain the accurate values of λ_i [46].

Finally, we also notice that for qubit states the l_1 norm of coherence, the robustness of coherence, the coherence of formation, the geometric measure of coherence, etc. are all monotonic functions of the absolute value of the off-diagonal element $|\rho_{01}|=|\langle 0|\rho|1\rangle|$. In the next section, we show that it is not the case for coherent weight, which depends on the specific form of the given qubit state and thus exhibits a richer structure.

III. C_w FOR SINGLE-QUBIT STATES

In this section, we present the analytical formula of coherence weight for single-qubit states. Before we begin, we recall some important definitions and results initially associated with the notion of BSA (or so called Lewenstein-Sanpera decomposition) [15,18].

Definition 1. A non-negative parameter Λ is called maximal with respect to a density matrix ρ and the projection operator $P=|\psi\rangle\langle\psi|$ iff $\rho-\Lambda P\succeq 0$, and for every $\epsilon\geqslant 0$, the matrix $\rho-(\Lambda+\epsilon)P$ is not positive definite.

Definition 2. A pair of non-negative parameters (Λ_1,Λ_2) is called maximal with respect to ρ and a pair of projection operators $P_1=|\psi_1\rangle\langle\psi_1|, P_2=|\psi_2\rangle\langle\psi_2|$ if and only if $\rho-\Lambda_1P_1-\Lambda_2P_2\succeq 0$, Λ_1 is maximal with respect to $\rho-\Lambda_2P_2$, Λ_2 is maximal with respect to $\rho-\Lambda_1P_1$, and the sum $\Lambda_1+\Lambda_2$ is maximal.

Lemma 4. A pair (Λ_1,Λ_2) is maximal with respect to ρ and a pair of projectors (P_1,P_2) if and only if

(i) if $|\psi_1\rangle,|\psi_2\rangle\notin r(\rho)$ [where $r(\rho)$ denotes the range of ρ] then $\Lambda_1=\Lambda_2=0$;

(ii) if $|\psi_1\rangle\notin r(\rho)$ while $|\psi_2\rangle\in r(\rho)$ then $\Lambda_1=0$, $\Lambda_2=\langle\psi_2|\rho^{-1}|\psi_2\rangle^{-1}$;

(iii) if $|\psi_1\rangle,|\psi_2\rangle\in r(\rho)$ and $\langle\psi_1|\rho^{-1}|\psi_2\rangle=0$ then $\Lambda_i=\langle\psi_i|\rho^{-1}|\psi_i\rangle^{-1}$, $i=1,2$;

(iv) if $|\psi_1\rangle,|\psi_2\rangle\in r(\rho)$ and $\langle\psi_1|\rho^{-1}|\psi_1\rangle,\langle\psi_2|\rho^{-1}|\psi_2\rangle\geqslant|\langle\psi_1|\rho^{-1}|\psi_2\rangle|\neq 0$, then

$$\Lambda_1=(\langle\psi_2|\rho^{-1}|\psi_2\rangle-|\langle\psi_1|\rho^{-1}|\psi_2\rangle|)/D,$$
$$\Lambda_2=(\langle\psi_1|\rho^{-1}|\psi_1\rangle-|\langle\psi_1|\rho^{-1}|\psi_2\rangle|)/D,$$

where $D=\langle\psi_1|\rho^{-1}|\psi_1\rangle\langle\psi_2|\rho^{-1}|\psi_2\rangle-|\langle\psi_1|\rho^{-1}|\psi_2\rangle|^2$.

(v) if $|\psi_1\rangle,|\psi_2\rangle\in r(\rho)$ and $\langle\psi_1|\rho^{-1}|\psi_1\rangle\geqslant|\langle\psi_1|\rho^{-1}|\psi_2\rangle|\geqslant\langle\psi_2|\rho^{-1}|\psi_2\rangle$, then $\Lambda_1=0$, $\Lambda_2=\langle\psi_2|\rho^{-1}|\psi_2\rangle^{-1}$.

It is worth emphasizing that small typo mistakes in Ref. [15,18] have been corrected here. Besides the original proof of Lemma 4 in Ref. [15], we refer the readers to an alternative derivation via SDP method [47]. A key observation in proving Lemma 4 lies in that although within the context of BSA the projectors are all pure product states such as $|\psi\rangle=|e\rangle\otimes|f\rangle$, actually this point has not been taken into account in the proof. Obviously, the above lemma can also been exploited in single-partite system through Eq. (9), where for qubit states the projectors are pure incoherent basis states $\{|0\rangle\langle 0|,|1\rangle\langle 1|\}$. Now we have the toolkit to present the first main result of this work.

Theorem 1. For an arbitrary qubit state ρ, the coherence weight can be evaluated as

$$C_w(\rho)=\begin{cases}2|\rho_{01}|, & \rho_{00},\rho_{11}\geqslant|\rho_{01}|\\ 1-\frac{\det\rho}{\min\{\rho_{00},\rho_{11}\}}, & \text{otherwise}\end{cases} \tag{10}$$

where $\rho_{ij}=\langle i|\rho|j\rangle$ are elements of ρ in the incoherent basis.

Proof. For convenience, we also adopt the Bloch representation of ρ, that is

$$\rho_u=\tfrac{1}{2}(\mathbb{1}+\vec{u}\cdot\vec{\sigma}), \tag{11}$$

where $\vec{u}=(u_1,u_2,u_3)$ denotes the Bloch vector and $\vec{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ are standard Pauli matrices. Using Eq. (11), one can easily verify that the inverse matrix of ρ can be expressed as

$$\rho_u^{-1}=\frac{4}{1-|\vec{u}|^2}\rho_{-u}=\frac{1}{\det\rho}\rho_{-u}. \tag{12}$$

Therefore, up to the factor $1/\det\rho$, the elements of ρ_u^{-1} in the incoherent basis are just that of ρ_{-u}. Meanwhile, note that $\langle i|\rho_{-u}|i\rangle=\rho_{jj}$ for $i\neq j=0,1$.

To utilize Lemma 4, we first assume $\rho_{00},\rho_{11}\geqslant|\rho_{01}|$. In this case, we can directly employ item (iv) of Lemma 4

$$\begin{aligned}C_w(\rho)&=1-\frac{\langle 0|\rho^{-1}|0\rangle+\langle 1|\rho^{-1}|1\rangle-2|\langle 0|\rho^{-1}|1\rangle|}{\langle 0|\rho^{-1}|0\rangle\langle 1|\rho^{-1}|1\rangle-|\langle 0|\rho^{-1}|1\rangle|^2}\\ &=1-\frac{\rho_{11}+\rho_{00}-2|\rho_{01}|}{\rho_{11}\rho_{00}-|\rho_{01}|^2}\det\rho\\ &=2|\rho_{01}|,\end{aligned} \tag{13}$$

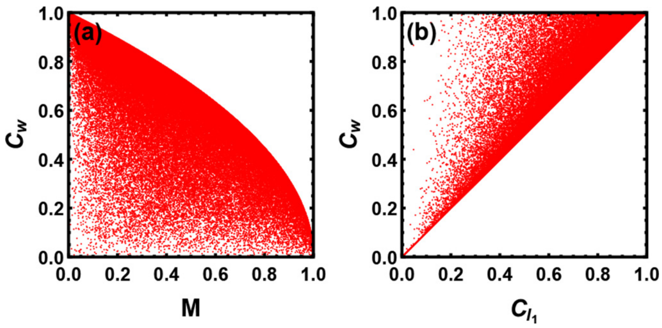

FIG. 2. The numerical simulation (e.g., 10^5 randomly generated qubit states) shows that (a) there exists a tradeoff relationship between $C_w(\rho)$ and the mixedness $M(\rho)$; (b) $C_w(\rho)$ is always larger than or equal to the l_1 norm of coherence $C_{l_1}(\rho)$ for qubit states.

where the relation $\rho_{00}\rho_{11} - |\rho_{01}|^2 = \det\rho$ is used. On the other hand, if the value of $|\rho_{01}|$ lies between ρ_{00} and ρ_{11}, item (v) of Lemma 4 can be applied

$$C_w(\rho) = 1 - \frac{\det\rho}{\min\{\rho_{00}, \rho_{11}\}}. \tag{14}$$

Finally, notice that the combined formula is also valid for pure or incoherent qubit states. ■

To gain a deeper insight into $C_w(\rho)$, we perform a numerical simulation for 10^5 randomly generated qubit states (see Fig. 2). The following two corollaries encapsulate the intriguing observations and analytical proofs.

Corollary 1. For any qubit state ρ, there exists a tradeoff relationship between the coherence weight $C_w(\rho)$ and the mixedness $M(\rho)$

$$C_w(\rho)^2 + M(\rho) \leqslant 1, \tag{15}$$

where the mixedness $M(\rho) = 2(1 - \mathrm{Tr}\rho^2)$ is characterized by the linear entropy of ρ [48].

Proof. In the Bloch representation, this inequality is equivalent to $C_w(\rho) \leqslant |\vec{u}|$, i.e., $C_w(\rho)$ should be less than or equal to the length of the Bloch vector of ρ. If $\rho_{00}, \rho_{11} \geqslant |\rho_{01}|$, this inequality is true since in this case $C_w(\rho) = 2|\rho_{01}| = (u_1^2 + u_2^2)^{1/2} \leqslant |\vec{u}|$. Therefore, without loss of generality, we can assume $\rho_{00} \geqslant |\rho_{01}| \geqslant \rho_{11}$, that is, $1 + u_3 \geqslant (u_1^2 + u_2^2)^{1/2} \geqslant 1 - u_3$, and the following equivalence relations hold:

$$\begin{aligned} C_w(\rho) &= 1 - \frac{2}{1-u_3}\frac{1-|\vec{u}|^2}{4} \leqslant |\vec{u}| \\ &\Leftrightarrow 1 - |\vec{u}| \leqslant \frac{1-|\vec{u}|^2}{2(1-u_3)} \\ &\Leftrightarrow 1 - 2u_3 \leqslant |\vec{u}| \end{aligned}$$

The last inequality is valid since $1 - 2u_3 \leqslant 1 - u_3 \leqslant (u_1^2 + u_2^2)^{1/2} \leqslant |\vec{u}|$ by assumption. ■

In fact, the inequality Eq. (15) is stronger than the inequality $C_{l_1}(\rho)^2 + M(\rho) \leqslant 1$ proved in Ref. [48] due to the fact $C_w(\rho) \geqslant C_{l_1}(\rho)$ for qubit states (see Lemma 3). In the following corollary, a more detailed proof is given starting from the analytical formula of $C_w(\rho)$ and as a byproduct we can show that the volume of the states on the line $C_w(\rho) = C_{l_1}(\rho) = 2|\rho_{01}|$ is precisely equal to that above this line [see Fig. 2(b)].

Corollary 2. For any qubit state ρ, $C_w(\rho) \geqslant C_{l_1}(\rho)$ holds. Further we have

$$\frac{\nu[C_w(\rho) > C_{l_1}(\rho)]}{\nu[C_w(\rho) = C_{l_1}(\rho)]} = 1, \tag{16}$$

where $\nu[\bullet]$ is the volume of states satisfying the corresponding condition.

Proof. See Appendix C.

To demonstrate the power of Corollary 2, we have independently generated two sets of random qubit states (e.g., 10^4 and 10^5 qubit states, respectively) and counted the number of states on the line [i.e., $C_w(\rho) = C_{l_1}(\rho)$] and off the line [i.e., $C_w(\rho) > C_{l_1}(\rho)$] with the accuracy of 10^{-10}, where the ratios are shown to be 4953 : 5047 and 49711 : 50289, respectively.

IV. MMCS AND NUMERICAL SIMULATIONS

From Corollary 1, one can infer that only pure qubit states achieve the maximum value of C_w. However, when we consider a Hilbert space of dimension $d \geqslant 3$, the situation is totally different. Here we introduce the notion of mixed maximally coherent states (MMCS), in the spirit of mixed maximally entangled states and mixed maximally steerable states in entanglement [38] and steering theories [28], respectively.

Definition 3. If a mixed coherent state has the same coherence value quantified by a certain coherence measure as pure maximally coherent states, we call it a mixed maximally coherent state. In particular, for coherence weight, a mixed state ρ is a MMCS if and only if $C_w(\rho) = 1$.

Since almost all papular coherence measures raised in the literature only assign a maximal value to the set of pure maximally coherent states [39], for these measures there never exist the notion of MMCS. Moreover, it is important to stress that a seemingly similar (but completely dissimilar) concept called maximally coherent mixed states (MCMS) was proposed to characterize the set of states with maximal coherence for a fixed purity [48–50]. First, we provide a necessary condition for the existence of MMCS in d-dimensional Hilbert space.

Corollary 3. In d-dimensional Hilbert space (e.g., $d \geqslant 3$), a MMCS must be rank-deficient, i.e., $\mathrm{rank}(\rho_{MMCS}) \leqslant d - 1$.

Proof. From the definition of the coherence weight and Lemma 2, if $C_w(\rho) = 1$ then it must be on the boundary of the set of density matrices, which implies that ρ is of deficient rank. ■

In fact, a significant class of MMCS has already been proposed although it has originally been raised for illustrating the (ir)reversibility of the coherence theory. More precisely, for a given state the reversibility indicates that its distillable coherence is equal to its coherence cost [7]. It is proved that this class of states satisfying reversibility requirement can only be of the following form [7]:

$$\rho = \oplus_j p_j |\phi_j\rangle\langle\phi_j|, \tag{17}$$

where the eigenvectors $\{|\phi_j\rangle\}$ are supported on the orthogonal subspaces spanned by a partition of the incoherent basis. From Lemma 1, we have substantially proved that the coherence weight has the property called the additivity of coherence for

TABLE I. For 10^5 randomly generated states, we have found the state with the largest coherence weight C_w in every dimension and also listed the corresponding participation ratio R, the second smallest eigenvalue $\lambda_{\rm sec}$, the minimum eigenvalue $\lambda_{\rm min}$, and the coherence rank r_c of the eigenvector $|\psi\rangle_{\rm min}$ associated with $\lambda_{\rm min}$.

d	C_w	R	$\lambda_{\rm sec}$	$\lambda_{\rm min}$	$r_c(\lvert\psi\rangle_{\rm min})$
3	0.999992	1.59051	0.246295	9.93186×10^{-7}	3
4	0.999997	2.30158	0.129657	5.64599×10^{-8}	4
5	0.999999	2.61211	0.060884	3.99851×10^{-8}	5
6	0.999999	2.91176	0.020337	3.32934×10^{-8}	6

subspace-independent states [51]

$$C_w(\oplus_j p_j \rho_j) = \sum_j p_j C_w(\rho_j). \tag{18}$$

If we additionally require all coherence ranks $r_c(|\phi_j\rangle) \geqslant 2$, combining Eqs. (17) and (18), we obtain

$$C_w(\oplus_j p_j |\phi_j\rangle\langle\phi_j|) = \sum_j p_j C_w(|\phi_j\rangle\langle\phi_j|) = \sum_j p_j = 1. \tag{19}$$

Here the coherence rank r_c of a pure state is defined as its number of nonzero terms in the incoherent basis [52]. In the next theorem, we present another interesting family of the MMCS.

Theorem 2. If ρ is rank deficient and an eigenvector $|\psi\rangle$ corresponding to zero eigenvalue has full coherence rank (i.e., $|\psi\rangle = \sum_{j=0}^{d-1} \psi_j |j\rangle$ with all $\psi_j > 0$), then ρ belongs to the MMCS.

Proof. From Definition 1 or directly the SDP form of Eq. (9), we explicitly know that $\rho \in$ MMCS is tantamount to the condition that no incoherent projector $\{|i\rangle\langle i|\}$ can be subtracted from ρ but still maintaining the positivity of the reminder. Therefore, if we can prove that ρ fulfills this equivalence condition then $\rho \in$ MMCS. Indeed, a square matrix M is said to be positive semidefinite iff $\langle\psi|M|\psi\rangle \geqslant 0$ for any vector $|\psi\rangle$. Using the assumption of the theorem, we have

$$\langle\psi|\,(\rho - \lambda_i |i\rangle\langle i|)\,|\psi\rangle = -\lambda_i |\langle i|\psi\rangle|^2 < 0, \tag{20}$$

where λ_i is a positive parameter and $|\psi\rangle$ is chosen to be the eigenvector corresponding to zero eigenvalue. Note that $|\langle i|\psi\rangle| > 0$ for all $i = 0, \ldots, d-1$ since $|\psi\rangle$ has full coherence rank. ■

In Fig. 3, we have plotted the distributions of $C_w(\rho)$ according to the purities of 10^5 randomly generated states in $d = 3, 4, 5, 6$ dimensions, where the participation ratio $R(\rho) = 1/\mathrm{Tr}\rho^2$ is introduced [53]. Intriguingly, from our numerical simulations it is found that in every dimension the state with the largest coherent weight (i.e., closest to 1) falls into the category described in Theorem 2 (see Table I). One step further, in fact we can prove that Theorem 2 is a necessary and sufficient condition for qutrit states and in this case the MMCS can only exist when the participation ratio $R(\rho) \leqslant 2$ [see Fig. 3(a)].

Corollary 4. A mixed qutrit state ρ is a MMCS if and only if it is of the form

$$\rho = \lambda_1 |\psi_1\rangle\langle\psi_1| + \lambda_2 |\psi_2\rangle\langle\psi_2|, \tag{21}$$

where $\lambda_1, \lambda_2 > 0$ with $\lambda_1 + \lambda_2 = 1$, $\langle\psi_1|\psi_2\rangle = 0$ and the eigenvector $|\psi_0\rangle$ associated with zero eigenvalue has full coherence rank. Moreover, the qutrit MMCS can only exist for states with $R(\rho) \leqslant 2$.

Proof. The "if" part is obviously valid owing to Theorem 2. On the other hand, if $C_w(\rho) = 1$ for a mixed qutrit state, it can be drawn from Corollary 3 that ρ has two strictly positive eigenvalues. We consider the spectral decomposition of ρ

$$\rho = \lambda_1 |\psi_1\rangle\langle\psi_1| + \lambda_2 |\psi_2\rangle\langle\psi_2|, \tag{22}$$

where $\lambda_1, \lambda_2 > 0$ with $\lambda_1 + \lambda_2 = 1$ and $\langle\psi_1|\psi_2\rangle = 0$.

Without loss of generality, we assume that $r_c(|\psi_1\rangle) \leqslant r_c(|\psi_2\rangle)$ and consider all possible options concerning the coherence ranks of $|\psi_1\rangle$ and $|\psi_2\rangle$.

(i) If $r_c(|\psi_1\rangle) = r_c(|\psi_2\rangle) = 1$, then ρ is incoherent, which contradicts $C_w(\rho) = 1$.

(ii) If $r_c(|\psi_1\rangle) = 1$, $r_c(|\psi_2\rangle) = 2$, from Eq. (18) we have $C_w(\rho) = \lambda_2 < 1$, which also contradicts $C_w(\rho) = 1$.

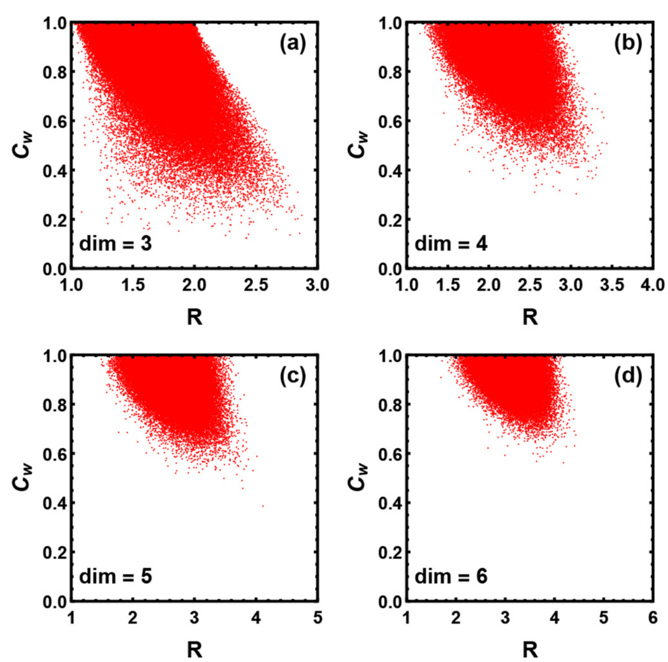

FIG. 3. The coherence weight $C_w(\rho)$ versus the participation ratio $R(\rho) = 1/\mathrm{Tr}\rho^2$ for 10^5 randomly generated states in $d = 3, 4, 5, 6$ dimensions. For qutrit states, it is evident that the MMCS exist only when $R(\rho) \leqslant 2$.

(iii) If $r_c(|\psi_1\rangle) = r_c(|\psi_2\rangle) = 2$, then ρ is reduced to a mixed qubit state while there does not exist MMCS for qubit system.

(iv) If $r_c(|\psi_1\rangle) = 2$, $r_c(|\psi_2\rangle) = 3$, a typical example can be expressed as

$$|\psi_1\rangle = \alpha|0\rangle + \beta|1\rangle,$$
$$|\psi_2\rangle = -\gamma\beta^*|0\rangle + \gamma\alpha^*|1\rangle + \sqrt{1-|\gamma|^2}|2\rangle,$$

where α, β, γ are nonzero complex numbers and $|\alpha|^2 + |\beta|^2 = 1$, $|\gamma| \neq 1$. Since $|\psi_0\rangle$ is also orthogonal to $|\psi_1\rangle$, it must have the same form as $|\psi_2\rangle$

$$|\psi_0\rangle = -\gamma_0\beta^*|0\rangle + \gamma_0\alpha^*|1\rangle + \sqrt{1-|\gamma_0|^2}|2\rangle.$$

The condition $\langle\psi_0|\psi_2\rangle = 0$ will lead to the equation

$$|\gamma|^2 + |\gamma_0|^2 = 1, \tag{23}$$

which is impossible when $|\gamma_0| = 0$ or 1 [i.e., $r_c(|\psi_0\rangle) = 1$ or 2]. Thus in this case we have $r_c(|\psi_0\rangle) = 3$.

(v) If $r_c(|\psi_1\rangle) = r_c(|\psi_2\rangle) = 3$, we first consider the probability $r_c(|\psi_0\rangle) = 2$. More precisely, if $r_c(|\psi_0\rangle) = 2$, the role of $|\psi_0\rangle$ played in this case is the same as $|\psi_1\rangle$ in the above case. Typically, we can assume $|\psi_0\rangle = \alpha|0\rangle + \beta|1\rangle$ then $|\psi_1\rangle$ and $|\psi_2\rangle$ can be expressed as $(0 < |\gamma_1|, |\gamma_2| < 1)$

$$|\psi_1\rangle = -\gamma_1\beta^*|0\rangle + \gamma_1\alpha^*|1\rangle + \sqrt{1-|\gamma_1|^2}|2\rangle,$$
$$|\psi_2\rangle = -\gamma_2\beta^*|0\rangle + \gamma_2\alpha^*|1\rangle + \sqrt{1-|\gamma_2|^2}|2\rangle.$$

Next, for instance we can check the positive semidefiniteness of $\rho - x|2\rangle\langle 2|$ for some strictly positive coefficient x. For any vector $|\varphi\rangle$ in the three-dimensional space, $\rho - x|2\rangle\langle 2| \succeq 0$ is equivalent to the positivity of the following expression:

$$\langle\varphi|\,(\rho - x|2\rangle\langle 2|)\,|\varphi\rangle = \langle\varphi|\rho|\varphi\rangle - x|\langle 2|\varphi\rangle|^2. \tag{24}$$

Note that when $|\varphi\rangle$ is chosen to be $|\psi_0\rangle$, x can be an arbitrary positive number. Therefore, if we choose x to be a constant within the realm of $(0, x^\star]$ where

$$x^\star = \min_{|\varphi\rangle\neq|\psi_0\rangle} \frac{\langle\varphi|\rho|\varphi\rangle}{|\langle 2|\varphi\rangle|^2} > 0, \tag{25}$$

then the positive semidefiniteness of $\rho - x|2\rangle\langle 2|$ is guaranteed. Actually, one can further infer that x is upper bounded by

$$x \leqslant \frac{1}{\langle 2|\rho^{-1}|2\rangle} < 1, \tag{26}$$

where the upper bound is achieved when (unnormalized) $|\varphi\rangle$ is set to be $\rho^{-1}|2\rangle$ in Eq. (25) [15]. This implies that the projector $|2\rangle\langle 2|$ can be subtracted from ρ by some amount but still maintaining the positivity of the reminder, which contradicts with the assumption $\rho \in MMCS$. Finally it can be concluded that $r_c(|\psi_0\rangle) = 3$.

Moreover, the participation ratio $R(\rho)$ is restricted to

$$R(\rho) = \frac{1}{\lambda_1^2 + \lambda_2^2} \leqslant \frac{2}{(\lambda_1+\lambda_2)^2} = 2. \tag{27}$$

This result is clearly illustrated in Fig. 3(a). ■

V. DISCUSSION AND CONCLUSION

In this work, we begin with the notion of BFA in a general convex resource theory, which generalizes the concept of BSA [40]. By presenting three crucial lemmas, we have exhibited the universal properties of this resource measure. Concentrating on the specific resource theory of coherence, an analytical formula of coherence weight has been derived for any qubit state. In fact, the value of coherent weight for a given qubit state relies on the relationship between the diagonal and off-diagonal elements in the incoherent basis, which is in sharp contrast with other popular coherence monotones. Furthermore, as another particular feature of weight-based resource measure, we have introduced the notion of MMCS, in the spirit of mixed maximally entangled states [38] and mixed maximally steerable states [28]. Combining with numerical simulations, we have presented two families of MMCS in arbitrary dimension (e.g., $d \geqslant 3$) and completely characterized the form of qutrit MMCS.

Although recently an operational interpretation has been proposed for the convex weight in general quantum resource theories [36,37], there still exist many open questions, especially focusing on the computability of weight-based quantifiers. For instance, while the coherence weight can be solved effectively by the SDP method, it is still worth making the effort to find analytical results for high-dimensional states. Moreover, we notice that at present there is no universal and efficient algorithm to determine the BSA of arbitrary states, mainly due to the fact that the set of separable states is not a polytope [54]. However, recently Lu *et al.* established a separability-entanglement classifier by using an iterative algorithm of convex hull approximation in Ref. [55]. Actually, we realize that such a method can also be adopted to compute the entanglement weight and our numerical simulations show that it is less time consuming than that of Refs. [26,27]. Subsequent work is already underway concerning these considerations.

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APPENDIX A: PROOF OF LEMMA 1

Indeed, owing to the similarity between the definitions of the robustness measure $\mathcal{R}(\rho)$ and BFA(ρ), one can readily mimic the proof presented in Ref. [9]. Here we take (C3) (i.e., strong monotonicity) for example. If we assume that the optimal mixture for ρ with respect to the BFA is given by $\rho = [1-\mathrm{BFA}(\rho)]\rho_f^\star + \mathrm{BFA}(\rho)\rho_r^\star$ and apply the (sub)channel Θ_i to both sides, then we have

$$\Theta_i(\rho) = [1-\mathrm{BFA}(\rho)]\Theta_i(\rho_f^\star) + \mathrm{BFA}(\rho)\Theta_i(\rho_r^\star). \tag{A1}$$

Since $\Theta_i(\rho_f^\star)/\mathrm{Tr}[\rho_f^\star] \in \mathcal{F}$, the definition (2) implies

$$\mathrm{BFA}\left[\frac{\Theta_i(\rho)}{\mathrm{Tr}[\Theta_i(\rho)]}\right] \leqslant \mathrm{BFA}(\rho)\frac{\mathrm{Tr}[\Theta_i(\rho_r^\star)]}{\mathrm{Tr}[\Theta_i(\rho)]}. \tag{A2}$$

Taking the sum of the above equations over all $\{\Theta_i\}$, finally we obtain

$$\sum_i \mathrm{Tr}[\Theta_i(\rho)]\mathrm{BFA}\left[\frac{\Theta_i(\rho)}{\mathrm{Tr}[\Theta_i(\rho)]}\right] \leqslant \mathrm{BFA}(\rho), \tag{A3}$$

where we have used the fact that $\sum_i \Theta_i$ constitutes a completely positive trace-preserving map.

APPENDIX B: GEOMETRIC INTERPRETATION OF BFA

The geometric interpretation is already illustrated in Fig. 1, where $\rho_f \in \mathcal{F}$ and $\rho_r \in \mathcal{D}/\mathcal{F}$ can be viewed as points on the straight line across the fixed point ρ. Note that any convex decomposition in the definition of Eq. (2) can be rewritten as

$$\rho - \rho_r = \lambda(\rho_f - \rho_r). \tag{B1}$$

By employing a valid distance metric, e.g., the Hilbert-Schmidt norm, we have

$$\lambda = \frac{\|\rho - \rho_r\|}{\|\rho_r - \rho_f\|} = \frac{l_{AB}}{l_{AC}}, \tag{B2}$$

where the lengths of the line segments of $\overline{AB}$ and $\overline{AC}$ are denoted by l_{AB} and l_{AC}, respectively.

To approach the maximum value of the weight λ, we can simply take two steps. First, for a given state ρ (i.e., the point B), we can fix ρ_r (i.e., the point A) in the interior of $\mathcal{D}$, then from Eq. (B2) it is obvious that ρ_f should be chosen on the boundary of $\mathcal{F}$ (i.e., the point C) in order to minimize the length l_{AC}. In fact, if ρ_f is in the interior region of $\mathcal{F}$ (i.e., the point D), apparently we have $l_{AD} > l_{AC}$. Second, when ρ_f is fixed on the boundary of $\mathcal{F}$, it is clear that λ is a monotonic increasing function of l_{AB} since

$$\lambda = \frac{l_{AB}}{l_{AC}} = \frac{l_{AB}}{l_{AB} + l_{BC}}. \tag{B3}$$

Therefore, ρ_r (i.e., the point A) should settle on the boundary of $\mathcal{D}$ for maximizing l_{AB}.

APPENDIX C: PROOF OF COROLLARY 2

To prove $C_w(\rho) \geqslant C_{l_1}(\rho)$, we only need to consider the case that the value of $|\rho_{01}|$ lies between ρ_{00} and ρ_{11}. Due to the perfect rotational symmetry of the Bloch sphere, we focus on a quarter of the unit disk shown in Fig. 4 and assume $\rho_{00} \geqslant |\rho_{01}| \geqslant \rho_{11}$, i.e., $u_3 \geqslant 1 - (u_1^2 + u_2^2)^{1/2}$. It is worth pointing out that the point A is actually the projection of ρ on the $x - y$ plane in the original Bloch sphere. Thus we have $l_{OA} = C_{l_1}(\rho) = (u_1^2 + u_2^2)^{1/2}$ and if we fix the length of l_{OA} then the allowed state ρ with constant $C_{l_1}(\rho)$ can move on the line segment connecting the point A and D. However, the condition $u_3 \geqslant 1 - (u_1^2 + u_2^2)^{1/2}$ results in the fact that ρ is further restricted on the line segment $\overline{CD}$, where the *critical* state on the point C satisfies the equality $u_3 = 1 - (u_1^2 + u_2^2)^{1/2}$.

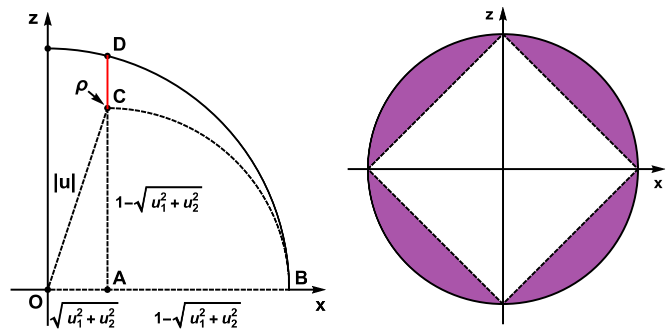

FIG. 4. The geometric interpretation of Corollary 2. The restriction $u_3 \geqslant 1 - (u_1^2 + u_2^2)^{1/2}$ renders the allowed state ρ on the line segment $\overline{CD}$. See the main text for more descriptions.

With this geometric representation in mind, now we deal with the inequality

$$C_w(\rho) = 1 - \frac{1 - |\vec{u}|^2}{2(1 - u_3)} \geqslant \sqrt{u_1^2 + u_2^2} = 2|\rho_{01}|. \tag{C1}$$

If we define the function of u_3

$$f(u_3) = 1 - \frac{1 - |\vec{u}|^2}{2(1 - u_3)} - \sqrt{u_1^2 + u_2^2}, \tag{C2}$$

then the validity of the inequality is equivalent to $f(u_3) \geqslant 0$ for $1 - (u_1^2 + u_2^2)^{1/2} \leqslant u_3 \leqslant [1 - (u_1^2 + u_2^2)]^{1/2}$. First, note that when ρ settles on the point C one can easily verify that $f(u_3) = 0$. Moreover, we have

$$f'(u_3) = \frac{u_3}{1 - u_3} - \frac{1 - u_3^2 - a^2}{2(1 - u_3)^2},$$

$$f''(u_3) = \frac{a^2}{(1 - u_3)^3} \geqslant 0,$$

where for simplicity we define $a = (u_1^2 + u_2^2)^{1/2}$. Since $f'(u_3 = 1 - a) = 0$ and $f''(u_3) \geqslant 0$, $f(u_3)$ is a convex function of u_3 for $1 - a \leqslant u_3 \leqslant (1 - a^2)^{1/2}$, and thus the minimum value of $f(u_3)$ is achieved at the boundary $u_3 = 1 - a$. Therefore we have $f(u_3) \geqslant f(u_3 = 1 - a) = 0$.

On the other hand, when $l_{OA} = (u_1^2 + u_2^2)^{1/2}$ varies the line segment $\overline{CD}$ evolves into the purple shaded regions of the Bloch sphere, implying that the qubit states satisfying $C_w(\rho) > C_{l_1}(\rho)$ occupy such regions (see Fig. 4). By use of the formula of the volume of a cone, we obtain

$$\frac{v[C_w(\rho) > C_{l_1}(\rho)]}{v[C_w(\rho) = C_{l_1}(\rho)]} = \frac{\frac{4}{3}\pi r^3 - 2 \times \frac{1}{3}\pi r^2 h}{2 \times \frac{1}{3}\pi r^2 h} = 1, \tag{C3}$$

where the height of the cone h is equal to the radius r of the Bloch sphere. The proof is complete.

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