Generalized coherence vector applied to coherence transformations and quantifiers

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One of the main problems in any quantum resource theory is the characterization of the conversions between resources by means of the free operations of the theory. In this work we advance on this characterization within the quantum coherence resource theory by introducing the generalized coherence vector of an arbitrary quantum state. The generalized coherence vector is a probability vector that can be interpreted as a concave roof extension of the pure states coherence vector. We show that it completely characterizes the notions of being incoherent, as well as being maximally coherent. Moreover, using this notion and the majorization relation, we obtain a necessary condition for the conversion of general quantum states by means of incoherent operations. These results generalize the necessary conditions of conversions for pure states given in the literature, and show that the tools of the majorization lattice are useful also in the general case. Finally, we introduce a family of coherence quantifiers by considering concave and symmetric functions applied to the generalized coherence vector. We compare this proposal with the convex roof measure of coherence and others quantifiers given in the literature.

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I. INTRODUCTION

Quantum coherence is one of the fundamental aspects of the quantum theory. It has practical relevance in numerous fields of quantum physics, particularly in quantum information processing. Moreover, quantum coherence is considered as a quantum resource that can be converted, manipulated, and quantified [1,2]. It admits a resource-theoretic formulation in terms of incoherent states (free states), coherent states (resources), and incoherent operations (free operations).

Since coherence is a basis dependent concept, the three components of the resource-theoretic formulation have to be defined for a given incoherent basis. In the standard approach, the incoherent basis is an orthonormal basis (see, e.g., [1,3]). There are also alternative resource-theoretic formulations based on nonorthonormal basis or positive-operator-valued measures (see, e.g., [4–6]).

In this work we follow the standard formulation. The incoherent states are diagonal in the incoherent basis, whereas coherent states have off-diagonal elements in this basis. Regarding the free operations, there is not a unique definition. Several definitions, often motivated by their operational interpretations, have been introduced (see, e.g., [3] for a review). In what follows, we restrict our attention to the definition of incoherent operation introduced in [1]. Within this definition, quantum coherence cannot be created from any incoherent input state by means of incoherent operations, not even in a probabilistic way.

One of the main problems in any resource theory is characterizing the conversion between states by means of free operations [7]. In the quantum coherence case, this problem has been completely solved for incoherent transformations from pure to pure states (see Refs. [8–12] or Lemma 4), as well as for transformations from pure to mixed states (see Refs. [12,13] or Prop. 5). This characterization is given in terms of the majorization relation [14] between the coherence vectors of the pure states. Motivated by this fact, we propose a generalization of the coherence vector applicable to arbitrary quantum states, and we advance on the characterization of the state conversion by means of incoherent operations by appealing to the majorization lattice theory [15–18]. More precisely, given a pure state decomposition of a quantum state, we define the coherence vector of the decomposition in terms of the coherence vectors of the pure states. Then, we define the coherence vector of a general quantum state as the supremum (in terms of the majorization order relation) of the coherence vectors of all pure-state decompositions. In this way our proposal can be interpreted as a concave roof extension of the pure state case. Alternatively, the generalized coherence vector of an arbitrary state ρ can be also defined as the supremum of all coherence vectors of the pure states that can be converted into ρ by means of an incoherent operation. Hence, our definition also acquires an operational meaning.

We prove that the generalized coherence vector characterizes the notions of being incoherent, as well as being maximally coherent. In addition, we extend the necessary condition of Prop. 5 (see Refs. [12,13]) to the case of initial mixed states, which is also given in terms of the majorization relation of the corresponding coherence vectors. This result is

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a step forward on the characterization of conversions between general quantum states under incoherent operations, whose complete solution is only known for the single qubit system [19,20]. Indeed, in higher dimensions ($d \geqslant 4$) it was recently shown that a finite number of conditions in terms of coherence measures are not sufficient to fully characterize coherence transformations between general quantum states [13]. Thus, the complete characterization of the general case remains open.

Another main problem in any resource theory is to quantify the resource amount of any state [10]. There are several coherence quantifiers and each of them captures different operational aspects of coherence, for instance, the distillable coherence, the coherence cost [21,22], the relative entropy of coherence, and the ℓ_1 norm of coherence [1], among others (see, e.g., [3]). Providing new quantifiers of coherence is an ongoing topic in the resource theory of coherence. A common strategy for obtaining a coherence quantifier is to define a suitable function on the pure states and then extend it to the entire set of quantum states. The extension can be done in different ways. The most frequently used is the convex roof construction [11,12], which was originally applied in the entanglement theory [23,24]. A recent proposal was given in [25], based on the state conversion process from pure to arbitrary quantum states by means of incoherent operations. In this work we also present a different approach to obtain a family of coherence quantifiers, based on the generalized coherence vector.

This paper is organized as follows. In Sec. II we recall the basics elements of the resource theory of quantum coherence. In particular, we review the notions of incoherent and coherent states, and incoherent operations. In addition, we present some important results about conversions of coherent states, as well as its axiomatic quantification, focusing on coherence measures based on the convex roof construction and on coherence monotones recently introduced. In Sec. III we introduce the notion of a generalized coherence vector, valid for arbitrary quantum states. We show that it is a good definition, since it allows us to characterize the notions of being incoherent and maximally coherent. In Sec. IV we apply the generalized coherence vector to provide a necessary condition, in terms of a majorization relation, for the conversion of general quantum states. In Sec. V we introduce a family of monotones based on the coherence vector, and we compare it with the convex roof construction and other monotones introduced in the literature. In Sec. VI we applied this family of monotones to quantify the coherence of a qubit system and a maximally coherent qutrit going through a depolarizing channel. Finally, some concluding remarks are given in Sec. VII. For the sake of readability, auxiliary lemmas and proofs are presented separately in Appendixes A and B, respectively.

II. PRELIMINARIES: RESOURCE THEORY OF QUANTUM COHERENCE

In this section we review the resource theory of quantum coherence introduced in [1]. In what follows, we consider a quantum system represented by a d-dimensional Hilbert space $\mathcal{H}$. Moreover, we denote as $\mathcal{S}(\mathcal{H})$ the set of density operators and as $\mathcal{P}(\mathcal{H})$ the set of pure states. Since the coherence of a quantum state is a basis dependent notion, it is necessary to choose a reference basis in order to formulate its resource theory, which is usually called *incoherent basis*. In the rest of this work we will choose the computational basis $\mathcal{B} = \{|i\rangle\}_{i=0}^{d-1}$ as the incoherent basis.

A. Free states, resources, and free operations

Any resource theory is built from the basic notions of free states, resources, and free operations. In the case of the resource theory of coherence, the free states are quantum states with diagonal density matrix in the incoherent basis, i.e., a state ρ is incoherent if and only if $\rho = \sum_{i=0}^{d-1} p_i \, |i\rangle \, \langle i|$, with $\sum_{i=0}^{d-1} p_i = 1$ and $p_i \geqslant 0$ for all $i \in \{0, \dots, d-1\}$. We call them *incoherent states*, and we denote the set of incoherent states as $\mathcal{I}$. The resources of a theory are the states which are not free. In the coherence case, the resources are quantum states represented by nondiagonal density matrices in the incoherent basis. We call them *coherent states*. Regarding the free operations, several definitions have been introduced [3]. For each definition we obtain different resource theories for coherence. In what follows, we focus on the incoherent operations introduced in [1].

In order to define the free operations, we consider completely positive and trace-preserving maps (CPTP) defined on the set of density operators $\mathcal{S}(\mathcal{H})$. If $\Lambda : \mathcal{S}(\mathcal{H}) \mapsto \mathcal{S}(\mathcal{H})$ is a CPTP map, it has an operator-sum representation in terms of Kraus operators $\{K_n\}_{n=1}^{N}$ of the form $\Lambda(\rho) = \sum_{n=1}^{N} K_n \rho K_n^{\dagger}$, where Kraus operators are such that $\sum_{n=1}^{N} K_n^{\dagger} K_n = I$ (with I the identity of the Hilbert space). The free operations for any resource theory of coherence have to be CPTP maps satisfying, at least, the additional condition of not creating coherence from an incoherent state. More precisely, $\Lambda(\rho) \in \mathcal{I}$ for any $\rho \in \mathcal{I}$. All operations of this type form the set of maximally incoherent operations (MIO).

In this work we are interested in a subset of the maximally incoherent operations, the so-called *incoherent operations* (IO), which were introduced in [1]. IO can be defined in terms of Kraus operations as follows [22,26,27]:

Definition 1 (Incoherent operation). A CPTP map Λ is an incoherent operation if it admits a Kraus representation $\{K_n\}_{n=1}^{N}$, such that the Kraus operators are incoherent, that is, $K_n \, |i\rangle \propto |f_n(i)\rangle$, for all $n \in \{1, \dots, N\}$, with f_n a relabeling function of the set $\{0, \dots, d-1\}$.

B. Necessary and sufficient conditions for coherent transformations

In this subsection we recall some important results about state transformations under incoherent operations. We denote as $\rho \underset{\mathrm{IO}}{\rightarrow} \sigma$ whenever a state ρ can be transformed into an state σ by means of an incoherent operation, i.e., when there is an incoherent operation Λ such that $\sigma = \Lambda(\rho)$.

We note that any incoherent state can be reached by any other state by means of a suitable incoherent operation, that is, for any state $\sigma \in \mathcal{I}$ there exists a state ρ such that $\rho \underset{\mathrm{IO}}{\rightarrow} \sigma$. Moreover, there are some states that can be converted into any other state (not necessarily incoherent) by means of incoherent operations. More precisely, there exist states

ρ called *maximally coherent state* (MCS), such that $\rho \underset{\text{IO}}{\to} \sigma$ for any $\sigma \in \mathcal{S}(\mathcal{H})$. The canonical MCS state is a pure state of the form $\rho^{\text{mcs}} = |\Psi^{\text{mcs}}\rangle\langle\Psi^{\text{mcs}}|$ with $|\Psi^{\text{mcs}}\rangle = \sum_{i=0}^{d-1}\frac{1}{\sqrt{d}}|i\rangle$. The set of all MCSs can be obtained from the orbit of ρ^{mcs} under the set of unitary incoherent operations, which are given by operators of the form $U_{\text{IO}} = \sum_{i=0}^{d-1} e^{\imath\theta_i}|\pi(i)\rangle\langle i|$, where π is a permutation acting on the set $\{0,\dots,d-1\}$ and $\theta_i \in \mathbb{R}$ [28].

In order to address the general problem of state transformation, we need the following notions. Let Δ_d be the set of d-dimensional probability vectors, i.e.,

$$\Delta_d = \left\{(u_0,\dots,u_{d-1}) \in \mathbb{R}^d : u_i \geqslant 0, \sum_{i=0}^{d-1} u_i = 1\right\}, \quad (1)$$

and let $\Delta_d^{\downarrow} \subseteq \Delta_d$ be the set of d-dimensional probability vectors with their entries decreasingly ordered. The *coherence vector of a pure state* of a d-dimensional Hilbert space is a probability vector in Δ_d defined as follows:

Definition 2 (Coherence vector). Let $\mathcal{B} = \{|i\rangle\}_{i=0}^{d-1}$ be the incoherent basis. The coherence vector of a pure state $|\psi\rangle\langle\psi|$ is defined as

$$\mu(|\psi\rangle\langle\psi|) = (|\langle 0|\psi\rangle|^2,\dots,|\langle d-1|\psi\rangle|^2). \quad (2)$$

We also define the ordered coherence vector $\mu^{\downarrow}(|\psi\rangle\langle\psi|) \in \Delta_d^{\downarrow}$, which is given by the entries of the vector $\mu(|\psi\rangle\langle\psi|)$, but in a nonincreasing order.

The state transformations between quantum states is related to the *majorization relation of probability vectors*. The majorization relation is defined as follows (see, e.g., [14]).

Definition 3 (Majorization relation). Given $u, v \in \Delta_d$, it is said that u is majorized by v (denoted as $u \preceq v$) if and only if $\sum_{i=0}^{k} u_{\pi_u(i)} \leqslant \sum_{i=0}^{k} v_{\pi_v(i)}$, for all $k \in \{0,\dots,d-1\}$, where π_u and π_v are permutations acting on the set $\{0,\dots,d-1\}$ that sort the entries of u and v, respectively, in a nonincreasing order.

The majorization relation is a preorder on the set Δ_d and a partial order on the set $\Delta_d^{\downarrow}$. Moreover, the set $\Delta_d^{\downarrow}$ endowed with the majorization relation $\preceq$ is a complete lattice[1] [15,16], and it is called the *majorization lattice*.

The algorithms to obtain the supremum and infimum of any subset of the majorization lattice can be found in [16–18]. In particular, the supremum of a set $\mathcal{U} \subseteq \Delta_d^{\downarrow}$, denoted as $\bigvee\mathcal{U}$, can be computed as follows. First, we obtain the *Lorenz curve*[2] of $\bigvee\mathcal{U}$, denoted as $L_{\bigvee\mathcal{U}}$. In [16] it has been shown that $L_{\bigvee\mathcal{U}}$ is equal to the upper envelope[3] of the polygonal curve given by the linear interpolation of the set of points $\{(j, S_j)\}_{j=0}^{d}$, where $S_j = \sup\{s_j(u) : u \in \mathcal{U}\}$ and $s_j(u) = \sum_{i=0}^{j-1} u_i$, with the convention $S_0 = 0$. Finally, we have $\bigvee\mathcal{U} = (L_{\bigvee\mathcal{U}}(1), L_{\bigvee\mathcal{U}}(2) - L_{\bigvee\mathcal{U}}(1),\dots,L_{\bigvee\mathcal{U}}(d) - L_{\bigvee\mathcal{U}}(d-1))$.

We remark that $\bigvee\mathcal{U}$ may or may not belong to $\mathcal{U}$. When $\bigvee\mathcal{U} \in \mathcal{U}$, $\bigvee\mathcal{U}$ is a maximum. In this case we have $S_k = L_{\bigvee\mathcal{U}}(k) = s_k(\bigvee\mathcal{U})$ for all $k \in \{1,\dots,d-1\}$. In other words, the Lorenz curve of $\bigvee\mathcal{U}$ is just the linear interpolation of $\{(j, S_j)\}_{j=0}^{d}$.

The majorization relation is intimately related to *Schur-concave functions* (see, e.g., [14, I.3]), which are functions that antipreserves the preorder relation. More precisely, a function $f : \Delta_d \to \mathbb{R}$ is Schur concave if for all $u, v \in \Delta_d$ such that $u \preceq v$, $f(u) \geqslant f(v)$. Moreover, if the function f also satisfies that $f(u) > f(v)$ whenever u is strictly majorized by v (i.e., when $u \preceq v$ and $u \neq \Pi v$, with Π a permutation matrix), we say that it is strictly Schur concave. In particular, the generalized entropies, including Shannon, Rény, and Tsallis entropies, are examples of strictly Schur-convave functions (see, e.g., [30]).

Taking into account these definitions, we present the following results about necessary and sufficient conditions for coherent transformations. The first result completely characterizes the incoherent transformations between pure states in terms of the majorization relation between their corresponding coherence vectors (see [8–12]).

Proposition 4. Let $|\psi\rangle\langle\psi|$ and $|\phi\rangle\langle\phi|$ be two arbitrary pure states, and let Λ be an incoherent operation. Then

$$|\psi\rangle\langle\psi| \underset{\text{IO}}{\to} |\phi\rangle\langle\phi| \iff \mu(|\psi\rangle\langle\psi|) \preceq \mu(|\phi\rangle\langle\phi|). \quad (3)$$

Notice that if both transformations are possible, we have $|\psi\rangle\langle\psi| \underset{\text{IO}}{\leftrightarrow} |\phi\rangle\langle\phi| \iff \mu(|\psi\rangle\langle\psi|) = \Pi(\mu(|\phi\rangle\langle\phi|))$, with Π a permutation matrix. As a consequence, the coherence vector $\mu(|\psi\rangle\langle\psi|)$ of the pure state $|\psi\rangle\langle\psi|$ and its ordered probability vector $\mu^{\downarrow}(|\psi\rangle\langle\psi|)$ are equivalent for the coherence resource theory.

The next result, given in [13, Th. 4], is a generalization of the previous proposition. It provides necessary and sufficient conditions for transformations from pure states to arbitrary states by means of incoherent operations.

Proposition 5. Let $|\psi\rangle\langle\psi|$ be an arbitrary pure state and σ be an arbitrary quantum state. Then

$$|\psi\rangle\langle\psi| \underset{\text{IO}}{\to} \sigma \iff \exists\{p_n, |\phi_n\rangle\}_{n=1}^{N} \text{ such that}$$
$$\begin{array}{l} (1)\ \sigma = \sum_{n=1}^{N} p_n|\phi_n\rangle\langle\phi_n| \text{ and} \\ (2)\ \mu(|\psi\rangle\langle\psi|) \preceq \sum_{n=1}^{N} p_n\mu^{\downarrow}(|\phi_n\rangle\langle\phi_n|). \end{array} \quad (4)$$

A related result, given in [12, Lemma 4], provides a particular decomposition of the final state σ given in Prop. 5,

$$|\psi\rangle\langle\psi| \underset{\text{IO}}{\to} \sigma \Rightarrow \mu(|\psi\rangle\langle\psi|) \preceq \sum_{n=1}^{N} p_n\mu^{\downarrow}(|\phi_n\rangle\langle\phi_n|), \quad (5)$$

[1] A preorder relation is a reflexive and transitive binary relation, and a partial order relation is a preorder that it is also antisymmetric. A set P endowed with a partial order relation is a complete lattice if the supremum and infimum of any subset of P exist (see, e.g., [29]).

[2] The Lorenz curve of a probability vector $u \in \Delta_d$ is an increasing and concave function $L_u : [0, d] \to [0, 1]$ formed by the linear interpolation of the points $\{(j, s_j(u^{\downarrow}))\}_{j=0}^{d}$. It can be shown that $u \preceq v \iff L_u \leqslant L_v$ (see, e.g., [14]).

[3] We recall that the upper envelope of a continuous function $f : \mathbb{R} \to \mathbb{R}$ is defined as $\inf\{g : f \leqslant g$ and g is continuous and concave$\}$ (see, e.g., [31, Def.4.1.5]).

where $p_n = \mathrm{Tr}(K_n |\psi\rangle\langle\psi| K_n^\dagger)$, $|\phi_n\rangle\langle\phi_n| = K_n |\psi\rangle\langle\psi| K_n^\dagger / p_n$, and $\{K_n\}_{n=1}^N$ are the incoherent Kraus operators of the incoherent operation Λ, which satisfies $\sigma = \Lambda(|\psi\rangle\langle\psi|)$.

The result given in Prop. 4 is a particular case of Prop. 5, but in the former the incoherent transformations are fully characterize by the majorization relation between the corresponding coherence vectors of the pure states.

C. Coherence measures

In this subsection we introduce the notion of *coherence measures*, mainly based on the axiomatic formulation given in [1].

Definition 6 (Coherence measure). A coherence measure is a function $C : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ satisfying the following conditions:

(C_1) *Vanishing on incoherent states:* $C(\rho) = 0$ for any ρ incoherent.

(C_2) *Monotonicity under incoherent operations:* $C(\rho) \geqslant C(\Lambda(\rho))$ for any incoherent operation Λ and any state ρ.

(C_3) *Monotonicity under selective incoherent operation:* $C(\rho) \geqslant \sum_{n=1}^N p_n C(\sigma_n)$, for any state ρ and any incoherent operation Λ, with incoherent Kraus operators $\{K_n\}_{n=1}^N$, where $p_n = \mathrm{Tr}\, K_n \rho K_n^\dagger$ and $\sigma_n = K_n \rho K_n^\dagger / p_n$.

(C_4) *Maximal coherence:* $\arg\max_{\rho\in\mathcal{S}(\mathcal{H})} C(\rho)$ is reached at maximally coherent states.

(C_5) *Convexity:* $C(\sum_{k=1}^M q_k \rho_k) \leqslant \sum_{k=1}^M q_k C(\rho_k)$.

Condition (C_1) guarantees that the measure is well defined for the incoherent states. Condition (C_2) ensures that it is consistent with incoherent operations. Both are the minimal requirements for any quantifier of the coherence resource. Condition (C_3) guarantees that coherence does not increase under incoherent measurements, even if one has access to the individual measurement outcomes. When a quantifier satisfies the conditions (C_1)–(C_3), it is called *coherence monotone*. We have included the condition (C_4) because maximally coherent states are the golden unit of the coherence resource theory with the incoherent operations given in Def. 1 (the golden unit does not necessary exist for other set of free operations, see, e.g., [3]). The relevance of this condition is discussed in [28]. Finally, condition (C_5) is often related to the fact that mixing states does not increase the amount of coherence. Although the convexity condition (C_5) is a desirable property for coherence quantifiers, it is not considered essential. Indeed, there are important quantifiers of coherence that do not satisfy (C_5), such as the maximum relative entropy of coherence [32]. Finally, we note that when conditions (C_2) and (C_5) are satisfied, condition (C_3) is automatically satisfied.

There are several quantifiers of coherence that satisfy some or all of the conditions given in Def. 6. In this work we are interested in families of coherence measures constructed from quantifiers of pure states. Before introducing an important result for coherence measures restricted to pure states (see, e.g., [11,12]), we need to define the following set of functions:

$$\mathcal{F} = \{f : \mathbb{R}^d \to [0,1] : f \text{ is symmetric and concave}, \\ f(1,0,\dots,0) = 0 \text{ and } \arg\max_{u\in\mathbb{R}^d} f(u) = (1/d,\dots,1/d)\}. \tag{6}$$

Since a symmetric and concave function is also Schur concave [14], then all functions in $\mathcal{F}$ are Schur concave.

The following result guarantees that the restriction of any coherence monotone to pure states can be written in terms of a function belonging to $\mathcal{F}$ evaluated on the coherence vectors of the pure states (see, e.g., [11,12]). We will call as f_C to the associated function of the coherence monotone C.

Proposition 7. Given a coherence monotone $C : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ satisfying conditions (C_1)–(C_4), there exists a function $f_C \in \mathcal{F}$, such that the restriction of C to the pure states, denoted as $C|_{\mathcal{P}(\mathcal{H})}$, can be written as

$$C|_{\mathcal{P}(\mathcal{H})}(|\psi\rangle\langle\psi|) = f_C(\mu(|\psi\rangle\langle\psi|)). \tag{7}$$

Conversely, given a function $f \in \mathcal{F}$, it is possible to define a coherence monotone. In the literature there are at least two proposals to do this. One was introduced in [11,12], whereas the other was recently developed in [25].

The first proposal appeals to the convex roof construction (see, e.g., [33]). Before introducing the *convex roof measure of coherence*, we define the set of all pure state decompositions of a given state ρ,

$$\mathcal{D}(\rho) = \left\{ \{q_k, |\psi_k\rangle\}_{k=1}^M : \rho = \sum_{k=1}^M q_k |\psi_k\rangle\langle\psi_k| \right\}, \tag{8}$$

where $(q_1,\dots,q_M) \in \Delta_M$ and $|\psi_k\rangle \in \mathcal{H}$ are unit-normed vectors (but not necessarily orthogonal to each other).

A complete characterization of this set is given by the *Schrödinger mixture theorem* (also known as *classification theorem for ensembles*, see, e.g., [34,35]). More precisely, $\{p_k, |\psi_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)$ if and only if there exists a unitary matrix U of $M \times M$ ($M \geqslant d$) such that

$$|\psi_k\rangle = \frac{1}{\sqrt{q_k}} \sum_{j=1}^d \sqrt{\lambda_j} U_{k,j} |e_j\rangle, \tag{9}$$

where λ_j and $|e_j\rangle$ are the eigenvalues and eigenstates of ρ, respectively.

Now we introduce the convex roof measure of coherence (see [11,12]).

Definition 8 (Convex roof measure). For any function $f \in \mathcal{F}$, the convex roof measure of coherence $C_f^{\mathrm{cr}} : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ is defined as

$$C_f^{\mathrm{cr}}(\rho) = \inf_{\{q_k,|\psi_k\rangle\}_{k=1}^M \in\mathcal{D}(\rho)} \sum_{k=1}^M q_k f(\mu(|\psi_k\rangle\langle\psi_k|)). \tag{10}$$

The convex roof measure C_f^{cr} is a good quantifier of coherence since it satisfies conditions (C_1)–(C_5). Moreover, the infimum in (10) can be replaced by a minimum, since there is always an optimal pure state decomposition of ρ that reaches the infimum (see, e.g., [36]).

The name of the measure C_f^{cr} is based on the fact that it is the convex roof extension of any coherence monotone with an associated function equal to f. An important property of this measure is the following.

Proposition 9. Let $C : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ be a coherence measure. Then

$$C \leqslant C_{f_C}^{\mathrm{cr}}, \tag{11}$$

where f_C is the associated function of C.

The convex roof construction is widely used, especially in the context of entanglement measures [23,24]. However, as we mentioned before, it is not the only way to define a coherence measure from a function $f \in \mathcal{F}$. Recently, an alternative construction was proposed [25]. Before introducing this measure of coherence, we need to define the set of all pure states that can be converted into a state ρ by means of incoherent operations,

$$\mathcal{O}(\rho) = \{|\psi\rangle\langle\psi| : |\psi\rangle\langle\psi| \underset{\mathrm{IO}}{\to} \rho\}. \tag{12}$$

Now we introduce the coherence measure given in [25]. In this work we will call it *top monotone of coherence*.

Definition 10 (Top monotone). For any function $f \in \mathcal{F}$, the top monotone of coherence $C_f^{\mathrm{top}} : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ is defined as

$$C_f^{\mathrm{top}}(\rho) = \inf_{|\psi\rangle\langle\psi| \in \mathcal{O}(\rho)} f(\mu(|\psi\rangle\langle\psi|)). \tag{13}$$

The top monotone C_f^{top} satisfies conditions (C_1)–(C_4), whereas condition (C_5) holds if and only if $C_f^{\mathrm{top}} = C_f^{\mathrm{cr}}$ [25, Th.4]. The chosen name for this measure is based on the following property given in [25].

Proposition 11. Let $C : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ be a coherence monotone. Then

$$C \leqslant C_{f_C}^{\mathrm{top}}, \tag{14}$$

where f_C is the associated function of C.

As in the case of coherence measures based on the convex roof construction, the infimum in (13) can be replaced by a minimum, since there always exists a pure state that reaches the infimum. This is a consequence of the continuity of f on Δ_d (concave functions on $\mathbb{R}^d$ are continuous on any subset of $\mathbb{R}^d$ [37, Th.10.1]) and the compactness of the set $\mathcal{O}(\rho)$, a fact that we will show in Lemma 36. In some proofs given in [25] it is assumed the existence of the minimum in (13), but its existence is not proven in general (see for instance the proofs of monotonicity and strong monotonicity of C_f^{top}, or the converse part of the proof of Th. 3 regarding the convexity of C_f^{top}, or the proof of Th. 7 regarding the continuity of C_f^{top}). Therefore, our Lemma 36 fills these gaps.

III. GENERALIZED COHERENT VECTOR: DEFINITION AND PROPERTIES

In this section we introduce the *generalized coherence vector* for arbitrary quantum states. This definition generalizes the one given in (2), and it connects the notion of coherence with the majorization lattice theory. Moreover, it allows us to introduce a new family of coherence quantifiers, alternative to C_f^{cr} and C_f^{top}.

Inspired by the definitions of C_f^{cr} and C_f^{top}, we define two sets of probability vectors associated with a given quantum state ρ. The first one is obtained from the pure state decompositions of ρ. We denote it as $\mathcal{U}^{\mathrm{psd}}(\rho)$, where the acronym "psd" refers to *pure state decompositions of* ρ.

Definition 12 (Pure state decompositions set). For any quantum state ρ, the pure state decompositions set of ρ is defined as

$$\mathcal{U}^{\mathrm{psd}}(\rho) = \left\{ \sum_{k=1}^{M} q_k \mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) : \{q_k, |\psi_k\rangle\}_{k=1}^{M} \in \mathcal{D}(\rho) \right\}. \tag{15}$$

The second set of probability vectors associated with a quantum state ρ is obtained from the set of all pure states that can be converted into ρ. We denote it as $\mathcal{U}^{\mathrm{psc}}(\rho)$, where the acronym "psc" refers to *pure states connected to* ρ.

Definition 13 (Connected pure states set). For any quantum state ρ, the connected pure states set of ρ is defined as

$$\mathcal{U}^{\mathrm{psc}}(\rho) = \{\mu^{\downarrow}(|\psi\rangle\langle\psi|) : |\psi\rangle\langle\psi| \in \mathcal{O}(\rho)\}. \tag{16}$$

An interesting property of these sets is that both are convex sets.

Proposition 14. The sets $\mathcal{U}^{\mathrm{psd}}(\rho)$ and $\mathcal{U}^{\mathrm{psc}}(\rho)$ are convex.

Another observation that will be useful for characterizing quantum coherence is the following. For a given ρ, $\mathcal{U}^{\mathrm{psd}}(\rho), \mathcal{U}^{\mathrm{psc}}(\rho) \subseteq \Delta_d^{\downarrow}$, and, since the majorization lattice is complete (see, e.g., [15,16]), the supremum and infimum (with respect to majorization partial order) of both sets always exist. Moreover, the supremum of both sets coincide. This result is stated in the following proposition.

Proposition 15. $\bigvee \mathcal{U}^{\mathrm{psd}}(\rho) = \bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$.

This result allows us to define the coherence vector of a general quantum state, generalizing the definition given in (2).

Definition 16 (Generalized coherence vector). For any quantum state ρ, its generalized coherence vector $\nu(\rho)$ is defined as

$$\nu(\rho) = \bigvee \mathcal{U}^{\mathrm{psd}}(\rho), \tag{17}$$

or, equivalently as $\nu(\rho) = \bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$.

Notice that for a pure state, the generalized coherence vector is equal to the ordered coherence vector, i.e., $\nu(|\psi\rangle\langle\psi|) = \mu^{\downarrow}(|\psi\rangle\langle\psi|)$, which means that the Def. 16 is a suitable extension of Def. 2.

We observe that whenever $\bigvee \mathcal{U}^{\mathrm{psd}}(\rho) \in \mathcal{U}^{\mathrm{psd}}(\rho)$, $\bigvee \mathcal{U}^{\mathrm{psd}}(\rho)$ is a maximum. We call *optimal pure state decomposition* to the ensemble that reaches this maximum.

Definition 17 (Optimal pure state decomposition). An ensemble $\{\tilde{q}_k, |\tilde{\psi}_k\rangle\}_{k=1}^{M}$ is an optimal pure state decomposition of ρ if $\{\tilde{q}_k, |\tilde{\psi}_k\rangle\}_{k=1}^{M} \in \mathcal{D}(\rho)$ and $\sum_{k=1}^{M} \tilde{q}_k \mu^{\downarrow}(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|) = \nu(\rho)$.

In Ref. [25] it is stated that for a general quantum state it is not easy to prove whether an optimal pure state decomposition always exists. In Sec. VI we will provide a method to check if the supremum is a maximum. In particular, we will show that there are qutrit states for which the optimal ensemble does not exist. This implies that in general the optimal pure state decomposition of a quantum state does not exist.

Whenever $\bigvee \mathcal{U}^{\mathrm{psc}}(\rho) \in \mathcal{U}^{\mathrm{psc}}(\rho)$, $\bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$ is also a maximum. We call *optimal pure state* to the state that reaches the maximum.

Definition 18 (Optimal pure state). A pure state $|\tilde{\psi}\rangle$ is optimal if $|\tilde{\psi}\rangle\langle\tilde{\psi}| \in \mathcal{O}(\rho)$ and $\mu^{\downarrow}(|\tilde{\psi}\rangle\langle\tilde{\psi}|) = \nu(\rho)$.

We have that when there exists an optimal pure state decomposition, there also exists an optimal pure state, and vice versa.

Proposition 19. $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho) \iff \nu(\rho) \in \mathcal{U}^{\rm psc}(\rho)$.

In what follows, we will show that the generalized coherence vector satisfies several properties that capture the main features of quantum. The first observation is that the generalized coherence vector completely characterizes the notion of incoherent state.

Proposition 20. ρ is incoherent $\iff \nu(\rho) = (1, 0, \ldots, 0)$.

This result justifies Def. 16 for the generalized coherence vector.

We also have that the generalized coherence vector fully characterizes maximally coherent states.

Proposition 21. ρ is maximally coherent $\iff \nu(\rho) = (\frac{1}{d}, \ldots, \frac{1}{d})$.

We observe that, by definition, for any pure state decomposition of ρ, the following majorization relation is satisfied.

Proposition 22. Let $\rho = \sum_{k=1}^{M} p_k |\psi_k\rangle\langle\psi_k|$. Then

$$\sum_{k=1}^{M} p_k \nu(|\psi_k\rangle\langle\psi_k|) \preceq \nu(\rho). \tag{18}$$

This result allows us to interpret the definition $\nu(\rho) = \bigvee \mathcal{U}^{\rm psd}(\rho)$ as a kind of concave roof extension of the pure state coherence vector.[4] However, the question whether the above statement is valid for any mixed state decomposition of ρ remains open.

Alternatively, the equivalence $\bigvee \mathcal{U}^{\rm psd}(\rho) = \bigvee \mathcal{U}^{\rm psc}(\rho)$ gives the generalized coherent vector an operational interpretation in terms of pure state transformations. In this sense, our definition is physically and mathematically well motivated, and it is a suitable extension of the pure state coherence vector given in Def. 2.

IV. NECESSARY CONDITIONS FOR INCOHERENT TRANSFORMATIONS

In this section we apply the notion of generalized coherence vector, given in (16), for characterizing state transformations between arbitrary quantum states.

Proposition 23. Let ρ and σ be two arbitrary quantum states. Then

$$\rho \underset{\rm IO}{\rightarrow} \sigma \Rightarrow \forall \{q_k, |\psi_k\rangle\}_{k=1}^{M} \in \mathcal{D}(\rho), \exists \{r_l, |\phi_l\rangle\}_{l\in L} \in \mathcal{D}(\sigma):$$

$$\sum_{k=1}^{M} q_k \mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{l\in L} r_l \mu^{\downarrow}(|\phi_l\rangle\langle\phi_l|). \tag{19}$$

Notice that this result generalizes the necessary condition of Prop. 5. In addition, we have the following consequences.

[4]Indeed, our proposal can be stated in a more abstract framework, generalizing the notion of concave roof extension of a function. More precisely, let Ω be a compact convex set and $\Omega^{\rm pure}$ be the set formed by its extremal points. The concave roof $f^{\rm cr}: \Omega \to \mathbb{R}$ of the function $f: \Omega^{\rm pure} \to \mathbb{R}$ is defined as $f^{\rm cr}(\omega) = \sup \sum_k q_k f(\omega_k)$, where the supremum is taken over all extremal convex decompositions of $\omega = \sum_k q_k \omega_k$, $\omega_k \in \Omega^{\rm pure}$ (see, e.g., [33]). This construction can be extended to functions from a compact convex set to the majorization lattice. The concave roof $\vec{f}^{\rm cr}: \Omega \to \Delta_d^{\downarrow}$ of the function $\vec{f}: \Omega^{\rm pure} \to \Delta_d^{\downarrow}$ is defined as $\vec{f}^{\rm cr}(\omega) = \bigvee \sum_k q_k \vec{f}(\omega_k)$, where, in this case, the supremum is the one of the majorization lattice.

Corollary 24. Let ρ and σ be two quantum states. Then

$$\rho \underset{\rm IO}{\rightarrow} \sigma \Rightarrow \nu(\rho) \preceq \sum_{n=1}^{N} p_n \nu(\sigma_n), \tag{20}$$

with $p_n = {\rm Tr}\,(K_n \rho K_n^\dagger)$ and $\sigma_n = K_n \rho K_n^\dagger / p_n$, where $\{K_n\}_{n=1}^{N}$ are incoherent Kraus operators such that $\sigma = \sum_{n=1}^{N} K_n \rho K_n^\dagger$.

We observe that the majorization relation (20) generalizes the necessary condition for incoherent transformations from pure to arbitrary states, given in (5), to the general case, i.e., from arbitrary states to arbitrary states.

Another consequence of Prop. 23 is that the generalized coherence vectors of two states ρ and σ satisfy a majorization whenever ρ can be transformed into σ.

Corollary 25. Let ρ and σ be two quantum states. Then

$$\rho \underset{\rm IO}{\rightarrow} \sigma \Rightarrow \nu(\rho) \preceq \nu(\sigma). \tag{21}$$

Notice that the right-hand side (r.h.s.) condition is not sufficient even for qubit systems. In fact, a qubit state ρ with Bloch vector (r_x, r_y, r_z) can be converted into another state σ with Bloch vector (s_x, s_y, s_x) by means of incoherent operations if and only if two conditions are satisfied: (i) $s_x^2 + s_y^2 \leqslant r_x^2 + r_y^2$, and (ii) $(1 - s_z^2)/(s_x^2 + s_y^2) \geqslant (1 - r_z^2)/(r_x^2 + r_y^2)$ (see [19,20]). By using the result given in Eq. (25) (or in [25]), it can be shown that only condition (i) is equivalent to the r.h.s. of (21). Moreover, in higher dimensions ($d \geqslant 4$), a finite number of conditions in terms of coherence measures are not enough to completely characterizes the coherence transformations [13].

V. A FAMILY OF COHERENCE MONOTONES

In this section we introduce a new family of coherence monotones, alternative to $C_f^{\rm cr}$ and $C_f^{\rm top}$. We adopt a different approach to the ones given in Defs. 8 and 10. Our proposal is based on the generalized coherence vector introduced in Def. 16. The fact that this definition satisfies the properties given in Props. 20–23 allows us to introduce the following family of coherence quantifiers, which we call *coherence vector monotone*.

Definition 26 (Coherence vector monotone). For any function $f \in \mathcal{F}$, the coherence vector monotone $C_f^{\rm cv}: \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ is defined as

$$C_f^{\rm cv}(\rho) = f(\nu(\rho)), \tag{22}$$

where $\nu(\rho)$ is the generalized coherence vector of ρ.

We observe that this family of quantifiers is well defined. The following result states that it satisfies the first four conditions of a coherence measure.

Proposition 27. For any function $f \in \mathcal{F}$, the coherence vector monotone $C_f^{\rm cv}$ satisfies conditions (C_1)–(C_4).

We observe that a coherence vector monotone $C_f^{\rm cv}$ can only be convex if $C_f^{\rm cv} \leqslant C_f^{\rm cr}$, as in the case of Eq. (23).

We stress that any function $f \in \mathcal{F}$ gives a coherence monotone. In others words, the function f can be arbitrarily chosen from the set $\mathcal{F}$ as in the cases of the convex roof measures and the top monotones.

In what follows, we are going to characterize the order relation among the coherence quantifiers $C_f^{\rm cr}$, $C_f^{\rm top}$, and $C_f^{\rm cv}$. First, we note that, due to Prop. 11, $C_f^{\rm top} \geqslant C_f^{\rm cr}$ and $C_f^{\rm top} \geqslant C_f^{\rm cv}$. Moreover, for some $\rho \in \mathcal{S}(\mathcal{H})$, we have $C_f^{\rm top}(\rho) = C_f^{\rm cv}(\rho)$. The following result characterizes this situation.

Proposition 28. The following statements are equivalent:

(1) There exists an optimal pure state decomposition of ρ, i.e., $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho)$.

(2) $C_f^{\rm cv}(\rho) = C_f^{\rm top}(\rho)$ for all $f \in \mathcal{F}$.

(3) $C_f^{\rm cv}(\rho) = C_f^{\rm top}(\rho)$ for some $f \in \mathcal{F}$, with f strictly Schur concave.

This result gives us a method to address the question about the existence of an optimal pure state decomposition of a general quantum state. In Sec. VI we will use it to show that for some qutrit states there exist an optimal pure state decomposition.

In general, there is not a defined order relation between $C_f^{\rm cv}$ and $C_f^{\rm cr}$. However, when there exists an optimal pure state decomposition of a state, we have the following result.

Proposition 29. If there exists an optimal pure state decomposition of ρ, then $C_f^{\rm cv}(\rho) \geqslant C_f^{\rm cr}(\rho)$.

On the contrary, for affine functions, we have the opposite relation between $C_f^{\rm cv}$ and $C_f^{\rm cr}$.

Proposition 30. Let $f \in \mathcal{F}$ be such that $f|_{\Delta_d^{\downarrow}} = c + \ell$, where $c \in \mathbb{R}$ and $\ell : \Delta_d^{\downarrow} \to \mathbb{R}$ is a linear function. Then $C_f^{\rm cv} \leqslant C_f^{\rm cr} = C_f^{\rm top}$.

Examples of this class of functions are $f(u) = 1 - u_1^{\downarrow}$, $f(u) = u_d^{\downarrow}$, and $f(u) = 1 - u_1^{\downarrow} + u_d^{\downarrow}$, where $u_i^{\downarrow} = (u^{\downarrow})_i$. In particular, for the former function, we have that all quantifiers coincide and are equal to the geometric measure of coherence [38], i.e., for the function $f(u) = 1 - u_1^{\downarrow}$ we have

$$C_f^{\rm cv}(\rho) = C_f^{\rm cr}(\rho) = C_f^{\rm top}(\rho) = \min_{\{q_k,|\psi_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)} \sum_{k=1}^{M} q_k \left(1 - \max_{0\leqslant i\leqslant d-1} |\langle i|\psi_k\rangle|^2\right). \tag{23}$$

Moreover, whenever there exists the optimal pure state decomposition of ρ, $C_f^{\rm cv}(\rho)$ and $C_f^{\rm cr}(\rho)$ are equal for a subclass of functions of $\mathcal{F}$.

Proposition 31. If there exists an optimal pure state decomposition of ρ, i.e., $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho)$, then

$$C_{f_k}^{\rm cv}(\rho) = C_{f_k}^{\rm cr}(\rho), \tag{24}$$

with $f_k(u) = 1 - \sum_{i=0}^{k-1} u_i^{\downarrow} \in \mathcal{F}$, for all $k \in \{1, \dots, d-1\}$.

The scheme of Fig. 1 summarizes the relationships among the three families of coherence quantifiers.

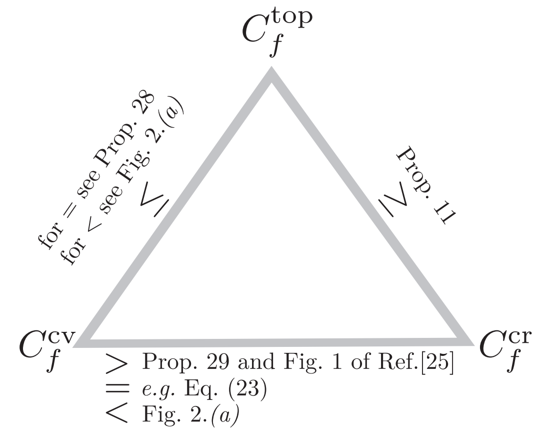

FIG. 1. Scheme of the relationships among $C_f^{\rm cr}$, $C_f^{\rm top}$, and $C_f^{\rm cv}$.

VI. EXAMPLES

In this section we calculate the coherence vector for two simple models. First, we consider a qubit state, and we obtain its generalized coherence vector. Second, we consider a maximally coherent qutrit going through a depolarizing channel, and we compute the value of $C_f^{\rm cr}(\rho)$, $C_f^{\rm top}(\rho)$, and $C_f^{\rm cv}(\rho)$ for a given state ρ and $f \in \mathcal{F}$.

A. Qubit case

Let us consider a qubit system in a state $\rho = \frac{1+\vec{r}\cdot\vec{\sigma}}{2}$, with $\vec{r} = (r_x, r_y, r_z)$ the Bloch vector ($\|\vec{r}\| \leqslant 1$), and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ the vector formed by the Pauli matrices.

In a previous work [25] it has been shown that the supremum of $\mathcal{U}^{\rm psd}(\rho)$ is a maximum, and it is given by

$$\nu(\rho) = \left(\frac{1+r}{2}, \frac{1-r}{2}\right), \tag{25}$$

where $r = \sqrt{1 - r_x^2 - r_y^2}$. An optimal pure state decomposition of ρ is given by $\{q, |\psi^+\rangle; 1-q, |\psi^-\rangle\}$ where $|\psi^{\pm}\rangle\langle\psi^{\pm}| = \frac{1+\vec{s}^{\pm}\cdot\vec{\sigma}}{2}$, with $\vec{s}^{\pm} = (r_x, r_y, \pm r)$ and $q = (r_z + r)/2r \in [0, 1]$. As a consequence of Prop. 28, we have that $C_f^{\rm cv} = C_f^{\rm top}$.

Furthermore, it has been shown that for any function $f(\nu(\rho)) = \tilde{f}(r)$, such that $\tilde{f}$ is a convex function on r, $C_f^{\rm top}$ is a convex monotone of coherence and $C_f^{\rm top} = C_f^{\rm cr}$ [25]. For the qubit case, most of the well-known coherence measures, like ℓ_1 norm, relative entropy, geometric coherence admit a formulation in terms of a convex function of r. This means that we have the triple equivalence among the families $C_f^{\rm cv}$, $C_f^{\rm top}$, and $C_f^{\rm cr}$ in this case.

Due to Prop. 28, to observe a difference between $C_f^{\rm cv}$ and $C_f^{\rm top}$, we need an example where $\nu(\rho)$ is not a maximum. This could be possible, in principle, in higher dimensions ($d \geqslant 3$). In what follows, we provide an example for $d = 3$.

B. Qutrit case

Let us consider a qutrit system in the maximally coherent state $|\psi^{\rm mcs}\rangle = (|0\rangle + |1\rangle + |2\rangle)/\sqrt{3}$, going through a depolarizing channel with depolarization probability p. The final state after the depolarizing channel is given by

$$\rho_p = \Lambda_p(|\psi^{\rm mcs}\rangle\langle\psi^{\rm mcs}|) = p\,\frac{I}{3} + (1-p)\,|\psi^{\rm mcs}\rangle\langle\psi^{\rm mcs}|. \tag{26}$$

Also, we consider the function $f(u) = 1 - u_1^{\downarrow} + u_d^{\downarrow}$. Clearly f satisfies the conditions of Prop. 30. Therefore, we have that for this function both measures $C_f^{\rm cr}$ and $C_f^{\rm top}$ are equal.

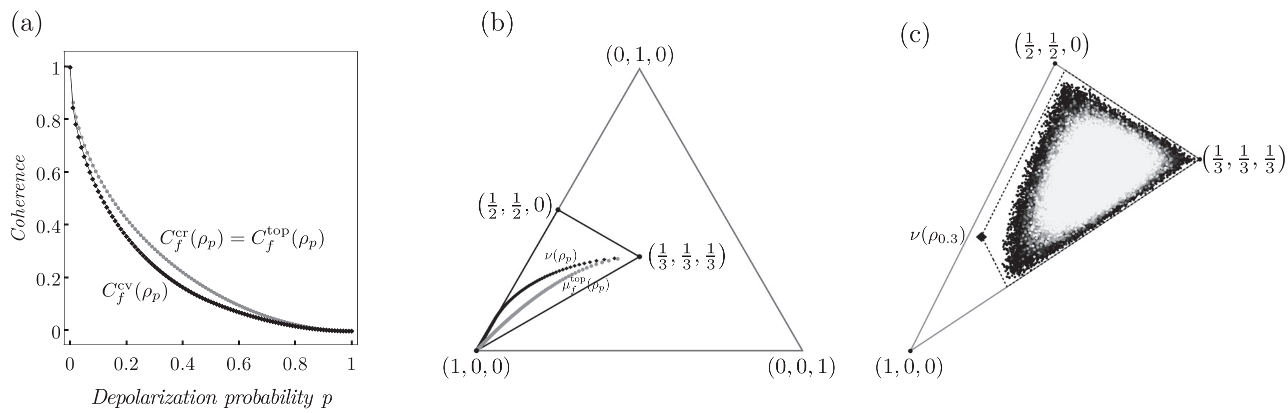

FIG. 2. Let $\rho_p = \Lambda_p(|\psi_3^{\mathrm{mcs}}\rangle\langle\psi_3^{\mathrm{mcs}}|)$ and $f(u) = 1 - u_1^{\downarrow} + u_d^{\downarrow}$. (a) $C_f^{\mathrm{cr}}(\rho_p)$ [or $C_f^{\mathrm{top}}(\rho_p)$] (gray circle) and $C_f^{\mathrm{cv}}(\rho_p)$ (black diamond) in function of depolarization probability p. (b) The big triangle represents the Δ_3, whereas that the small triangle depicts the set $\Delta_3^{\downarrow}$. We plot $\nu(\rho_p)$ (black diamond) and $u_f^{\mathrm{top}}(\rho_p) = \arg\min_{u \in \mathcal{U}^{\mathrm{psc}}(\rho)} f(u)$ (gray circle) for several values of $p \in [0, 1]$. (c) For $p = 0.3$ we plot $\nu(\rho_p) \approx (0.777, 0.2, 0.0223)$ (black diamond) and the region $\{u \in \Delta_3^{\downarrow} : u \preceq \nu(\rho_p)\}$ (enclosed by the black dashed lines). In addition, we generate 10^5 random unitary matrices of dimensions from 3 to 9. For each unitary matrix U, we use the Schrödinger theorem (see, e.g., [34,35]) to generate an ensemble compatible with ρ_p ($p = 0.3$), i.e., $\sqrt{p_k}\,|\phi_k\rangle = \sum_{j=1}^{3} \sqrt{\lambda_j} U_{k,j} |e_j\rangle$, where λ_j and $|e_j\rangle$ are the eigenvalues and eigenstates of ρ_p. For each ensemble, we plot its coherence vector in grayscale representing the dimension of the unitary matrix (from 3 to 9) used to generate the ensemble. The darkest gray corresponds to dimension 3, whereas the lightest gray corresponds to dimension 9. This plot evidences that the optimal set of this state does not exist (which can be inferred from the left figure and Prop. 28).

In Fig. 2(a) we plot $C_f^{\mathrm{cr}}(\rho_p)$ [or, equivalently $C_f^{\mathrm{top}}(\rho_p)$] and $C_f^{\mathrm{cv}}(\rho_p)$ as functions of $p \in [0, 1]$. Both functions are monotonically decreasing in terms of p, and in the open interval (0, 1), we have $C_f^{\mathrm{cr}}(\rho_p) = C_f^{\mathrm{top}}(\rho_p) > C_f^{\mathrm{cv}}(\rho_p)$. Equivalently, this means that the supremum is not a maximum (see Prop. 28). In Fig. 2(b) we plot $\nu(\rho_p)$ and $u_f^{\mathrm{top}}(\rho_p) = \arg\min_{u \in \mathcal{U}^{\mathrm{psc}}(\rho)} f(u)$. It is shown that $u_f^{\mathrm{top}}(\rho_p) \preceq \nu(\rho_p)$ and $u_f^{\mathrm{top}}(\rho_p) \neq \nu(\rho_p)$ for several values of p in the open interval (0, 1). Finally, in Fig. 2(c) we consider ρ_p for $p = 0.3$ and we depict $\nu(\rho_p)$ and the region $\{u \in \Delta_3^{\downarrow} : u \preceq \nu(\rho_p)\}$. In addition, we generate 10^5 random unitary matrices of dimensions from 3 up to 9.[5] For each unitary matrix we use the Schrödinger theorem (see Eq. (B12) or [35]) to generate an ensemble compatible with ρ_p and we plot its coherence vector. This plot depicts that the optimal pure state decomposition of this state does not exist (which can be inferred from the left figure and Prop. 28).

VII. CONCLUDING REMARKS

In this work we have advanced on the characterization of the quantum coherence resource theory by defining the generalized coherence vector of an arbitrary quantum state. This probability vector can be interpreted as a concave roof extension of the coherence vector defined for pure states. We showed that it is a good definition, since it allows us to characterize the notions of being incoherent, as well as being maximally coherent. Using this definition and the majorization relation, we obtain a necessary condition for the conversion of general quantum states by means of incoherent operations. This generalizes the result for pure states given in the literature, and shows that the tools of the majorization lattice are useful also in the general case.

Moreover, based on the generalized coherence vector, we introduced a family of monotones, called coherence vector monotones. In order to do this, we considered concave and symmetric functions applied to the generalized coherence vector of a quantum state. In this way, our approach is an alternative method to construct extended coherence measures from pure to mixed states. This family of monotone was compared with the families of the convex roof measure and the top monotone. We obtain that the coherence vector monotone is lower than or equal to the top monotone, and the equality is only satisfied when the generalized coherence vector of the state is a maximum. In addition, we have obtained that there is not a definite order between the convex roof measure and the coherence vector monotone. We provided several examples showing that our quantifier can be strictly greater than, equal to, or strictly lower than the convex roof measure. We have also applied the coherence vector monotone to quantify the coherence of a qubit system and a maximally coherent qutrit going through a depolarizing channel.

Finally, we stress that our framework, which is mainly based on the majorization lattice theory, could also be used in other majorization-based resource theories. Moreover, it would be interesting to study whether this approach can be extend to more general resource theories of coherence, such as the ones based on nonorthonormal basis or on positive-operator-valued measures.

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[5]The upper bound 9 is not arbitrary. According to Lemma 1 in [36], the optimal $C_f^{\mathrm{cr}}(\rho_p)$ requires at most nine terms. It is conjectured in [39, Conjecture and Lemma 7] that three terms are enough.

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APPENDIX A: AUXILIARY LEMMAS

The following result is necessary for Prop. 23. It states that any convex combination of ordered probability vectors preserves the majorization relation.

Lemma 32. Let $u_0,\dots,u_m \in \Delta_d^{\downarrow}$ and $v_0,\dots,v_m \in \Delta_d^{\downarrow}$ be two sequences of ordered probability vectors, such that $u_\ell \preceq v_\ell$, for all $0\leqslant \ell \leqslant m$. For any probability vector $q=(q_0,\dots,q_m)\in\Delta_{m+1}$, the vectors $u=\sum_{\ell=0}^m q_\ell u_\ell$ and $v=\sum_{\ell=0}^m q_l v_l$ belong to $\Delta_d^{\downarrow}$ and $u\preceq v$.

Proof. Let $q=(q_0,\dots,q_m)$ be an arbitrary probability vector in Δ_{m+1}. First, we note that $(u)_i=\sum_{\ell=0}^m q_\ell (u_\ell)_i \geqslant 0$ for all $0\leqslant i\leqslant d-1$, and $\sum_{i=0}^{d-1}(u)_i=\sum_{i=0}^{d-1}\sum_{\ell=0}^m q_\ell(u_\ell)_i=\sum_{\ell=0}^m q_\ell \sum_{i=0}^{d-1}(u_\ell)_i=1$, i.e., $u\in\Delta_d$. Moreover, since $(u_\ell)_{i+1}\leqslant (u_\ell)_i$ for all $0\leqslant i\leqslant d-2$ and for all $0\leqslant \ell\leqslant m$, we have $(u)_{i+1}=\sum_{\ell=0}^m q_\ell (u_\ell)_{i+1}\leqslant \sum_{\ell=0}^m q_\ell(u_\ell)_i=(u)_i$. Hence, $u\in\Delta_d^{\downarrow}$. Analogously, $v\in\Delta_d^{\downarrow}$.

Second, since $u_\ell\preceq v_\ell$, for all $0\leqslant\ell\leqslant m$, then we have $\sum_{i=0}^k (u_\ell)_i\leqslant\sum_{i=0}^k(v_\ell)_i$, for all $0\leqslant k\leqslant d-1$. Therefore, for all $0\leqslant k\leqslant d-1$, we have $\sum_{i=0}^k(u)_i=\sum_{i=0}^k\sum_{\ell=0}^m q_\ell(u_\ell)_i=\sum_{\ell=0}^m q_\ell\sum_{i=0}^k(u_\ell)_i\leqslant \sum_{\ell=0}^m q_\ell\sum_{i=0}^k(v_\ell)_i=\sum_{i=0}^k(v)_i$. Hence, $u\preceq v$. ■

The following result is necessary for Prop 28.

Lemma 33. Let $f:\Delta_d\to\mathbb{R}$ be a strictly Schur-concave function, and $u,v\in\Delta_d$. If $f(u)=f(v)$, then either (i) $u\npreceq v$ and $v\npreceq u$ (incomparable) or (ii) $u=\Pi v$, with Π a permutation matrix.

Proof. Given $u,v\in\Delta_d$, we suppose that $f(u)=f(v)$. Then there are two options: (i) u and v are incomparable or (ii) u and v are comparable. If (i) is the case, there is nothing to prove. If (ii) is the case, without loss of generality, we can assume $u\preceq v$. Since $f(u)=f(v)$, and f is strictly Schur concave, we conclude $u=\Pi v$, with Π a permutation matrix. ■

The following two lemmas will be necessary to prove that the sets $\mathcal{U}^{\rm psd}(\rho)$ and $\mathcal{U}^{\rm psc}(\rho)$ have the same supremum (see Prop.15).

Lemma 34. $\mathcal{U}^{\rm psd}(\rho)\subseteq\mathcal{U}^{\rm psc}(\rho)$.

Proof. Given an arbitrary $u\in\mathcal{U}^{\rm psd}(\rho)$, there exists a pure state decomposition $\{q_k,|\psi_k\rangle\}_{k=1}^M$ of ρ such that $\sum_{k=1}^M q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|)=u$. Moreover, always exists a pure state $|\psi\rangle\langle\psi|$ such that $\mu^{\downarrow}(|\psi\rangle\langle\psi|)=u$.

Since the majorization relation is reflexive, $\mu^{\downarrow}(|\psi\rangle\langle\psi|)\preceq\sum_k q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|)$. Finally, from Prop. 5 we have that $|\psi\rangle\langle\psi|\underset{\rm IO}{\to}\rho$ and $\mu\in\mathcal{U}^{\rm psc}(\rho)$. Therefore, $\mathcal{U}^{\rm psd}(\rho)\subseteq\mathcal{U}^{\rm psc}(\rho)$. ■

Lemma 35. For each $u\in\mathcal{U}^{\rm psc}(\rho)$, there exists an element $u'\in\mathcal{U}^{\rm psd}(\rho)$, such that $u\preceq u'$.

Proof. Given an arbitrary $u\in\mathcal{U}^{\rm psc}(\rho)$, there exists a pure state $|\psi\rangle\langle\psi|$ such that $\mu^{\downarrow}(|\psi\rangle\langle\psi|)=u$ and $|\psi\rangle\langle\psi|\underset{\rm IO}{\to}\rho$.

From Prop. 5 there exists a pure state decomposition $\{q_k,|\psi_k\rangle\}_{k=1}^M$ of ρ such that $u\preceq\sum_{k=1}^M q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|)$.

Since $\rho=\sum_{k=1}^M q_k|\psi_k\rangle\langle\psi_k|$, then $u'=\sum_k q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|)$ belongs to $\mathcal{U}^{\rm psd}(\rho)$.

Therefore, $u\preceq u'$. ■

The next result shows the compactness of the set $\mathcal{O}(\rho)$. This result will be used for the proof of Prop. 20. In addition, Lemma 36 together with the continuity of f allows us to replace the infimum in (13) by a minimum. In addition, this allows us to fill the gaps of some proofs given in [25], where the existence of an optimal state in (13) is assumed, but not proved.

Lemma 36. The set $\mathcal{O}(\rho)=\{|\psi\rangle\langle\psi| : |\psi\rangle\langle\psi|\underset{\rm IO}{\to}\rho\}$ is a compact set.

Proof. According to [19], there exists a fixed N such that any pure state $|\psi\rangle\langle\psi|\in\mathcal{O}(\rho)$ satisfies $\sum_{n=1}^N K_n|\psi\rangle\langle\psi|K_n^\dagger=\rho$, where K_n are incoherent Kraus operators. By Def. 1, the Kraus operators satisfy the two following conditions:

$$\sum_n K_n^\dagger K_n=I. \tag{A1}$$

$$K_n|i\rangle\propto|f_n(i)\rangle,\ \text{with } f_n \text{ a relabeling of } \{0,\dots,d-1\}. \tag{A2}$$

On the one hand, from Eq. (A1), it follows that each incoherent Kraus operator is bounded, i.e, $\|K_n\|_{HS}=\mathrm{Tr}(K_n^\dagger K_n)\leqslant d$. On the other hand, condition (A2) is equivalent to

$$(K_n)_{j,i}=(K_n)_{j,i}\,\delta_{j,f_n(i)},\quad \forall i,j\in\{0,\dots,d-1\}. \tag{A3}$$

Notice that condition (A3) are d^2 equations for the entries of K_n.

We denote the set of all relabeling functions as $\mathcal{R}=\{f:\{0,\dots,d-1\}\to\{0,\dots,d-1\}\}$ and the N-Cartesian product as $\mathcal{R}^N$. Given $\vec{f}=(f_1,\dots,f_N)\in\mathcal{R}^N$, we define the set

$$K_{\vec{f}}=\Bigg\{(K_1,\dots,K_N)\in\mathbb{C}^{d\times d}\times\cdots\times\mathbb{C}^{d\times d}:\ \sum_{n=1}^N K_n^\dagger K_n=I,\quad (K_n)_{j,i}=(K_n)_{j,i}\,\delta_{j,f_n(i)}\quad \forall i,j\in\{0,\dots,d-1\}\Bigg\}, \tag{A4}$$

and the set

$$V_{\vec{f}}(\rho)=\Bigg\{(|\psi\rangle\langle\psi|,K_1,\dots,K_N)\in\mathcal{P}(\mathcal{H})\times\mathbb{C}^{d\times d}\times\cdots\times\mathbb{C}^{d\times d}:\ (K_1,\dots,K_N)\in K_{\vec{f}},\quad \sum_{n=1}^N K_n|\psi\rangle\langle\psi|K_n^\dagger=\rho\Bigg\}. \tag{A5}$$

Finally, we consider the set $V(\rho)=\bigcup_{\vec{f}\in\mathcal{R}^N}V_{\vec{f}}(\rho)$. Since $\mathcal{R}$ is a finite set, $V(\rho)$ is a finite union of sets. Notice that

$$|\psi\rangle\langle\psi|\in\mathcal{O}(\rho)\iff\exists(K_1,\dots,K_N)\in\mathbb{C}^{d\times d}\times\cdots\times\mathbb{C}^{d\times d}:\ (|\psi\rangle\langle\psi|,K_1,\dots,K_N)\in V(\rho). \tag{A6}$$

Since $\mathcal{P}(\mathcal{H})$ is closed and the set $V_{\vec{f}}(\rho)$ is given by a finite number of equations,[6] then we have that $V_{\vec{f}}(\rho)$ is a closed set. Moreover, $V_{\vec{f}}(\rho)$ is bounded, since $\mathcal{P}(\mathcal{H})$ is bounded and each incoherent Kraus operator has $\|K_n\|_{HS} \leqslant d$. Therefore, $V(\rho)$ is a compact set, since it is a finite union of compact sets.

Let us denote the projection of the set $\mathcal{P}(\mathcal{H}) \times \mathbb{C}^{d\times d} \times \cdots \times \mathbb{C}^{d\times d}$ onto the first coordinate as $\Pi : \mathcal{P}(\mathcal{H}) \times \mathbb{C}^{d\times d} \times \cdots \times \mathbb{C}^{d\times d} \to \mathcal{P}(\mathcal{H})$. Since Π is a continuous function and $V(\rho)$ is compact, then $\Pi(V(\rho))$ is compact.

We are going to show that $\mathcal{O}(\rho) = \Pi(V(\rho))$. On the one hand, let $|\psi\rangle\langle\psi| \in \Pi(V(\rho))$. Then there is an element $(|\psi\rangle\langle\psi|, K_1, \dots, K_N) \in V(\rho)$. Therefore, using equivalence (A6), we have $|\psi\rangle\langle\psi| \in \mathcal{O}(\rho)$. On the other hand, if $|\psi\rangle\langle\psi| \in \mathcal{O}(\rho)$, there exists $(K_1, \dots, K_N) \in \mathbb{C}^{d\times d} \times \cdots \times \mathbb{C}^{d\times d}$ such that $(|\psi\rangle\langle\psi|, K_1, \dots, K_N) \in V(\rho)$. Then $|\psi\rangle\langle\psi| \in \Pi(V(\rho))$. Therefore, we conclude that $\mathcal{O}(\rho) = \Pi(V(\rho))$ and it is a compact set. ■

APPENDIX B: PROOFS OF PROPOSITIONS GIVEN IN THE MAIN TEXT

For the sake of readability we repeat the statements of the propositions given in the main text and we provide their corresponding proofs.

Proposition 9. Let $C : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ be a coherence measure. Then

$$C \leqslant C^{\mathrm{cr}}_{f_C}, \tag{B1}$$

where f_C is a function associated with C.

Proof. Given an arbitrary quantum state ρ, we consider a pure state decomposition $\{q_k, |\psi_k\rangle\}_{k=1}^M$ of the state, i.e., $\rho = \sum_{k=1}^M q_k |\psi_k\rangle\langle\psi_k|$. Since $C : \mathcal{S}(\mathcal{H}) \to \mathbb{R}$ satisfies conditions (C$_1$)–(C$_4$), from Prop. 7, there exists a function $f_C \in \mathcal{F}$, such that

$$C(|\psi\rangle\langle\psi|) = f_C(\mu(|\psi\rangle\langle\psi|)), \quad \forall\, |\psi\rangle\langle\psi| \in \mathcal{P}(\mathcal{H}). \tag{B2}$$

In addition, C satisfies condition (C$_5$), hence

$$C(\rho) \leqslant \sum_{k=1}^M q_k C(|\psi_k\rangle\langle\psi_k|) = \sum_{k=1}^M q_k f_C(\mu(|\psi_k\rangle\langle\psi_k|)). \tag{B3}$$

The inequality (B3) is valid for any pure state decomposition of ρ, then

$$C(\rho) \leqslant \inf_{\{q_k,|\psi_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)} \sum_{k=1}^M q_k f_C(\mu(|\psi_k\rangle\langle\psi_k|)). \tag{B4}$$

By definition, the r.h.s. of (B4) is the convex roof measure for the function f_C. Therefore, we obtain $C(\rho) \leqslant C^{\mathrm{cr}}_{f_C}(\rho)$, for all ρ. ■

Proposition 14. The sets $\mathcal{U}^{\mathrm{psd}}(\rho)$ and $\mathcal{U}^{\mathrm{psc}}(\rho)$ are convex.

Proof. We start with the set $\mathcal{U}^{\mathrm{psd}}(\rho)$. Let $u, u' \in \mathcal{U}^{\mathrm{psd}}(\rho)$. Given $t \in (0, 1)$, we consider the ordered probability vector $u_t = tu + (1 - t)u'$.

By definition of $\mathcal{U}^{\mathrm{psd}}(\rho)$, we have $\{q_k, |\psi_k\rangle\}_{k=1}^M$ and $\{q'_k, |\psi'_k\rangle\}_{k=1}^{M'}$, two pure state decompositions of ρ, such that $u = \sum_{k=1}^M q_k \mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|)$ and $u' = \sum_{k=1}^{M'} q'_k \mu^{\downarrow}(|\psi'_k\rangle\langle\psi'_k|)$. Since $\rho = \sum_{k=1}^M q_k |\psi_k\rangle\langle\psi_k| = \sum_{k=1}^{M'} q'_k |\psi'_k\rangle\langle\psi'_k|$, we have

$$t \sum_{k=1}^M q_k |\psi_k\rangle\langle\psi_k| + (1 - t) \sum_{k=1}^{M'} q'_k |\psi'_k\rangle\langle\psi'_k| = \rho. \tag{B5}$$

Therefore, the join $\{tq_k, |\psi_k\rangle\}_{k=1}^M \cup \{(1 - t)q'_k, |\psi'_k\rangle\}_{k=1}^{M'}$ is also a pure state decomposition of ρ, and $u_t = \sum_{k=1}^M tq_k \mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) + \sum_{k=1}^{M'} (1 - t)q'_k \mu^{\downarrow}(|\psi'_k\rangle\langle\psi'_k|) \in \mathcal{U}^{\mathrm{psd}}(\rho)$. Hence, $\mathcal{U}^{\mathrm{psd}}(\rho)$ is a convex set.

Now, we consider the set $\mathcal{U}^{\mathrm{psc}}(\rho)$. Let $u, u' \in \mathcal{U}^{\mathrm{psc}}(\rho)$. Again, given $t \in (0, 1)$, we consider the ordered probability vector $u_t = tu + (1 - t)u'$. Also, we consider a pure state $|u_t\rangle\langle u_t|$, such that $\mu^{\downarrow}(|u_t\rangle\langle u_t|) = u_t$.

From Lemma 35 we know that there are two probability vectors $v, v' \in \mathcal{U}^{\mathrm{psd}}(\rho)$, such that $u \preceq v$ and $u' \preceq v'$. If we define the ordered probability vector $v_t = tv + (1 - t)v'$, then, from Lemma 32, we have $u_t = tu + (1 - t)u' \preceq tv + (1 - t)v' = v_t$. Since $\mathcal{U}^{\mathrm{psd}}(\rho)$ is convex, $v_t \in \mathcal{U}^{\mathrm{psd}}(\rho)$. By definition of the set $\mathcal{U}^{\mathrm{psd}}(\rho)$, there is a pure state decomposition $\{q_k, |\phi_k\rangle\}_{k=1}^M$ of ρ, such that $v_t = \sum_{k=1}^M q_k \mu^{\downarrow}(|\phi_k\rangle\langle\phi_k|)$.

Summing up, given the pure state $|u_t\rangle\langle u_t|$, we have that $u_t = \mu^{\downarrow}(|u_t\rangle\langle u_t|) \preceq v_t = \sum_{k=1}^M q_k \mu^{\downarrow}(|\phi_k\rangle\langle\phi_k|)$, with $\rho = \sum_{k=1}^M q_k |\phi_k\rangle\langle\phi_k|$. Finally, from Prop. 5, we conclude $|u_t\rangle\langle u_t| \underset{\mathrm{IO}}{\to} \rho$, which implies $u_t = tu + (1 - t)u' \in \mathcal{U}^{\mathrm{psc}}(\rho)$. Hence, $\mathcal{U}^{\mathrm{psc}}(\rho)$ is a convex set. ■

Proposition 15. $\bigvee \mathcal{U}^{\mathrm{psd}}(\rho) = \bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$.

Proof. From Lemma 34 we have $\mathcal{U}^{\mathrm{psd}}(\rho) \subseteq \mathcal{U}^{\mathrm{psc}}(\rho)$. Then $\bigvee \mathcal{U}^{\mathrm{psd}}(\rho) \preceq \bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$. In addition, from Lemma 35 we have $\bigvee \mathcal{U}^{\mathrm{psc}}(\rho) \preceq \bigvee \mathcal{U}^{\mathrm{psd}}(\rho)$. Therefore, since the majorization relation is antisymmetric, we obtain $\bigvee \mathcal{U}^{\mathrm{psd}}(\rho) = \bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$. ■

Proposition 19. $\nu(\rho) \in \mathcal{U}^{\mathrm{psd}}(\rho) \iff \nu(\rho) \in \mathcal{U}^{\mathrm{psc}}(\rho)$.

Proof. ($\Longrightarrow$) Suppose $\nu(\rho) \in \mathcal{U}^{\mathrm{psd}}(\rho)$. Then, from Lemma 34, it follows that $\nu(\rho) \in \mathcal{U}^{\mathrm{psc}}(\rho)$.

($\Longleftarrow$) Suppose $\nu(\rho) \in \mathcal{U}^{\mathrm{psc}}(\rho)$. From Lemma 35, exists $u' \in \mathcal{U}^{\mathrm{psd}}(\rho)$ such that $\nu(\rho) \preceq u'$. From Prop. 15 we also have that $u' \preceq \nu(\rho)$. Then $u' = \nu(\rho) \in \mathcal{U}^{\mathrm{psd}}(\rho)$. ■

Proposition 20. ρ is incoherent $\iff \nu(\rho) = (1, 0, \dots, 0)$.

Proof. ($\Longrightarrow$) Let $\rho \in \mathcal{I}$ be an incoherent state. By definition, ρ is diagonal in the incoherent basis, that is, $\rho = \sum_{i=0}^{d-1} p_i |i\rangle\langle i|$. Since $\{p_i, |i\rangle\} \in \mathcal{D}(\rho)$ and $\sum_i p_i \mu^{\downarrow}(|i\rangle\langle i|) = (1, 0, \dots, 0) \in \mathcal{U}^{\mathrm{psd}}(\rho)$, then $\nu(\rho) = (1, 0, \dots, 0)$.

($\Longleftarrow$) Let $\rho \in \mathcal{S}(\mathcal{H})$ be such that $\nu(\rho) = (1, 0, \dots, 0)$. To prove the converse statement, we appeal to *reductio ad absurdum* by assuming that ρ is a coherent state. From Prop. 15 we have that $\nu(\rho) = \bigvee \mathcal{U}^{\mathrm{psc}}(\rho)$.

According to the formula of the supremum [16], the first entry of $\nu(\rho)$ is given by the supremum of the first entries of the vectors of $\mathcal{U}^{\mathrm{psc}}(\rho)$, i.e.,

$$(\nu(\rho))_1 = \bigvee\{(\mu^{\downarrow}(|\psi\rangle\langle\psi|))_1 : |\psi\rangle\langle\psi| \in \mathcal{O}(\rho)\}, \tag{B6}$$

where

$$(\mu^{\downarrow}(|\psi\rangle\langle\psi|))_1 = \max_{0\leqslant i\leqslant d-1} |\langle i|\psi\rangle|^2. \tag{B7}$$

[6] For any continuous function h the set $\{x : h(x) = 0\}$ is closed.

Then

$$(\nu(\rho))_1 = \max_{0\leqslant i\leqslant d-1} \bigvee\{|\langle i|\psi\rangle|^2 : |\psi\rangle\langle\psi| \in \mathcal{O}(\rho)\}. \tag{B8}$$

For each $0 \leqslant i \leqslant d-1$ we consider the function $f_i : \mathcal{O}(\rho) \to \mathbb{R}$, given by $f_i(|\psi\rangle\langle\psi|) = |\langle i|\psi\rangle|^2$. Since $\mathcal{O}(\rho)$ is compact (see Lemma 36) and f_i is continuous, there exists a pure state $|\psi_i\rangle\langle\psi_i| \in \mathcal{O}(\rho)$ which is the maximum of f_i in $O(\rho)$, i.e.,

$$f_i(|\psi_i\rangle\langle\psi_i|) = \max\{|\langle i|\psi\rangle|^2 : |\psi\rangle\langle\psi| \in \mathcal{O}(\rho)\}. \tag{B9}$$

Therefore, if we define $f_{i^*}(|\psi_{i^*}\rangle\langle\psi_{i^*}|) = \max_{0\leqslant i\leqslant d-1} f_i(|\psi_i\rangle\langle\psi_i|)$, we have

$$(\nu(\rho))_1 = f_{i^*}(|\psi_{i^*}\rangle\langle\psi_{i^*}|), \tag{B10}$$

with $|\psi_{i^*}\rangle\langle\psi_{i^*}| \in \mathcal{O}(\rho)$. By hypothesis, $\nu(\rho) = (1, 0, \ldots, 0)$, then $f_{i^*}(|\psi_{i^*}\rangle\langle\psi_{i^*}|) = |\langle i^*|\psi_{i^*}\rangle|^2 = 1$. This implies that $|\psi_{i^*}\rangle\langle\psi_{i^*}| \in \mathcal{I}$.
Summing up, $|\psi_{i^*}\rangle\langle\psi_{i^*}|$ is an incoherent pure state that can be transformed into the coherent state ρ by means of an incoherent operation, but this is absurd. Therefore, ρ has to be incoherent. ■

Proposition 21. ρ is maximally coherent $\iff \nu(\rho) = (\frac{1}{d}, \ldots, \frac{1}{d})$.

Proof. ($\Longrightarrow$) Let $\rho \in \mathcal{S}(\mathcal{H})$ be an arbitrary maximally coherent state, that is, $\rho = U_{\rm IO}|\Psi^{\rm mcs}\rangle\langle\Psi^{\rm mcs}|U_{\rm IO}^\dagger$, with $|\Psi^{\rm mcs}\rangle = \sum_{i=0}^{d-1}\frac{1}{\sqrt{d}}|i\rangle$ and $U_{\rm IO} = \sum_{i=0}^{d-1} e^{\imath\theta_i}|\pi(i)\rangle\langle i|$, where $\theta_i \in \mathbb{R}$ and π is a permutation acting on the set $\{0, \ldots, d-1\}$. Since $|\langle i|U_{\rm IO}|\Psi^{\rm mcs}\rangle|^2 = 1/d$ for all $i \in \{0, \ldots, d-1\}$, we have $\nu(\rho) = \mu(U_{\rm IO}|\Psi^{\rm mcs}\rangle\langle\Psi^{\rm mcs}|U_{\rm IO}^\dagger) = (1/d, \ldots, 1/d)$.
($\Longleftarrow$) Let $\rho \in \mathcal{S}(\mathcal{H})$ be such that $\nu(\rho) = (\frac{1}{d}, \ldots, \frac{1}{d})$.

First, we consider the pure state case, i.e., $\rho = |\psi\rangle\langle\psi|$. The coherence vector of ρ is given by $\nu(\rho) = \mu^\downarrow(|\psi\rangle\langle\psi|) = (\frac{1}{d}, \ldots, \frac{1}{d})$. From Def. 2 it follows $|\langle i|\psi\rangle|^2 = 1/d$ for all $i \in \{0, \ldots, d-1\}$. Therefore, $|\psi\rangle = U_{\rm IO}|\Psi^{\rm mcs}\rangle$, with $U_{\rm IO} = \sum_{i=0}^{d-1} e^{\imath\theta_i}|i\rangle\langle i|$ and $\theta_i \in \mathbb{R}$. This implies that ρ is a maximally coherent state.

Second, we are going to show that ρ has to be a pure state. We appeal to *reductio ad absurdum* by assuming that ρ is a mixed state. Let $\{q_k, |\psi_k\rangle\}_{k=1}^M$ be an arbitrary pure state decomposition of ρ, i.e., $\rho = \sum_{k=1}^M q_k|\psi_k\rangle\langle\psi_k|$. On the one hand, by definition of $\nu(\rho)$, we have $\sum_{k=1}^M q_k\mu^\downarrow(|\psi_k\rangle\langle\psi_k|) \preceq (1/d, \ldots, 1/d)$. On the other hand, since $(1/d, \ldots, 1/d)$ is the bottom of the majorization lattice, we have $(1/d, \ldots, 1/d) \preceq \sum_{k=1}^M q_k\mu^\downarrow(|\psi_k\rangle\langle\psi_k|)$. Then $\sum_{k=1}^M q_k\mu^\downarrow(|\psi_k\rangle\langle\psi_k|) = (1/d, \ldots, 1/d)$. Moreover, the probability vector $(1/d, \ldots, 1/d)$ is an extreme point of the $d-1$ simplex, which implies that $\mu^\downarrow(|\psi_k\rangle\langle\psi_k|) = (1/d, \ldots, 1/d)$ for all $k \in \{1, \ldots, M\}$. Then states $|\psi_k\rangle\langle\psi_k|$ have to be maximally coherent states. Therefore, we conclude that any pure state decomposition of ρ has to be formed by maximally coherent pure states.

In particular, we consider the spectral decomposition of ρ,

$$\rho = \sum_{j=1}^d \lambda_j|e_j\rangle\langle e_j|. \tag{B11}$$

The eigenvectors have to be maximally coherent pure states. Since by hypothesis ρ is a mixed state, there are at least two eigenvalues different from zero. Without loss of generality, we consider $\lambda_1, \lambda_2 > 0$. In terms of the incoherent basis we have $|e_1\rangle = \sum_{i=0}^{d-1}\frac{e^{\imath\alpha_i}}{\sqrt{d}}|i\rangle$ and $|e_2\rangle = \sum_{i=0}^{d-1}\frac{e^{\imath\beta_i}}{\sqrt{d}}|i\rangle$, with $\alpha_i, \beta_i \in \mathbb{R}$, for all $i \in \{0, \ldots, d-1\}$.

According to the Schrödinger mixture theorem (see, e.g., [34,35]), any ensemble $\{p_k, |\phi_k\rangle\}_{k=1}^M$ is a pure state decomposition of ρ if and only if there exists a unitary matrix U such that

$$|\phi_k\rangle = \frac{1}{\sqrt{p_k}}\sum_{j=1}^d \sqrt{\lambda_j}U_{k,j}|e_j\rangle. \tag{B12}$$

We consider a $d \times d$ unitary matrix of the form

$$U = \left(\begin{array}{cc|c} U_{11} & U_{1,2} & \multirow{2}{*}{$\mathbf{0}$} \\ -U_{12}^* & U_{1,1} & \\ \hline \multicolumn{2}{c|}{\mathbf{0}} & I_{d-2}\end{array}\right), \tag{B13}$$

with $U_{1,1} = \sqrt{\frac{\lambda_2}{\lambda_1+\lambda_2}}$ and $U_{1,2} = -e^{\imath(\alpha_0-\beta_0)}\sqrt{\frac{\lambda_1}{\lambda_1+\lambda_2}}$. Then the first state takes the form

$$|\phi_1\rangle = \frac{1}{\sqrt{p_1}}(\sqrt{\lambda_1}U_{1,1}|e_1\rangle + \sqrt{\lambda_2}U_{1,2}|e_2\rangle), \tag{B14}$$

and, taking into account the expression of $|e_1\rangle$ and $|e_2\rangle$ in the incoherent basis, we obtain

$$\langle 0|\phi_1\rangle = \frac{1}{\sqrt{dp_1}}(e^{\imath\alpha_0}\sqrt{\lambda_1}U_{1,1} + e^{\imath\beta_0}\sqrt{\lambda_2}U_{1,2}) = 0, \tag{B15}$$

which is in contradiction with $|\phi_1\rangle$ being a maximally coherent state. Therefore, ρ cannot be a mixed state, it has to be a pure state.

Proposition 22. Let $\rho = \sum_{k=1}^M p_k|\psi_k\rangle\langle\psi_k|$. Then

$$\sum_{k=1}^M p_k\nu(|\psi_k\rangle\langle\psi_k|) \preceq \nu(\rho). \tag{B16}$$

Proof. Let $\rho = \sum_{k=1}^M p_k|\psi_k\rangle\langle\psi_k|$. We have $\sum_{k=1}^M p_k\mu^\downarrow(|\psi_k\rangle\langle\psi_k|) = \sum_{k=1}^M p_k\nu(|\psi_k\rangle\langle\psi_k|) \in \mathcal{U}^{\rm psd}(\rho)$. Then, by definition of the supremum, $\sum_{k=1}^M p_k\nu(|\psi_k\rangle\langle\psi_k|) \prec \nu(\rho)$. ■

Proposition 23. Let ρ and σ be two arbitrary quantum states. Then

$$\rho \underset{\rm IO}{\to} \sigma \Rightarrow \forall\{q_k, |\psi_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho), \exists\{r_l, |\phi_l\rangle\}_{l\in L} \in \mathcal{D}(\sigma):$$
$$\sum_{k=1}^M q_k\mu^\downarrow(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{l\in L} r_l\mu^\downarrow(|\phi_l\rangle\langle\phi_l|). \tag{B17}$$

Proof. Let Λ be an incoherent operation, with incoherent Kraus operators $\{K_n\}_{n=1}^N$, such that $\sigma = \Lambda(\rho) = \sum_{n=1}^N K_n\rho K_n^\dagger$. Let $\{q_k, |\psi_k\rangle\}_{k=1}^M$ be an arbitrary pure state decomposition of ρ, that is, $\rho = \sum_{k=1}^M q_k|\psi_k\rangle\langle\psi_k|$. Then we have $\sigma = \Lambda(\rho) = \sum_{n=1}^N\sum_{k=1}^M q_k p_{n,k}|\phi_{n,k}\rangle\langle\phi_{n,k}|$, with $p_{n,k} = {\rm Tr}(K_n|\psi_k\rangle\langle\psi_k|K_n^\dagger)$ and $|\phi_{n,k}\rangle = K_n|\psi_k\rangle/\sqrt{p_{n,k}}$.

In particular, for each $|\psi_k\rangle\langle\psi_k|$, we have $|\psi_k\rangle\langle\psi_k| \underset{\rm IO}{\to} \sum_{n=1}^N p_{n,k}|\phi_{n,k}\rangle\langle\phi_{n,k}|$. Then, according to Eq. (5) [12, Lemma 4],

$$\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{n=1}^{N} p_{n,k}\mu^{\downarrow}(|\phi_{n,k}\rangle\langle\phi_{n,k}|). \tag{B18}$$

Applying Lemma 32 for the sequences of ordered probability vectors $\{\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|)\}_{k=1}^{M}$ and $\{\sum_n p_{n,k}\mu^{\downarrow}(|\phi_{n,k}\rangle\langle\phi_{n,k}|)\}_{k=1}^{M}$, we obtain

$$\sum_{k=1}^{M} q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{n=1}^{N}\sum_{k=1}^{M} q_k p_{n,k}\mu^{\downarrow}(|\phi_{n,k}\rangle\langle\phi_{n,k}|), \tag{B19}$$

where $q_k \geqslant 0$ and $\sum_{k=1}^{M} q_k = 1$. Defining $r_l = q_k p_{n,k}$, $|\phi_l\rangle = |\phi_{n,k}\rangle$ and $L = \{(n,k) : 1 \leqslant n \leqslant N, 1 \leqslant k \leqslant M\}$, we can rewrite expression (B19) as

$$\sum_{k=1}^{M} q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{l\in L} r_l\mu^{\downarrow}(|\phi_l\rangle\langle\phi_l|), \tag{B20}$$

with $\{r_l, |\phi_l\rangle\}_{l\in L} \in \mathcal{D}(\sigma)$. Since the majorization relation (B20) is valid for any pure state decomposition of ρ, we conclude that for each $\{q_k, |\psi_k\rangle\}_{k=1}^{M} \in \mathcal{D}(\rho)$, there exists a pure state decomposition $\{r_l, |\phi_l\rangle\}_{l\in L} \in \mathcal{D}(\sigma)$, such that relation (B20) is satisfied. ■

Corollary 24. Let ρ and σ be two arbitrary quantum states. Then

$$\rho \underset{\text{IO}}{\rightarrow} \sigma \Rightarrow \nu(\rho) \preceq \sum_{n=1}^{N} p_n\nu(\sigma_n), \tag{B21}$$

with $p_n = \mathrm{Tr}\,(K_n\rho K_n^{\dagger})$ and $\sigma_n = K_n\rho K_n^{\dagger}/p_n$, where $\{K_n\}_{n=1}^{N}$ are incoherent Kraus operators such that $\sigma = \sum_{n=1}^{N} K_n\rho K_n^{\dagger}$.

Proof. Let Λ be an incoherent operation, with incoherent Kraus operators $\{K_n\}_{n=1}^{N}$, such that $\sigma = \Lambda(\rho) = \sum_{n=1}^{N} K_n\rho K_n^{\dagger}$, and define $p_n = \mathrm{Tr}\,(K_n\rho K_n^{\dagger})$ and $\sigma_n = K_n\rho K_n^{\dagger}/p_n$.

For any arbitrary pure state decomposition $\{q_k, |\psi_k\rangle\}_{k=1}^{M}$ of ρ, we can write $\sigma_n = \sum_{k=1}^{M} q_k p_{n,k}|\phi_{n,k}\rangle\langle\phi_{n,k}|/p_n$, with $p_n = \sum_k q_k p_{n,k}$. Since $\sum_{k=1}^{M} q_k p_{n,k}\mu^{\downarrow}(|\phi_{n,k}\rangle\langle\phi_{n,k}|)/p_n \in \mathcal{U}^{\text{psd}}(\sigma_n)$, then

$$\sum_{k=1}^{M}\frac{q_k p_{n,k}}{p_n}\mu^{\downarrow}(|\phi_{n,k}\rangle\langle\phi_{n,k}|) \preceq \nu(\sigma_n). \tag{B22}$$

Multiplying by p_n, summing over n, and using (B19), we obtain

$$\sum_{k=1}^{M} q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{n=1}^{N}\sum_{k=1}^{M} q_k p_{n,k}\mu^{\downarrow}(|\phi_{n,k}\rangle\langle\phi_{n,k}|) \tag{B23}$$

$$\preceq \sum_{n=1}^{N} p_n\nu(\sigma_n). \tag{B24}$$

The last majorization relation does not depend on the pure state decomposition of ρ, then $\sum_{n=1}^{N} p_n\nu(\sigma_n)$ is also an upper bound of $\mathcal{U}^{\text{psd}}(\rho)$. Therefore, by definition of supremum, we conclude that $\nu(\rho) \preceq \sum_n p_n\nu(\sigma_n)$. ■

Corollary 25. Let ρ and σ be two arbitrary quantum states. Then

$$\rho \underset{\text{IO}}{\rightarrow} \sigma \Rightarrow \nu(\rho) \preceq \nu(\sigma). \tag{B25}$$

Proof. Since $\rho \underset{\text{IO}}{\rightarrow} \sigma$, from Prop. 23, we have that, for all $\{q_k, |\psi_k\rangle\}_{k=1}^{M} \in \mathcal{D}(\rho)$, there is a $\{r_l, |\phi_l\rangle\}_{l\in L} \in \mathcal{D}(\sigma)$, such that

$$\sum_{k=1}^{M} q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \sum_{l\in L} r_l\mu^{\downarrow}(|\phi_l\rangle\langle\phi_l|). \tag{B26}$$

Then, from the definition of the supremum, we have

$$\sum_{k=1}^{M} q_k\mu^{\downarrow}(|\psi_k\rangle\langle\psi_k|) \preceq \nu(\sigma). \tag{B27}$$

This implies that $\nu(\sigma)$ is an upper bound of the set $\mathcal{U}^{\text{psd}}(\rho)$. Therefore, by definition of $\nu(\rho)$, we have $\nu(\rho) \preceq \nu(\sigma)$. ■

Proposition 27. For any function $f \in \mathcal{F}$, the coherence vector measure C_f^{cv} satisfies conditions (C_1)–(C_4).

Proof. (C_1) By Prop. 20, if $\rho \in \mathcal{I}$, then $\nu(\rho) = (1, 0, \ldots, 0)$. Therefore, $C_f^{\text{cv}}(\rho) = f(1, 0, \ldots, 0) = 0$.

(C_2) Since $\rho \underset{\text{IO}}{\rightarrow} \Lambda(\rho)$, from Cor. 25, we obtain $\nu(\rho) \preceq \nu(\Lambda(\rho))$. Moreover, f is symmetric and concave, then f is also Schur concave, which implies that $f(\nu(\rho)) \geqslant f(\nu(\Lambda(\rho)))$. Finally, we conclude that $C_f^{\text{cv}}(\rho) \geqslant C_f^{\text{cv}}(\Lambda(\rho))$.

(C_3) Let $\rho \in \mathcal{S}(\mathcal{H})$ be an arbitrary quantum state and Λ an incoherent operation, with incoherent Kraus operators $\{K_n\}_{n=1}^{N}$, $p_n = \mathrm{Tr}\,(K_n\rho K_n^{\dagger})$ and $\sigma_n = K_n\rho K_n^{\dagger}/p_n$. If we define $\sigma = \Lambda(\rho)$, from Cor. 24, Eq. (20), we obtain $\nu(\rho) \preceq \sum_{n=1}^{N} p_n\nu(\sigma_n)$. Then we have

$$\sum_{n=1}^{N} p_n f(\nu(\sigma_n)) \leqslant f\left(\sum_{n=1}^{N} p_n\nu(\sigma_n)\right) \leqslant f(\nu(\rho)),$$

where in the first inequality we have used the concavity of f and in the second one the Schur concavity. Finally, taking into account the coherence vector definition, we conclude

$$\sum_{n=1}^{N} p_n C_f^{\text{cv}}(\sigma_n) \leqslant C_f^{\text{cv}}(\rho).$$

(C_4) Let ρ a maximally coherent state and σ an arbitrary state. Due to Prop. 21, $\nu(\rho) = (1/d, \ldots, 1/d)$. Moreover, since $\arg\max_{u\in\mathbb{R}^d} f(u) = (1/d, \ldots, 1/d)$, we have $f(\nu(\rho)) = f(1/d, \ldots, 1/d) \geqslant f(\nu(\sigma))$. This implies that $C_f(\rho) \geqslant C_f(\sigma)$. Therefore, we conclude that $\arg\max_{\rho\in S(\mathcal{H})} C_f(\rho)$ is reached at maximally coherent states. ■

Proposition 28. The following statements are equivalent:

(1) There exists an optimal pure state decomposition of ρ, i.e., $\nu(\rho) \in \mathcal{U}^{\text{psd}}(\rho)$.

(2) $C_f^{\text{cv}}(\rho) = C_f^{\text{top}}(\rho)$ for all $f \in \mathcal{F}$.

(3) $C_f^{\text{cv}}(\rho) = C_f^{\text{top}}(\rho)$ for some $f \in \mathcal{F}$ strictly Schur concave.

Proof. ($1 \Rightarrow 2$) Let $f \in \mathcal{F}$. On the one hand, by Prop. 11, we have $C_f^{\text{top}}(\rho) \geqslant C_f^{\text{cv}}(\rho)$. On the other hand, if there exists an optimal pure state decomposition of ρ, then $\nu(\rho) \in \mathcal{U}^{\text{psd}}(\rho)$. From Lemma 34 we have $\nu(\rho) \in \mathcal{U}^{\text{psc}}(\rho)$. By definition of the top measure, $C_f^{\text{top}}(\rho) \leqslant f(u)$ for all $u \in \mathcal{U}^{\text{psc}}(\rho)$. In particular, $C_f^{\rm top}(\rho) \leqslant f(\nu(\rho)) = C_f^{\rm cv}(\rho)$. Finally, we conclude $C_f^{\rm cv}(\rho) = C_f^{\rm top}(\rho)$, which is valid for all $f \in \mathcal{F}$.

($2 \Rightarrow 3$) Trivial.

($3 \Rightarrow 1$) Let $f \in \mathcal{F}$ be a strictly Schur-concave function such that $C_f^{\rm cv}(\rho) = C_f^{\rm top}(\rho)$.

Notice that $C_f^{\rm top}$ can be written as

$$C_f^{\rm top}(\rho) = \min_{u \in \mathcal{U}^{\rm psc}(\rho)} f(u). \tag{B28}$$

We denote the probability vector where the minimum is reached as $\tilde{u}$. Then $f(\nu(\rho)) = C_f^{\rm cv}(\rho) = C_f^{\rm top}(\rho) = f(\tilde{u})$. Since f is strictly Schur concave, then by Lemma 33 we have $\nu(\rho) = \tilde{u} \in \mathcal{U}^{\rm psc}(\rho)$. Finally, by Lemma 19, $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho)$, i.e., there exists an optimal pure state decomposition of ρ. ■

Proposition 29. If there exists an optimal pure state decomposition of ρ, then $C_f^{\rm cv}(\rho) \geqslant C_f^{\rm cr}(\rho)$.

Proof. Let $\{\tilde{q}_k, |\tilde{\psi}_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)$ be an optimal pure state decomposition of ρ. Thus, $\nu(\rho) = \sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)$. Let $f \in \mathcal{F}$, then

$$C_f^{\rm cv}(\rho) = f(\nu(\rho)) = f\left(\sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)\right) \tag{B29}$$

$$\geqslant \sum_{k=1}^M \tilde{q}_k f(\mu(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)) \tag{B30}$$

$$\geqslant \inf_{\{q_k,|\psi_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)} \sum_{k=1}^M q_k f(\mu(|\psi_k\rangle\langle\psi_k|)) \tag{B31}$$

$$= C_f^{\rm cr}(\rho), \tag{B32}$$

where the first inequality comes from the concavity and symmetric properties of f, and the second one comes from the definition of the convex roof measure. ■

Proposition 30. Let $f \in \mathcal{F}$ be such that $f|_{\Delta_d^\downarrow} = c + \ell$, where $c \in \mathbb{R}$ and $\ell : \Delta_d^\downarrow \to \mathbb{R}$ is a linear function. Then $C_f^{\rm cv} \leqslant C_f^{\rm cr} = C_f^{\rm top}$.

Proof. Let $\rho \in \mathcal{S}(\mathcal{H})$. On the one hand, by definition of the convex roof measure, we have

$$C_f^{\rm cr}(\rho) = \inf_{\{q_k,|\psi_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)} \sum_{k=1}^M q_k f(\mu(|\psi_k\rangle\langle\psi_k|)) \tag{B33}$$

$$= \sum_{k=1}^M \tilde{q}_k f(\mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)), \tag{B34}$$

with $\{\tilde{q}_k, |\tilde{\psi}_k\rangle\}_{k=1}^M \in \mathcal{D}(\rho)$ the pure state decomposition of ρ where the minimum is reached. Taking into account the form of f, we get

$$C_f^{\rm cr}(\rho) = \sum_{k=1}^M \tilde{q}_k[c + \ell(\mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|))] \tag{B35}$$

$$= c + \ell\left(\sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)\right) \tag{B36}$$

$$= f\left(\sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)\right), \tag{B37}$$

where we have used the linearity of ℓ and the condition $\sum_{k=1}^M q_k = 1$.

On the other hand, by definition of $\nu(\rho)$ and Schur concavity of f, we have

$$C_f^{\rm cv}(\rho) = f(\nu(\rho)) \leqslant f\left(\sum_{k=1}^M q_k \mu^\downarrow(|\psi_k\rangle\langle\psi_k|)\right), \quad \forall\{q_k, |\psi\rangle_k\}_{k=1}^M \in \mathcal{D}(\rho). \tag{B38}$$

In particular,

$$C_f^{\rm cv}(\rho) \leqslant f\left(\sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)\right). \tag{B39}$$

Therefore, we conclude $C_f^{\rm cv}(\rho) \leqslant C_f^{\rm cr}(\rho)$.

In order to prove the equality part of the proposition, first we note that $C_f^{\rm cr}(\rho) \leqslant C_f^{\rm top}(\rho)$, see Eq. (14). Moreover, by definition of the top measure, we have

$$C_f^{\rm top}(\rho) \leqslant f(\mu^\downarrow(|\psi\rangle\langle\psi|)), \quad \forall\, |\psi\rangle\langle\psi| \in \mathcal{O}(\rho). \tag{B40}$$

Since $\mathcal{U}^{\rm psd}(\rho) \subseteq \mathcal{U}^{\rm psc}(\rho)$ (see Lemma 34), we have that $\sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|) \in \mathcal{U}^{\rm psc}(\rho)$. Then there is $|\tilde{\psi}\rangle\langle\tilde{\psi}| \in \mathcal{O}(\rho)$, such that $\mu^\downarrow(|\tilde{\psi}\rangle\langle\tilde{\psi}|) = \sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)$. Therefore,

$$C_f^{\rm top}(\rho) \leqslant f(\mu^\downarrow(|\tilde{\psi}\rangle\langle\tilde{\psi}|)) = f\left(\sum_{k=1}^M \tilde{q}_k \mu^\downarrow(|\tilde{\psi}_k\rangle\langle\tilde{\psi}_k|)\right). \tag{B41}$$

Then, from (B35) and (B41), we have $C_f^{\rm top}(\rho) \leqslant C_f^{\rm cr}(\rho)$. Finally, we conclude that $C_f^{\rm top}(\rho) = C_f^{\rm cr}(\rho)$. ■

Proposition 31. If there exists an optimal pure state decomposition of ρ, i.e., $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho)$, then

$$C_{f_k}^{\rm cv}(\rho) = C_{f_k}^{\rm cr}(\rho), \tag{B42}$$

with $f_k(u) = 1 - \sum_{i=0}^{k-1} u_i^\downarrow \in \mathcal{F}$, for all $k \in \{1, \dots, d-1\}$.

Proof. On the one hand, let us recall that if $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho)$, then $S_k(\rho) = s_k(\nu(\rho))$ for all $k \in \{1, \dots, d-1\}$, where $S_k(\rho) = \sup_{u \in \mathcal{U}^{\rm psd}(\rho)} s_k(u)$ and $s_j(u) = \sum_{i=0}^{j-1} u_i$, with $u = (u_0, \dots, u_{d-1})$.

On the other hand, we note that $f_k(u) = 1 - s_k(u^\downarrow)$. Therefore,

$$C_{f_k}^{\rm cr}(\rho) = 1 - S_k(\rho) \quad \text{and} \tag{B43}$$

$$C_{f_k}^{\rm cv}(\rho) = 1 - s_k(\nu(\rho)). \tag{B44}$$

Summarizing, $\nu(\rho) \in \mathcal{U}^{\rm psd}(\rho)$ implies $C_{f_k}^{\rm cr}(\rho) = C_{f_k}^{\rm cv}(\rho)$ for all $k \in \{1, \dots, d-1\}$. ■

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