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Maximal coherence and the resource theory of purity

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Abstract

The resource theory of quantum coherence studies the off-diagonal elements of a density matrix in a distinguished basis, whereas the resource theory of purity studies all deviations from the maximally mixed state. We establish a direct connection between the two resource theories, by identifying purity as the maximal coherence which is achievable by unitary operations. The states that saturate this maximum identify a universal family of maximally coherent mixed states. These states are optimal resources under maximally incoherent operations, and thus independent of the way coherence is quantified. For all distance-based coherence quantifiers the maximal coherence can be evaluated exactly, and is shown to coincide with the corresponding distance-based purity quantifier. We further show that purity bounds the maximal amount of entanglement and discord that can be generated by unitary operations, thus demonstrating that purity is the most elementary resource for quantum information processing.

1. Introduction

A number of different quantum features are considered as important resources for applications of quantum information theory. Entanglement [1–4], quantum discord [5–10], and quantum coherence [11–16] have been identified as necessary ingredients for the successful implementation of tasks, such as quantum cryptography [17], quantum algorithms [17, 18] and quantum metrology [19–23]. Quantum resources can be formally classified in the framework of resource theories [24, 25], where the state space is divided into free states and resource states. Moreover, a set of free operations, which cannot turn a free state into a resource state, is identified⁹. The possibility of conversion between two resource states via free operations is a central issue within a resource theory, as it introduces a natural order of the resource states. A suitable measure for the resource must be non-increasing under free operations. Equipped with suitable measures, one is able to quantify the resource in any given quantum state.

States that maximize such measures are called extremal resource states¹⁰. Every quantum state can then be characterized by the minimal rate of extremal resource states needed to create it (resource cost), or the maximal rate for creating an extremal resource state from it (distillable resource), using the free operations¹¹. A number of different resource theories have been developed in the context of quantum information theory [24, 25], prominent examples being entanglement [1–4] and coherence [11–16].

⁹ Throughout this paper, a quantum operation (or just ‘operation’) is used as a synonym for a completely positive trace-preserving map.

¹⁰ Here, the term ‘extremal’ is not synonymous to extremal elements of convex sets.

¹¹ This has to be understood in the asymptotic setting, where ‘rate’ means the asymptotic fraction of required (distilled) resource states per copy of the desired (given) quantum state ρ . Widely used examples for such asymptotic rates are entanglement cost and distillable entanglement, we refer to [3] for their formal definition.

While the concept of coherence is basis-dependent by its very definition, both entanglement and quantum discord are locally basis-independent. However, entanglement and discord usually change if a global unitary is applied. It is clear, however, that the unitary activation of these resources must be limited in terms of some basis-independent quantity of the initial quantum state. As we will show in rigorous quantitative terms, this fundamental quantity is identified as purity. Specifically, we show how purity can be used to establish quantum coherence by a unitary operation. This further provides direct bounds on the amount of entanglement and discord that can be reached by unitary operations, since these quantities can be traced back to coherences in a specific many-body basis. These results hold for all suitable distance-based quantifiers.

A resource theory of purity was introduced in [26] for the asymptotic limit of infinitely many copies of the quantum state. The finite-copy scenario was considered more recently [27]. Our results relate both of these approaches directly to the resource theory of coherence. In general, purity can be interpreted as the maximal coherence, maximized over all unitaries. Depending on the chosen coherence monotone, we recover either the asymptotic or the finite-copy resource theory of purity, by maximizing over unitary operations, or even more generally, over all unital operations. As one of our main results, we are able to identify the states that maximize any given coherence monotone for a fixed spectrum of the density matrix. These states define a universal set of maximally coherent mixed states. The coherence of these states can be evaluated exactly for any distance-based coherence monotone, and is shown to coincide with its distance-based purity.

2. Resource theory of quantum coherence

In the following, we recall the resource theory of coherence [11–16] and then identify the family of maximally coherent mixed states. The free states of this resource theory are called *incoherent states*, these are states which are diagonal in a fixed basis $\{|i\rangle\}$, i.e.,

$$\sigma = \sum_i p_i |i\rangle\langle i|. \quad (1)$$

The set of all incoherent states will be denoted by \mathcal{I} . The definition of free operations is not unique, and several approaches have been presented in the literature [15, 16].

The historically first and most general approach was suggested in [11], where the set of *maximally incoherent operations* (MIO) was considered. These are all operations which cannot create coherence, i.e.,

$$\Lambda_{\text{MIO}}[\sigma] \in \mathcal{I} \quad (2)$$

for any incoherent state $\sigma \in \mathcal{I}$. Another important family is the set of *incoherent operations* (IO) [12]. These are operations which admit a Kraus decomposition

$$\Lambda_{\text{IO}}[\rho] = \sum_i K_i \rho K_i^\dagger \quad (3)$$

with incoherent Kraus operators K_i , i.e., $K_i|m\rangle \sim |n\rangle$, where the states $|m\rangle$ and $|n\rangle$ belong to the incoherent basis. We also note that IO is a strict subset of MIO [14, 28, 29]

$$\text{IO} \subset \text{MIO}, \quad (4)$$

and the inclusion is strict even for single-qubit states [30]. While we will focus on the sets MIO and IO in this work, other relevant sets of operations have been discussed in recent literature, based on physical or mathematical considerations [13–15, 28–33]. An extension of quantum coherence to multipartite systems has also been presented [34, 35], which made it possible to investigate the resource theory of coherence in distributed scenarios [36–41]. A review over alternative frameworks of coherence and their interpretation can be found in [16].

The amount of coherence in a given state can be quantified via *coherence monotones*. These are nonnegative functions \mathcal{C} which do not increase under the corresponding set of free operations, i.e., for a MIO monotone we have $\mathcal{C}(\Lambda_{\text{MIO}}[\rho]) \leq \mathcal{C}(\rho)$. Since MIO is the most general set of free operations for any resource theory of coherence, a MIO monotone is also a monotone in any other coherence theory. An important example are distance-based coherence monotones:

$$\mathcal{C}(\rho) = \inf_{\sigma \in \mathcal{I}} D(\rho, \sigma), \quad (5)$$

where D is a suitable distance on the space of quantum states. Such quantifiers were studied in [11, 12], the most prominent example being the relative entropy of coherence

$$\mathcal{C}_r(\rho) = \min_{\sigma \in \mathcal{I}} S(\rho||\sigma) \quad (6)$$

with the quantum relative entropy $S(\rho||\sigma) = \text{Tr}[\rho \log_2 \rho] - \text{Tr}[\rho \log_2 \sigma]$ ¹². Remarkably, this quantity admits a closed expression [12] and coincides with the distillable coherence under MIO and IO and also with the coherence cost under MIO [14]:

$$\mathcal{C}_r(\rho) = S(\Delta[\rho]) - S(\rho). \quad (7)$$

Here, $S(\rho) = -\text{Tr}[\rho \log_2 \rho]$ is the von Neumann entropy and $\Delta[\rho] = \sum_i \langle i|\rho|i\rangle |i\rangle\langle i|$ denotes dephasing in the incoherent basis.

For a general distance-based coherence quantifier as given in equation (5) one usually considers nonnegative distances D which are contractive under any quantum operation Λ :

$$D(\Lambda[\rho], \Lambda[\sigma]) \leq D(\rho, \sigma). \quad (8)$$

Any such distance gives rise to a MIO monotone [12, 16]. Examples for such distances are the relative Rényi entropy

$$D_\alpha(\rho||\sigma) = \frac{1}{\alpha - 1} \log_2 \text{Tr}[\rho^\alpha \sigma^{1-\alpha}] \quad (9)$$

and the quantum relative Rényi entropy

$$D_\alpha^q(\rho||\sigma) = \frac{1}{\alpha - 1} \log_2 \text{Tr}[(\sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}})^\alpha]. \quad (10)$$

While D_α is contractive for $\alpha \in [0, 2]$, the function D_α^q is contractive in the range $\alpha \in [\frac{1}{2}, \infty]$ [42, 43]. We can now define a family of coherence monotones in the following way:

$$\mathcal{C}_\alpha(\rho) = \begin{cases} \inf_{\sigma \in \mathcal{I}} D_\alpha(\rho||\sigma) & \text{for } 0 < \alpha < 1, \\ \inf_{\sigma \in \mathcal{I}} D_\alpha^q(\rho||\sigma) & \text{for } \alpha > 1. \end{cases} \quad (11)$$

This quantity is a MIO monotone in the range $\alpha \in [0, \infty]$. In the limit $\alpha \rightarrow 1$ both functions $D_\alpha(\rho||\sigma)$ and $D_\alpha^q(\rho||\sigma)$ coincide with the relative entropy $S(\rho||\sigma)$. Coherence quantifiers of this type were studied in [28, 29, 44]. A related approach based on Tsallis relative entropies has also been investigated [45].

Several MIO monotones have additional desirable properties such as strong monotonicity under IO and convexity [12, 16]. This is in particular the case for the relative entropy of coherence [12]. While any MIO monotone is also an IO monotone, the other direction is less clear. In particular, the l_1 -norm of coherence

$$\mathcal{C}_i(\rho) = \sum_{i \neq j} |\rho_{ij}| \quad (12)$$

is known to be an IO monotone [12], but violates monotonicity under MIO [46]. Another IO monotone which is not a MIO monotone is the coherence of formation

$$\mathcal{C}_f(\rho) = \min_i \sum_i p_i S(\Delta[|\psi_i\rangle\langle\psi_i|]), \quad (13)$$

where the minimum is taken over all pure state decompositions $\{p_i, |\psi_i\rangle\}$ of the state ρ [14, 47, 48].

We also note that coherence of formation is equal to coherence cost under IO [14], and l_1 -norm of coherence is related to the path information in multi-path interferometer [49, 50].

3. Maximally coherent mixed states

Since coherence is a basis-dependent concept, a unitary operation will in general change the amount of coherence in a given state. In the following, we will focus on the question: which unitary maximizes the coherence of a given state ρ ? The corresponding figure of merit is given as follows:

$$\mathcal{C}_{\max}(\rho) := \sup_U \mathcal{C}(U\rho U^\dagger). \quad (14)$$

If the supremum in equation (14) is realized for the unitary V , the corresponding state $\rho_{\max} = V\rho V^\dagger$ will be called *maximally coherent mixed state*. This definition is in full analogy to maximally entangled mixed states investigated in [51–54]. Maximally coherent mixed states were first introduced for specific measures of coherence in [55], and studied further more recently in [56].

While the relative entropy of coherence admits a closed formula, the evaluation of general coherence monotones is considered as a hard problem [16]. It is thus reasonable to believe that the maximization in equation (14) is out of reach. Quite surprisingly, we will now show that the supremum in equation (14) can be

¹² We note that the quantum relative entropy is not a distance in the mathematical sense, as it is not symmetric and does not fulfill the triangle inequality.

evaluated in a large number of relevant scenarios. In particular, we will see that there exists a *universal* maximally coherent mixed state, which does not depend on the particular choice of coherence monotone. These results will also lead us to a closed expression of \mathcal{C}_{\max} for all distance-based coherence monotones.

Theorem 1. *Among all states ρ with a fixed spectrum $\{p_n\}$, the state*

$$\rho_{\max} = \sum_{n=1}^d p_n |n_+\rangle \langle n_+| \quad (15)$$

is a maximally coherent mixed state with respect to any MIO monotone. Here, $\{|n_+\rangle\}$ denotes a mutually unbiased basis with respect to the incoherent basis $\{|i\rangle\}$, i.e., $|\langle i|n_+\rangle|^2 = \frac{1}{d}$, where d is the dimension of the Hilbert space.

Proof. We will actually prove an even stronger statement. In particular, we will show that for any unitary U , the transformation $\rho_{\max} \rightarrow U\rho_{\max}U^\dagger$ can be achieved via MIO, i.e.,

$$\Lambda_{\text{MIO}}[\rho_{\max}] = U\rho_{\max}U^\dagger. \quad (16)$$

The proof of the theorem then follows by using monotonicity of \mathcal{C} under MIO:

$$\mathcal{C}(U\rho_{\max}U^\dagger) = \mathcal{C}(\Lambda_{\text{MIO}}[\rho_{\max}]) \leq \mathcal{C}(\rho_{\max}). \quad (17)$$

The operation Λ_{MIO} which achieves this transformation has Kraus operators $K_n = U|n_+\rangle \langle n_+|$. Note that bases $\{|n_+\rangle\}$ and $\{|i\rangle\}$ are mutually unbiased, which implies that $\sum_n K_n \sigma K_n^\dagger = \mathbf{1}/d$ for any incoherent state σ . This means that the operation $\Lambda_{\text{MIO}}[\rho] = \sum_n K_n \rho K_n^\dagger$ is indeed maximally incoherent. In the final step, note that $\sum_n K_n \rho_{\max} K_n^\dagger = U\rho_{\max}U^\dagger$, and the proof is complete. \square

This theorem has several important implications. First, it implies that the state ρ_{\max} is a resource with respect to all states with the same spectrum. Second, this theorem provides an alternative simple proof for the fact that l_1 -norm of coherence can increase under MIO [46]. This can be seen by combining theorem 1 with the fact that the state in equation (15) is not a maximally coherent mixed state for the l_1 -norm of coherence [56]. Moreover, a unitary V for an arbitrary state ρ which achieves the supremum in equation (14) for any MIO monotone is given by $V = \sum_{n=1}^d |n_+\rangle \langle \psi_n|$, where $\{|\psi_n\rangle\}$ are the eigenstates of ρ .

We will now go one step further and give an explicit expression for \mathcal{C}_{\max} for any distance-based coherence monotone.

Theorem 2. *For any distance-based coherence monotone as given in equation (5) with a contractive distance D the following equality holds:*

$$\mathcal{C}_{\max}(\rho) = \mathcal{C}(\rho_{\max}) = D(\rho, \mathbf{1}/d). \quad (18)$$

We refer to appendix A for the proof. Note that theorem 2 also holds for all coherence quantifiers

$$\mathcal{C}_p = \min_{\sigma \in \mathcal{I}} \|\rho - \sigma\|_p \quad (19)$$

based on Schatten p -norms $\|M\|_p = (\text{Tr}[(M^\dagger M)^{p/2}])^{1/p}$ for all $p \geq 1$. Equipped with these results, we will show below in this paper that the resource theory of coherence is closely related to the resource theory of purity. Before we present these results, we review the main properties of the resource theory of purity in the following.

4. Resource theory of purity

We will now review resource theories of purity based on different sets of free operations. The discussion summarizes results previously presented in [27]. There exists a hierarchy of quantum operations which generalize classical bistochastic (purity non-increasing) maps. We distinguish three types of quantum operations:

- Mixture of unitary operations:

$$\Lambda_{\text{MU}}[\rho] = \sum_i p_i U_i \rho U_i^\dagger, \quad (20)$$

with $p_i \geq 0$, $\sum_i p_i = 1$, and unitary operations U_i .

- Noisy operations:

$$\Lambda_{\text{NO}}[\rho] = \text{Tr}_E[U(\rho \otimes \mathbf{1}_E/d)U^\dagger], \quad (21)$$

with a unitary operation U .

- Unital operations:

$$\Lambda_U[\mathbf{1}/d] = \mathbf{1}/d, \quad (22)$$

i.e., operations which preserve the maximally mixed state.

Note that in contrast to the discussion in [27], we only consider operations which preserve the dimension of the Hilbert space. It turns out that these operations form a subset hierarchy

$$\{\Lambda_{\text{MU}}\} \subset \{\Lambda_{\text{NO}}\} \subset \{\Lambda_U\}, \quad (23)$$

see, e.g., lemma 5 in [27].

We call two resource theories equivalent if their respective sets of free states, as well as their sets of all states coincide, and additionally if for each Λ_1 with $\Lambda_1(\rho) = \sigma$ there exists a Λ_2 , such that $\Lambda_2(\rho) = \sigma$, where Λ_1 (Λ_2) is a free operation of resource theory 1 (2). Due to lemma 10 in [27] the state conversion abilities are equivalent for the three cases Λ_{MU} , Λ_{NO} , and Λ_U . It follows that any resource theory which only deviates in the type of operations as defined above will be equivalent. If not stated otherwise, we will consider the resource theory of purity based on unital operations Λ_U in the following.

Within the resource theory of purity, the state conversion possibilities follow from the classical theory of bistochastic maps [27, 57], using the concept of majorization. A state ρ majorizes another state σ , i.e., $\rho \succ \sigma$, if their spectra are in majorization order:

$$\sum_{i=1}^k \lambda_i^\downarrow(\rho) \geq \sum_{j=1}^k \lambda_j^\downarrow(\sigma) \quad (24)$$

for all $k \geq 1$. Here, $\lambda_i^\downarrow(\rho)$ denotes the eigenvalues of ρ in non-increasing order. The aforementioned relation to the resource theory of purity is established via the following Lemma.

Lemma 3. *Given two states ρ and σ of the same dimension, ρ can be converted into σ via some unital operation Λ_U if and only if ρ majorizes σ :*

$$\Lambda_U[\rho] = \sigma \Leftrightarrow \rho \succ \sigma. \quad (25)$$

For the proof of this lemma we refer to theorem 4.1.1 in [58] (see also [59]). Due to the arguments mentioned above, it follows that the majorization relation is necessary and sufficient for state conversion via any set of operations presented above.

Fundamental questions in any resource theory address the number of extremal resource states that can be distilled from a state ρ . In the case of purity this poses the question, how many copies of a pure single-qubit state $|\psi\rangle_2$ can one extract via unital operations? We will call the corresponding figure of merit *single-shot distillable purity*. Its formal definition can be given as follows¹³:

$$\mathcal{P}_d^1(\rho) = \max \left\{ m: \exists \Lambda_U, \text{ s.t. } \Lambda_U \left[\rho \otimes \frac{\mathbf{1}}{d_2} \right] = \psi_2^{\otimes m} \otimes \frac{\mathbf{1}}{d_1} \right\}, \quad (26)$$

where Λ_U is a unital operation, $\psi_2 = |\psi\rangle \langle \psi|_2$ is a pure single-qubit state, and $\mathbf{1}/d_i$ is a maximally mixed state of dimension d_i . Correspondingly, we define the *single-shot purity cost* as the minimal number of pure single-qubit states which are required to create the state ρ via unital operations:

$$\mathcal{P}_c^1(\rho) = \min \left\{ m: \exists \Lambda_U, \text{ s.t. } \Lambda_U \left[\psi_2^{\otimes m} \otimes \frac{\mathbf{1}}{d_1} \right] = \rho \otimes \frac{\mathbf{1}}{d_2} \right\}. \quad (27)$$

Similar quantities were first studied in the asymptotic limit in [26], allowing for infinitely many copies of a quantum state and a finite error margin that only vanishes in this limit. It was found that in the asymptotic case, the distillable purity and the purity cost coincide, and are both equal to the relative entropy of purity

$$\mathcal{P}_r(\rho) = \log_2 d - S(\rho). \quad (28)$$

The single-copy scenario was considered in [27], under the label of ‘nonuniformity’. There the Rényi α -purities were identified as figures of merit using an approach based on Lorentz curves. We will discuss these results in more detail in the following, with particular focus on the resource theory of coherence.

¹³ Note that the dimensions d_1 and d_2 in equation (26) are arbitrary finite numbers, up to the requirement that $d \times d_2 = 2^m \times d_1$. This guarantees that the unital operation preserves the dimension of the Hilbert space. As we show in appendix C, the optimal choice is $d_1 = d$ and $d_2 = 2^{\lceil \log_2(d/r) \rceil}$, where r is the rank of ρ . This only applies if $\log_2(d/r) \geq 1$, as single-shot purity distillation does not work otherwise. By similar considerations, the optimal choice of dimensions in equation (27) is $d_1 = d$ and $d_2 = 2^{\lceil \log_2(d/\lambda_{\max}) \rceil}$, where λ_{\max} is the maximal eigenvalue of ρ , see appendix D for more details.

5. Relation between the resource theories of purity and coherence

Following established notions from the resource theories of entanglement [1–4] and coherence [11–16], we will now introduce a framework for purity quantification. In particular, we distinguish between *purity monotones* and *purity measures*. Any purity monotone \mathcal{P} should fulfill the following two requirements.

Nonnegativity: \mathcal{P} is nonnegative and vanishes for the state $\mathbb{1}/d$.

Monotonicity: \mathcal{P} does not increase under unital operations, i.e., $\mathcal{P}(\Lambda_U[\rho]) \leq \mathcal{P}(\rho)$ for any unital operation Λ_U .

Similar as in the resource theories of entanglement and coherence, we regard these two properties as the most fundamental for any quantity which aims to capture the performance of some purity based task. Purity measures will be monotones with the following additional properties.

Additivity: $\mathcal{P}(\rho \otimes \sigma) = \mathcal{P}(\rho) + \mathcal{P}(\sigma)$ for any two states ρ and σ .

Normalization: $\mathcal{P}(|\psi\rangle_d) = \log_2 d$ for all pure states $|\psi\rangle_d$ of dimension d .

A purity monotone/measure \mathcal{P} is further convex if it fulfills $\sum_i p_i \mathcal{P}(\rho_i) \geq \mathcal{P}(\sum_i p_i \rho_i)$. We note that purity monotones have also been previously studied in [27].

We can now introduce a family of coherence-based purity monotones as follows:

$$\mathcal{P}_C(\rho) := \sup_{\Lambda_U} \mathcal{C}(\Lambda_U[\rho]), \quad (29)$$

where the supremum is taken over all unital operations Λ_U and \mathcal{C} is an arbitrary MIO monotone. Clearly, \mathcal{P}_C is nonnegative, vanishes for $\mathbb{1}/d$, and does not increase under unital operations, i.e., it fulfills the requirements P1 and P2 for a purity monotone. Remarkably, as we show in appendix B, for any MIO monotone \mathcal{C} the corresponding purity monotone can be written as

$$\mathcal{P}_C(\rho) = \mathcal{C}(\rho_{\max}) \quad (30)$$

with the maximally coherent mixed state ρ_{\max} . If \mathcal{C} is a distance-based coherence monotone with a contractive distance D , we can apply theorem 2 to write the corresponding purity monotone explicitly as

$$\mathcal{P}_D(\rho) = D(\rho, \mathbb{1}/d). \quad (31)$$

Equation (31) represents a general distance-based purity quantifier, in direct analogy to similar approaches for entanglement [1–4], coherence [12, 16], and quantum discord [7–10, 60]. In contrast to these theories, a minimization over free states in equation (31) is not necessary due to the uniqueness of the free state in the resource theory of purity. For a single qubit the relation between coherence and purity can be visualized on the Bloch ball if coherence and purity are quantified via the trace norm, see figure 1.

Cases of particular interest can be derived from the coherence monotones introduced in equation (11). In these cases, equation (29) leads to the Rényi α -purity

$$\mathcal{P}_\alpha(\rho) = \log_2 d - S_\alpha(\rho) \quad (32)$$

with the Rényi α -entropy $S_\alpha(\rho) = \frac{1}{1-\alpha} \log_2(\text{Tr}[\rho^\alpha])$. This quantity was studied in [27], and it admits an operational interpretation in the resource theories of purity. In particular, the single-shot distillable purity \mathcal{P}_d^1 , which was introduced in equation (26), can be expressed in terms of \mathcal{P}_α as follows:

$$\mathcal{P}_d^1(\rho) = \left\lceil \lim_{\alpha \rightarrow 0} \mathcal{P}_\alpha(\rho) \right\rceil = \lceil \log_2(d/r) \rceil, \quad (33)$$

where r is the rank and d is the dimension of ρ . Also the single-shot purity cost \mathcal{P}_c^1 , introduced in equation (27), can be written in terms of \mathcal{P}_α as follows:

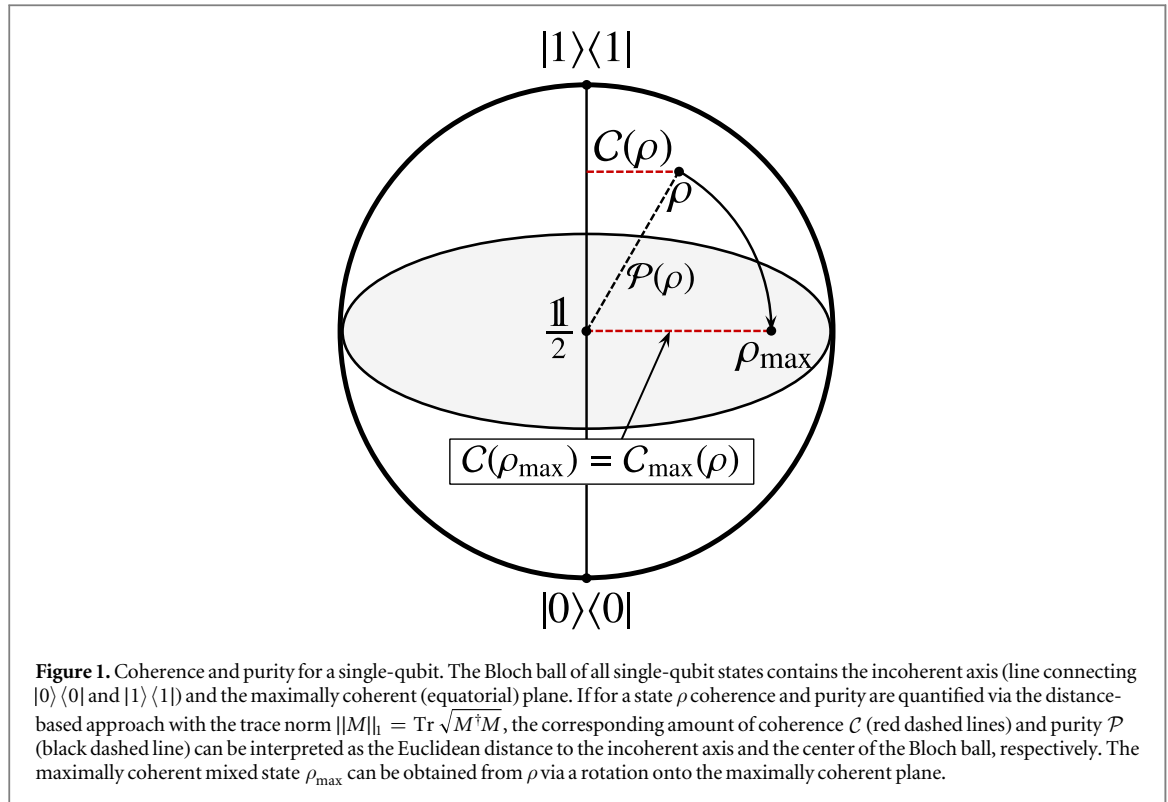
$$\mathcal{P}_c^1(\rho) = \left\lceil \lim_{\alpha \rightarrow \infty} \mathcal{P}_\alpha(\rho) \right\rceil = \lceil \log_2(d\lambda_{\max}) \rceil, \quad (34)$$

with the maximum eigenvalue λ_{\max} of ρ . These results for single-shot purity distillation and dilution were first found in [27]; we present alternative proofs in appendices C and D. Finally,

$$\mathcal{P}_r(\rho) = \lim_{\alpha \rightarrow 1} \mathcal{P}_\alpha(\rho) = \log_2 d - S(\rho) \quad (35)$$

is the *relative entropy of purity*. It coincides with both the distillable purity and the purity cost in the asymptotic limit, where the resource theory of purity becomes reversible [26].

As is summarized in appendix E, \mathcal{P}_α is a purity measure for all $\alpha \geq 0$, i.e., it fulfills all requirements P1–P4, and it is convex for $0 \leq \alpha \leq 1$. We further note that $\mathcal{P}_\alpha(\rho) \geq \mathcal{P}_\beta(\rho)$ for $\alpha \geq \beta$, since the Rényi entropy S_α is



non-increasing in α [61]. Aside from the cases discussed before, another case of interest is the Rényi 2-purity $\mathcal{P}_2(\rho) = \log_2(d \text{Tr}[\rho^2])$, a simple function of the linear purity $\text{Tr}[\rho^2]$ ¹⁴, which can be directly measured by letting two copies of the state ρ interfere with each other [62, 63]. In this way, the purity of a composite system of ultracold bosonic atoms in an optical lattice, as well as the purity of its subsystems, have been determined experimentally [64].

6. Relation to entanglement and quantum discord

Of particular interest for quantum information theory are non-classical properties of correlated quantum states in multipartite systems [4, 18]. Our results about purity have immediate consequences for quantities such as entanglement and discord. Certain relations between entanglement and purity have already been reported. Bipartite entangled states, e.g., must have a linear purity above a threshold value of $\text{Tr}[\rho^2] = 1/(d-1)$, with total dimension d , due to the existence of a finite-volume set of separable states around the maximally mixed state [65–67]. Furthermore, a bound for entanglement can be provided by comparing the purity of the composite system to the one of its subsystems [64, 68]. Similar investigations have also been performed for multipartite quantum systems [69, 70].

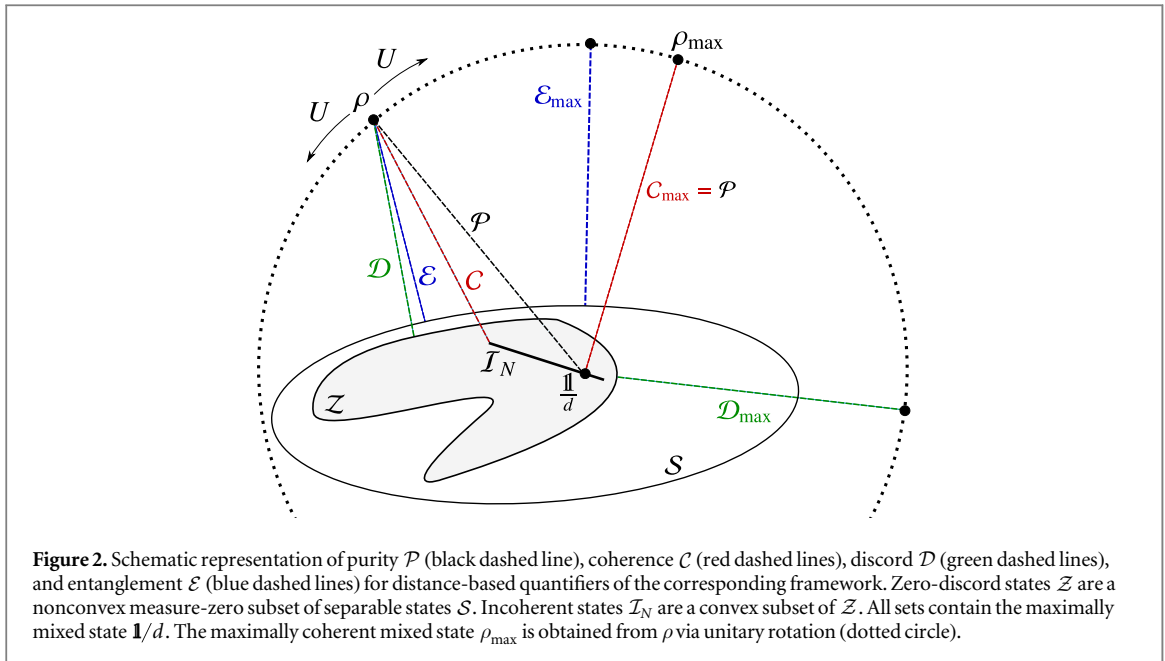
In the following we focus on distance-based quantifiers for discord \mathcal{D} and entanglement \mathcal{E} , in analogy to equations (5) and (31). In a multipartite system these can be defined as [1, 60]

$$\mathcal{D}(\rho) = \inf_{\sigma \in \mathcal{Z}} D(\rho, \sigma), \quad (36)$$

$$\mathcal{E}(\rho) = \inf_{\sigma \in \mathcal{S}} D(\rho, \sigma), \quad (37)$$

where \mathcal{Z} and \mathcal{S} denote the sets of zero-discord and separable states, respectively. The latter contains all convex combinations of arbitrary product states $\rho_1 \otimes \dots \otimes \rho_N$, whereas the set of zero-discord states can either be defined with respect to a particular subsystem, or symmetrically with respect to all subsystems. Here, we consider the symmetrical set \mathcal{Z} [7], encompassing all convex combinations of pure, locally orthonormal product states $|\varphi_1\rangle\langle\varphi_1| \otimes \dots \otimes |\varphi_N\rangle\langle\varphi_N|$. With this choice, $\mathcal{D}(\rho)$ provides an upper bound for the non-symmetric definitions of discord.

¹⁴Notice that $\text{Tr}[\rho^2] = 1/d$ corresponds to the purity monotone obtained from the squared Schatten 2-norm $\|\rho - \mathbf{1}/d\|_2^2$.



Our general distance-based approach leads to the following natural ordering of resources:

$$\mathcal{P}(\rho) \geq \mathcal{C}_N(\rho) \geq \mathcal{D}(\rho) \geq \mathcal{E}(\rho). \quad (38)$$

Here, $\mathcal{C}_N(\rho) = \inf_{\sigma \in \mathcal{I}_N} D(\rho, \sigma)$ denotes a coherence monotone with respect to an N -partite incoherent product basis, where \mathcal{I}_N is the set of N -partite incoherent states [34, 35]. This hierarchy holds true if purity, coherence, discord, and entanglement are defined via the same distance D . In this case, the statement follows directly by noting that $\mathbf{1}/d \in \mathcal{I}_N \subset \mathcal{Z} \subset \mathcal{S}$, see also figure 2. Based on the same argument, this hierarchy can be easily extended beyond entanglement to include the concepts of steering and non-locality [9, 71]. It holds that $\mathcal{D}(\rho) = \inf_{U_N} \mathcal{C}_N(U_N \rho U_N^\dagger)$ with product unitary U_N ; this was pointed out for the relative entropy in [72], but holds for general distance-based quantifiers.

A change of the *global* basis, or equivalently, application of a collective unitary operation can generate entanglement and discord. As we will see below, the maximal achievable amount is again directly bounded by the purity. For this we introduce $\mathcal{D}_{\max}(\rho) = \sup_U \mathcal{D}(U\rho U^\dagger)$ and similarly $\mathcal{E}_{\max}(\rho) = \sup_U \mathcal{E}(U\rho U^\dagger)$, in analogy to equation (14). As we prove in appendix F, these quantities obey the following relation

$$\mathcal{P}(\rho) = \mathcal{C}_{\max}(\rho) \geq \mathcal{D}_{\max}(\rho) \geq \mathcal{E}_{\max}(\rho), \quad (39)$$

which is visualized in figure 2. States related to \mathcal{D}_{\max} and \mathcal{E}_{\max} have been studied for the two-qubit case. For instance, the set of maximally entangled mixed states, i.e., states which maximize entanglement for a fixed spectrum, as well as states that maximize entanglement at a fixed value of purity, have been characterized for various quantifiers of entanglement and purity [51–54]. States satisfying $\mathcal{E}_{\max}(\rho) = 0$ are also known as absolutely separable states, and have been studied in [73–75]. Similar studies were performed for discord [76, 77], based on the original definition [5]. We also note that the relative entropy of purity \mathcal{P}_r coincides with the maximal mutual information $I_{\max}(\rho) = \max_U I(U\rho U^\dagger)$, where $I(\rho) = S(\rho^A) + S(\rho^B) - S(\rho)$ is the mutual information and both subsystems A and B have the same dimension \sqrt{d} [78]. As a direct consequence of theorem 2, purity further bounds the accessible entanglement under IO. This is discussed in more detail in appendix G.

7. Experimental relevance

In well-controllable quantum systems, quantum states with nearly maximal purity are usually easy to initialize but hard to maintain. Especially large quantum systems suffer immensely from purity losses due to noise. For example the linear purity $\text{Tr}[\rho^2]$ of the Greenberger–Horne–Zeilinger state decreases exponentially in time under global phase noise with a decay proportional to the number of particles squared [79]. A principal challenge of single photon experiments is the creation of the temporal purity, which is necessary for coherent interaction between photons of two independent sources [80].

In contrast to measures of entanglement, discord, or coherence, purity measures are rather easily accessible in experiments [62–64]. For example the Rényi α -purities (32) are essentially functions of the eigenvalue distribution $\{p_i\}$ of ρ . Any von Neumann measurement of ρ immediately provides a lower bound for this

distribution: if such a measurement is performed in a basis $\{|\varphi_i\rangle\}$, the measurement outcomes are distributed according to the probabilities $p'_i = \langle \varphi_i | \rho | \varphi_i \rangle$. Any purity monotone that is evaluated on the basis of the $\{p'_i\}$ is a lower bound for the true purity of ρ ¹⁵. The most easily accessible basis in experiments is the energy eigenbasis. In this case the measured bound coincides with the purity for all thermal states. By virtue of theorem 2, the measured purity also naturally provides an experimental bound on the amount of coherence, entanglement, and quantum discord.

8. Conclusions

As we have proven in this work, the resource theories of coherence and purity are closely connected. This connection was established by showing that any amount of purity can be converted into coherence by means of a suitable unitary operation. We further provided a closed expression for the optimal unitary operation, as well as the quantum states that achieve the maximal coherence. Remarkably, this set of maximally coherent mixed states is universal, i.e., these states maximize all coherence monotones for a fixed spectrum. For any distance-based coherence monotone the maximal coherence achievable via unitary operations can be evaluated exactly, and is shown to coincide with the corresponding distance-based purity monotone.

Based on these results, we defined a new family of coherence-based purity monotones which admit a closed expression and an operational interpretation in several relevant scenarios. We further proposed a general framework for quantifying purity, following related approaches for entanglement and coherence. This approach also provides quantitative bounds on the required amount of purity to achieve certain levels of entanglement and discord. Lower bounds for a large variety of purity measures are easily accessible in experiments.

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Appendix A. Proof of theorem 2

Here we will prove that

$$\mathcal{C}_{\max}(\rho) = \sup_U \mathcal{C}(U\rho U^\dagger) = \max_U \mathcal{C}(U\rho U^\dagger) = D(\rho, \mathbf{1}/d) \quad (\text{A1})$$

holds true for any distance-based coherence monotone $\mathcal{C}(\rho) = \inf_{\sigma \in \mathcal{I}} D(\rho, \sigma)$ with a contractive distance D , i.e.,

$$D(\Lambda[\rho], \Lambda[\sigma]) \leq D(\rho, \sigma) \quad (\text{A2})$$

for any quantum operation Λ .

Our proof will consist of two steps. In the first step, we will prove the inequality

$$\mathcal{C}_{\max}(\rho) \leq D(\rho, \mathbf{1}/d). \quad (\text{A3})$$

This follows by noting that the maximally mixed state $\mathbf{1}/d$ is incoherent, and thus gives an upper bound for any distance-based coherence monotone: $\mathcal{C}(\rho) \leq D(\rho, \mathbf{1}/d)$. By contractivity (A2) the distance D must be invariant under unitaries, which implies that $\mathcal{C}(U\rho U^\dagger) \leq D(\rho, \mathbf{1}/d)$ for any unitary U . This completes the proof of equation (A3).

To complete the proof of the theorem, we will now show the converse inequality

$$\mathcal{C}_{\max}(\rho) \geq D(\rho, \mathbf{1}/d). \quad (\text{A4})$$

For this, we introduce the unitary V with the property that $\rho_{\max} = V\rho V^\dagger$, where $\rho_{\max} = \sum_n p_n |n_+\rangle \langle n_+|$ is a maximally coherent mixed state. By definition of \mathcal{C}_{\max} , it must be that $\mathcal{C}_{\max}(\rho) \geq \mathcal{C}(V\rho V^\dagger)$. We further define Δ_+ as the dephasing operation in the maximally coherent basis:

$$\Delta_+[\rho] = \sum_n \langle n_+ | \rho | n_+ \rangle |n_+\rangle \langle n_+|. \quad (\text{A5})$$

¹⁵This is a direct consequence of the fact that nonselective von Neumann measurements are unital operations.

It is important to note that the application of Δ_+ to any incoherent state $\sigma \in \mathcal{I}$ leads to the maximally mixed state: $\Delta_+[\sigma] = \mathbf{1}/d$. If we further define $\tau \in \mathcal{I}$ to be the closest incoherent state to ρ_{\max} , we arrive at the following result:

$$\mathcal{C}_{\max}(\rho) \geq \mathcal{C}(\rho_{\max}) = D(\rho_{\max}, \tau) \geq D(\Delta_+[\rho_{\max}], \Delta_+[\tau]) = D(\rho_{\max}, \mathbf{1}/d) = D(\rho, \mathbf{1}/d). \quad (\text{A6})$$

In the second line we used contractivity (A2) and in the last equality we used unitary invariance of the distance D . This completes the proof of the theorem.

We note that the same proof also applies for all coherence quantifiers \mathcal{C}_p based on Schatten p -norms for $p \geq 1$. This can be seen by using the same arguments as above, together with the fact that Schatten p -norms are contractive under unital operations for all $p \geq 1$ [81].

Appendix B. Proof of equation (30)

Here, we will show that any MIO monotone \mathcal{C} fulfills the following inequality:

$$\sup_{\Lambda_U} \mathcal{C}(\Lambda_U[\rho]) = \max_{\Lambda_U} \mathcal{C}(\Lambda_U[\rho]) = \mathcal{C}(\rho_{\max}), \quad (\text{B1})$$

where $\rho_{\max} = \sum_n p_n |n_+\rangle \langle n_+|$ is a maximally coherent mixed state, $\{p_n\}$ is the spectrum of ρ , and the supremum is taken over all unital operations Λ_U .

In the first step of the proof, we recall that unital operations are equivalent to mixtures of unitaries with respect to state transformations, see lemma 10 in [27]. By using similar arguments as in appendix A, we will now show that for any mixture of unitaries $\Lambda_{\text{MU}}[\rho] = \sum_i q_i U_i \rho U_i^\dagger$ there exists a MIO Λ_{MIO} such that

$$\Lambda_{\text{MU}}[\rho_{\max}] = \Lambda_{\text{MIO}}[\rho_{\max}]. \quad (\text{B2})$$

The desired MIO will be given by $\Lambda_{\text{MIO}}[\rho] = \sum_{i,n} K_{i,n} \rho K_{i,n}^\dagger$ with Kraus operators $K_{i,n} = \sqrt{q_i} U_i |n_+\rangle \langle n_+|$. It is straightforward to verify that $\sum_{i,n} K_{i,n} \sigma K_{i,n}^\dagger = \mathbf{1}/d$ holds for any incoherent state σ , which means that the operation is indeed maximally incoherent. Moreover, it holds that

$$\sum_{i,n} K_{i,n} \rho_{\max} K_{i,n}^\dagger = \sum_i q_i U_i \rho_{\max} U_i^\dagger, \quad (\text{B3})$$

which completes the proof of equation (B2).

Together with lemma 10 in [27], this result implies that for any unital operation Λ_U there exists a MIO Λ_{MIO} such that $\Lambda_U[\rho_{\max}] = \Lambda_{\text{MIO}}[\rho_{\max}]$. To complete the proof of equation (B1), recall that the states ρ and ρ_{\max} are related via a unitary, i.e., $\rho = U \rho_{\max} U^\dagger$. This immediately implies that $\mathcal{C}(\rho_{\max}) \leq \sup_{\Lambda_U} \mathcal{C}(\Lambda_U[\rho])$. On the other hand, the results presented above imply the converse inequality:

$$\mathcal{C}(\rho_{\max}) \geq \sup_{\Lambda_U} \mathcal{C}(\Lambda_U[\rho_{\max}]) = \sup_{\Lambda_U} \mathcal{C}(\Lambda_U[\rho]), \quad (\text{B4})$$

where the last equality follows from the fact that ρ and ρ_{\max} are related via a unitary. This completes the proof.

Appendix C. Proof of equation (33)

For proving the statement, let m be an integer such that

$$\Lambda_U \left[\rho \otimes \frac{\mathbf{1}}{d_2} \right] = \psi_2^{\otimes m} \otimes \frac{\mathbf{1}}{d_1} \quad (\text{C1})$$

holds true for some unital operation Λ_U and some integers d_1 and d_2 . Since we require that the unital operation does not change the dimension of the system, we have the additional constraint

$$\frac{d_1}{d_2} = \frac{d}{2^m}. \quad (\text{C2})$$

From lemma 3, it follows that the rank of a state cannot decrease under unital operations. Thus, equation (C1) implies

$$\frac{d_1}{d_2} \geq r, \quad (\text{C3})$$

where r is the rank of ρ . The inequality (C3) implies the majorization relation

$$\rho \otimes \frac{\mathbf{1}}{d_2} \succ \psi_2^{\otimes m} \otimes \frac{\mathbf{1}}{d_1}, \quad (\text{C4})$$

as can be seen by recalling that the maximally mixed state is majorized by any other state of the same dimension. Thus, by lemma 3, equations (C2) and (C3) are necessary and sufficient conditions for the transformation in equation (C1).

Equations (C2) and (C3) further imply the inequality

$$m \leq \log_2(d/r), \quad (\text{C5})$$

which proves that single-shot distillable purity is bounded above by $\lfloor \log_2(d/r) \rfloor$. Moreover, it is straightforward to check that equations (C2) and (C3) hold true if we choose $m = \lfloor \log_2(d/r) \rfloor$, $d_1 = d$, and $d_2 = 2^m$. This completes the proof.

Appendix D. Proof of equation (34)

In the first step of the proof, let m be an integer such that m copies of a pure single-qubit state ψ_2 can be transformed into the desired state ρ via some unital operation Λ_U , i.e.,

$$\Lambda_U \left[\psi_2^{\otimes m} \otimes \frac{\mathbf{1}}{d_1} \right] = \rho \otimes \frac{\mathbf{1}}{d_2} \quad (\text{D1})$$

with some integers d_1 and d_2 . Since we require that Λ_U preserves the dimension of the Hilbert space, it must be that

$$\frac{d_1}{d_2} = \frac{d}{2^m}. \quad (\text{D2})$$

A necessary requirement for the existence of the unital operation in equation (D1) is that due to lemma 3 the maximal eigenvalue of $\rho \otimes \mathbf{1}/d_2$ —which is λ_{\max}/d_2 —is smaller or equal than the maximal eigenvalue of the resource state $\psi_2^{\otimes m} \otimes \mathbf{1}/d_1$, i.e.

$$\frac{\lambda_{\max}}{d_2} \leq \frac{1}{d_1}. \quad (\text{D3})$$

It is now crucial to note that due to the special form of the resource state, equation (D3) directly implies the majorization relation

$$\rho \otimes \frac{\mathbf{1}}{d_2} \prec \psi_2^{\otimes m} \otimes \frac{\mathbf{1}}{d_1}. \quad (\text{D4})$$

Thus, by lemma 3, equations (D2) and (D3) are necessary and sufficient for the transformation in equation (D1).

In the next step, we note that equations (D2) and (D3) imply the following inequality:

$$m \geq \log_2(d\lambda_{\max}), \quad (\text{D5})$$

which means that the single-shot purity cost is bounded below by $\lceil \log_2(d\lambda_{\max}) \rceil$. In the last step, it is straightforward to check that equations (D2) and (D3) hold true if we choose $m = \lceil \log_2(d\lambda_{\max}) \rceil$, $d_1 = d$, and $d_2 = 2^m$. This completes the proof.

Appendix E. Properties of Rényi α -purities

Here we will prove that the Rényi α -purity

$$\mathcal{P}_\alpha(\rho) = \log_2 d - S_\alpha(\rho) \quad (\text{E1})$$

is a purity measure, i.e., it fulfills the requirements P1–P4 stated in the main text. For this, we will use the fact that the Rényi entropy is Schur concave for all $\alpha \geq 0$ [82]:

$$\rho \succ \sigma \Rightarrow S_\alpha(\rho) \leq S_\alpha(\sigma). \quad (\text{E2})$$

We will now prove each of the conditions P1–P4.

$\mathcal{P}_\alpha(\mathbf{1}/d) = 0$ follows immediately from $S_\alpha(\mathbf{1}/d) = \log_2 d$ for all α . Furthermore equation (E2) and the fact that the maximally mixed state $\mathbf{1}/d$ is majorized by any other state of the same dimension imply nonnegativity:

$$\mathcal{P}_\alpha(\rho) \geq \mathcal{P}_\alpha(\mathbf{1}/d) = 0. \quad (\text{E3})$$

Due to lemma 3, we have $\rho \succ \Lambda_U[\rho]$ for any unital operation Λ_U . Equation (E2) then implies that $\mathcal{P}_\alpha(\rho) \geq \mathcal{P}_\alpha(\Lambda_U[\rho])$.

The Rényi entropy is additive: $S_\alpha(\rho \otimes \sigma) = S_\alpha(\rho) + S_\alpha(\sigma)$. This directly implies additivity of \mathcal{P}_α .

$\mathcal{P}_\alpha(|\psi\rangle_d) = \log_2 d$, since $S_\alpha(|\psi\rangle_d) = 0$ for all α .

The Rényi α -purity is convex for $0 \leq \alpha \leq 1$, since S_α is concave in this region [61]. For $\alpha > 1$ the Rényi entropy S_α is neither concave nor convex [83].

Appendix F. Proof of equation (39)

Let us denote with $U_{\mathcal{E}}$ the unitary operation that provides the maximum for $\mathcal{E}_{\max}(\rho)$. We find

$$\mathcal{E}_{\max}(\rho) = \mathcal{E}(U_{\mathcal{E}}\rho U_{\mathcal{E}}^\dagger) \leq \mathcal{D}(U_{\mathcal{E}}\rho U_{\mathcal{E}}^\dagger) \leq \sup_U \mathcal{D}(U\rho U^\dagger) = \mathcal{D}_{\max}(\rho). \quad (\text{F1})$$

Similarly, let $U_{\mathcal{D}}$ be the unitary that leads to $\mathcal{D}_{\max}(\rho)$. We obtain

$$\mathcal{D}_{\max}(\rho) = \mathcal{D}(U_{\mathcal{D}}\rho U_{\mathcal{D}}^\dagger) \leq \mathcal{C}_N(U_{\mathcal{D}}\rho U_{\mathcal{D}}^\dagger) \leq \sup_U \mathcal{C}_N(U\rho U^\dagger) = \sup_U \mathcal{C}(U\rho U^\dagger) = \mathcal{P}(\rho), \quad (\text{F2})$$

where we used theorem 2 as well as the fact that any two bases can be mapped onto each other by a unitary operation.

Appendix G. Purity bounds on entanglement by IO

The amount of entanglement which can be generated by an optimal IO is bounded by the coherence [35]:

$$\mathcal{C}_r(\rho^A) = \lim_{d_B \rightarrow \infty} \left\{ \sup_{\Lambda_i} \mathcal{E}_r^{A:B}(\Lambda_i[\rho^A \otimes |0\rangle \langle 0|^B]) \right\}, \quad (\text{G1})$$

where the supremum is performed over all bipartite IO Λ_i [35] and \mathcal{C}_r and \mathcal{E}_r are the relative entropy of coherence and entanglement respectively. Our results from theorem 2 allow us to further connect these results to the relative entropy of purity: using a unitary to rotate ρ^A into a maximally coherent basis followed by the application of the optimal IO, the generated entanglement amounts to

$$\mathcal{P}_r(\rho^A) = \sup_U \lim_{d_B \rightarrow \infty} \left\{ \sup_{\Lambda_i} \mathcal{E}_r^{A:B}(\Lambda_i[U\rho^A U^\dagger \otimes |0\rangle \langle 0|^B]) \right\} \quad (\text{G2})$$

with the relative entropy of purity \mathcal{P}_r .

A similar result can be established for the geometric entanglement $\mathcal{E}_g(\rho) = 1 - \max_{\sigma \in \mathcal{S}} F(\rho, \sigma)$ and the geometric coherence $\mathcal{C}_g(\rho) = 1 - \max_{\sigma \in \mathcal{I}} F(\rho, \sigma)$, recalling that equation (G1) also holds true for these quantities [35]. If we introduce the geometric purity as $\mathcal{P}_g(\rho) = 1 - F(\rho, \mathbf{1}/d) = 1 - \frac{1}{d}(\text{Tr} \sqrt{\rho})^2$, we immediately obtain the following result:

$$\mathcal{P}_g(\rho^A) = \sup_U \lim_{d_B \rightarrow \infty} \left\{ \sup_{\Lambda_i} \mathcal{E}_g^{A:B}(\Lambda_i[U\rho^A U^\dagger \otimes |0\rangle \langle 0|^B]) \right\}. \quad (\text{G3})$$

In [84] a CNOT-gate (U_{CNOT}) is used to create entanglement out of the two-qubit input state

$$\rho_{\text{in}} = \rho^A \otimes |0\rangle \langle 0|^B \quad (\text{G4})$$

with system A being the control qubit system and B being the target qubit, i.e. $\rho_{\text{out}} = U_{\text{CNOT}} \rho_{\text{in}} U_{\text{CNOT}}^\dagger$. In this two-qubit scenario the entanglement of the state ρ_{out} can be measured by the negativity $\mathcal{N}(\rho) = \sum_j |\lambda_j^-|$ where λ_j^- are the negative eigenvalues of the partial transpose of ρ [65, 85–87]. The negativity of ρ_{out} is closely related to the l_1 -norm of coherence of the state ρ^A [88]:

$$\mathcal{N}(\rho_{\text{out}}) = |\rho_{01}^A| = \frac{\mathcal{C}_{\ell_1}(\rho^A)}{2}, \quad (\text{G5})$$

with ρ_{01}^A being the off-diagonal element of the chosen qubit basis.

For a single-qubit there is a direct relation between \mathcal{C}_{ℓ_1} and the geometric coherence [35]:

$\mathcal{C}_{\ell_1} = \sqrt{1 - (1 - 2\mathcal{C}_g)^2}$. Using theorem 2 to bound the geometric coherence by the geometric purity, we obtain the following bound for the negativity

$$\mathcal{N}(\rho_{\text{out}}) \leq \sqrt{1 - (1 - 2\mathcal{P}_g)^2}, \quad (\text{G6})$$

where equality holds if the eigenstates of ρ^A form a maximally coherent basis.

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