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Geometric quantum discord with Bures distance

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New Journal of Physics **15** (2013) 103001 (18pp)

Received 10 April 2013

Published 2 October 2013

Online at <http://www.njp.org/>

doi:10.1088/1367-2630/15/10/103001

Abstract. We define a new measure of quantum correlations in bipartite quantum systems given by the Bures distance of the system state to the set of classical states with respect to one subsystem, that is, to the states with zero quantum discord. Our measure is a geometrical version of the quantum discord. As the latter it quantifies the degree of non-classicality in the system. For pure states it is identical to the geometric measure of entanglement. We show that for mixed states it coincides with the optimal success probability of an ambiguous quantum state discrimination task. Moreover, the closest zero-discord states to a state ρ are obtained in terms of the corresponding optimal measurements.

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Contents

1. Introduction	2
2. Definitions of the quantum discords and Bures distance	4
2.1. The quantum discord and the set of A -classical states	4
2.2. Distance measures of quantum correlations with the Bures distance	5
3. The Bures geometric quantum discord of pure states	7
4. The Bures geometric quantum discord of mixed states	9
4.1. Link with minimal error quantum state discrimination	9
4.2. Derivation of the variational formula (23)	13
4.3. Closest A -classical states	14
5. Conclusions	15
Acknowledgments	16
Appendix. Necessary and sufficient condition for the optimal success probability to be equal to the inverse number of states	16
References	17

1. Introduction

One of the basic questions in quantum information theory is to understand how quantum correlations in composite quantum systems can be used to perform tasks that cannot be performed classically, or that lead classically to much lower efficiencies [1]. These correlations have been long thought to come solely from the entanglement among the different subsystems. This is the case for quantum computation and communication protocols using pure states. For instance, in order to offer an exponential speedup over classical computers, a pure-state quantum computation must necessarily produce multi-partite entanglement which is not restricted to blocks of qubits of fixed size as the problem size increases [2]. For composite systems in mixed states, however, there is now increasing evidence that other types of quantum correlations, such as those captured by the quantum discord of Ollivier and Zurek [3] and Henderson and Vedral [4], could provide the main resource to exploit, in order to outperform classical algorithms [5–8] or in some quantum communication protocols [8–11]. The quantum discord quantifies the amount of mutual information not accessible by local measurements on one subsystem. One can generate mixed states with non-zero discord but no entanglement by preparing locally statistical mixtures of nonorthogonal states, which cannot be perfectly distinguished by measurements. The strongest hint so far suggesting that the discord may in certain cases quantify the resource responsible for quantum speedups is provided by the deterministic quantum computation with one qubit (DQC1) of Knill and Laflamme [12]. The DQC1 model leads to an exponential speedup with respect to known classical algorithms. It consists of a control qubit, which remains unentangled with n unpolarized target qubits at all stages of the computation. For other bipartitions of the $n + 1$ qubits, e.g. putting together in one subsystem the control qubit and half of the target qubits, one finds in general some entanglement, but its amount is bounded in n [13]. Hence, for large system sizes, the total amount of bipartite entanglement is a negligible fraction of the maximal entanglement possible. On the other hand, the DQC1 algorithm typically produces a non-zero quantum discord between the control

qubit and the target qubits [5], save in some special cases [14]. This has been demonstrated experimentally in optical [6] and liquid-state nuclear magnetic resonance [7] implementations of DQC1. This presence of non-zero discord can be nicely interpreted by using the monogamy relation [15] between the discord of a bipartite system AB and the entanglement of B with its environment E if ABE is in a pure state [16]. The precise role played by the quantum discord in the DQC1 algorithm is still, however, subject to debate (see [8] and references therein).

A mathematically appealing way to quantify quantum correlations in multi-partite systems is given by the minimal distance of the system state to a separable state [17]. The Bures metric [18, 19] provides a nice distance d_B on the convex cone of density matrices, which has better properties than the Hilbert–Schmidt distance d_2 from a quantum information perspective. In particular, d_B is monotonous and Riemannian [20] and its metric coincides with the quantum Fisher information [21] playing an important role in high precision interferometry. As a consequence, the minimal Bures distance to separable states satisfies all criteria of an entanglement measure [17], which is not the case for the distance d_2 . This entanglement measure has been widely studied in the literature [22–25]. By analogy with entanglement, a geometric measure of quantum discord has been defined by Dakić *et al* [14] as the minimal distance of the system state to the set of zero-discord states. This geometric quantum discord (GQD) has been evaluated explicitly for two qubits [14]. However, the aforementioned authors use the Hilbert–Schmidt distance d_2 , which leads to serious drawbacks [26].

The aim of this work is to study a similar GQD as in [14] but based on the Bures distance d_B , which seems to be a more natural choice. This distance measure of quantum correlations has a clearer geometrical interpretation than other measures [17, 27] based on the relative entropy, which is not a distance on the set of density matrices. We show that it shares many of the properties of the quantum discord. Most importantly, as in the description of quantum correlations using the relative entropy [27, 28], our geometrical approach provides further information not contained in the quantum discord itself. In fact, one can look for the closest state(s) with zero discord to a given state ρ , and hence learn something about the ‘position’ of ρ with respect to the set of zero-discord states. The main result of this paper shows that finding the Bures-GQD and the closest zero-discord state(s) to ρ is closely linked to a minimal error quantum state discrimination (QSD) problem.

The task of discriminating states pertaining to a known set $\{\rho_1, \dots, \rho_n\}$ of density matrices ρ_i with prior probabilities η_i plays an important role in quantum communication and quantum cryptography. For instance, the set $\{\rho_1, \dots, \rho_n\}$ can encode a message to be sent to a receiver. The sender chooses at random some states among the ρ_i ’s and gives them one by one to the receiver, who is required to identify them and henceforth to decode the message. With this goal, the receiver performs a measurement on each state given to him by the sender. If the ρ_i are non-orthogonal, they cannot be perfectly distinguished from each other by measurements, so that the amount of sent information is smaller than in the case of orthogonal states. The best the receiver can do is to find the measurement that minimizes in some way his probability of equivocation. Two distinct strategies have been widely studied in the literature (see the review paper [29]). In the first one, the receiver seeks for a generalized measurement with $(n + 1)$ outcomes, allowing him to identify perfectly each state ρ_i but such that one of the outcomes leads to an inconclusive result (unambiguous QSD). The probability of occurrence of the inconclusive outcome must be minimized. In the second strategy, the receiver looks for a measurement with n outcomes yielding the maximal success probability $P_S = \sum_{i=1}^n \eta_i P_{i|i}$, where $P_{i|i}$ is the probability of the measurement outcome i given that the state is ρ_i . This strategy is called minimal error

(or ambiguous) QSD. The maximal success probability P_S^{opt} and the optimal measurement(s) are known explicitly for $n = 2$ [30], but no general solution has been found so far for more than two states (see, however, [31]) except when the ρ_i are related to each other by some symmetry and have equal probabilities η_i (see [29, 32, 33] and references therein). However, several upper bounds on P_S^{opt} are known [34] and the discrimination task can be solved efficiently numerically [35, 36]. Let us also stress that unambiguous and ambiguous QSD have been implemented experimentally for pure states [37] and, more recently, for mixed states [38], by using polarized light.

Let ρ be any state of a bipartite system with a finite-dimensional Hilbert space. We will prove in what follows that the Bures-GQD of ρ is equal to the maximal success probability P_S^{opt} in the ambiguous QSD of a family of states $\{\rho_i\}$ and prior probabilities $\{\eta_i\}$ depending on ρ . Moreover, the closest zero-discord states to ρ are given in terms of the corresponding optimal von Neumann measurement(s). The number of states ρ_i to discriminate is equal to the dimension of the Hilbert space of the measured subsystem. When this subsystem is a qubit, the discrimination task involves only two states and can be solved exactly [29, 30]: P_S^{opt} and the optimal von Neumann projectors are given in terms of the eigenvalues and eigenvectors of the Hermitian matrix $\Lambda = \eta_0\rho_0 - \eta_1\rho_1$. In a companion paper [39], we use this approach to derive an explicit formula for the Bures-GDQ of a family of two-qubits states (states with maximally mixed marginals) and determine the corresponding closest zero-discord states.

This paper is organized as follows. The definitions of the quantum discords and of the Bures distance are given in section 2, together with their main properties. In section 3, we show that the Bures-GQD of a pure state coincides with the geometric measure of entanglement and is simply related to the highest Schmidt coefficient. We explain this fact by noting that the closest zero-discord states to a pure state are convex combinations of orthogonal pure product states. The link between the minimal Bures distance to the set of zero-discord states and ambiguous QSD is explained and proved in section 4. The last section contains some conclusive remarks and perspectives. The appendix contains a technical proof of an intuitively obvious fact in QSD.

2. Definitions of the quantum discords and Bures distance

2.1. The quantum discord and the set of A-classical states

In this work we consider a bipartite quantum system AB with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, the spaces \mathcal{H}_A and \mathcal{H}_B of the subsystems A and B having arbitrary finite dimensions n_A and n_B . The states of AB are given by density matrices ρ on \mathcal{H} (i.e. Hermitian positive $N \times N$ matrices $\rho \in \text{Mat}(\mathbb{C}, N)$ with unit trace $\text{tr}(\rho) = 1$, with $N = n_A n_B$). The reduced states of A and B are defined by partial tracing ρ over the other subsystem. They are denoted by $\rho_A = \text{tr}_B(\rho)$ and $\rho_B = \text{tr}_A(\rho)$.

Let us first recall the definition of the quantum discord [3, 4]. The total correlations of the bipartite system in the state ρ are described by the mutual information $I_{A:B}(\rho) = S(\rho_A) + S(\rho_B) - S(\rho)$, where $S(\cdot)$ stands for the von Neumann entropy. The amount $J_{B|A}(\rho)$ of classical correlations is given by the maximal reduction of entropy of the subsystem B after a von Neumann measurement on A . Such a measurement is described by an orthogonal family $\{\pi_i^A\}$ of projectors acting on \mathcal{H}_A (i.e. by self-adjoint operators π_i^A on \mathcal{H}_A satisfying $\pi_i^A \pi_j^A = \delta_{ij} \pi_i^A$). Hence $J_{B|A}(\rho) = \max_{\{\pi_i^A\}} \{S(\rho_B) - \sum_i q_i S(\rho_{B|i})\}$, where the maximum is over all von Neumann measurements $\{\pi_i^A\}$, $q_i = \text{tr}(\pi_i^A \otimes 1 \rho)$ is the probability of the measurement

outcome i , and $\rho_{B|i} = q_i^{-1} \text{tr}_A(\pi_i^A \otimes 1 \rho)$ is the corresponding post-measurement conditional state of B . The quantum discord is by definition the difference $\delta_A(\rho) = I_{A:B}(\rho) - J_{B|A}(\rho)$ between the total and classical correlations. It measures the amount of mutual information which is not accessible by local measurements on the subsystem A . Note that it is asymmetric under the exchange $A \leftrightarrow B$. It can be shown [40] that $\delta_A(\rho) \geq 0$ for any ρ . Moreover, $\delta_A(\sigma_{A\text{-cl}}) = 0$ if and only if

$$\sigma_{A\text{-cl}} = \sum_{i=1}^{n_A} q_i |\alpha_i\rangle\langle\alpha_i| \otimes \sigma_{B|i}, \quad (1)$$

where $\{|\alpha_i\rangle\}_{i=1}^{n_A}$ is an orthonormal basis of \mathcal{H}_A , $\sigma_{B|i}$ are some (arbitrary) states of B depending on the index i , and $q_i \geq 0$ are some probabilities, $\sum_i q_i = 1$. The fact that $\delta_A(\sigma_{A\text{-cl}}) = 0$ follows directly from $I_{A:B}(\sigma_{A\text{-cl}}) = S(\text{tr}_A(\sigma_{A\text{-cl}})) - \sum_i q_i S(\sigma_{B|i}) \leq J_{B|A}(\sigma_{A\text{-cl}})$ and from the non-negativity of the quantum discord. For a bipartite system in the state $\sigma_{A\text{-cl}}$, the subsystem A is in one of the orthogonal states $|\alpha_i\rangle$ with probability q_i , hence A behaves as a classical system. For this reason, we will call *A-classical states* the zero-discord states of the form (1). In the literature they are often referred to as the ‘classical quantum’ states. We denote by \mathcal{C}_A the set of all A -classical states. By using the spectral decompositions of the $\sigma_{B|i}$, any A -classical state $\sigma_{A\text{-cl}} \in \mathcal{C}_A$ can be decomposed as

$$\sigma_{A\text{-cl}} = \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} q_{ij} |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_{j|i}\rangle\langle\beta_{j|i}|, \quad (2)$$

where, for any fixed i , $\{|\beta_{j|i}\rangle\}_{j=1}^{n_B}$ is an orthonormal basis of \mathcal{H}_B , and $q_{ij} \geq 0$, $\sum_{ij} q_{ij} = 1$ (note that the $|\beta_{j|i}\rangle$ need not be orthogonal for distinct i 's). One defines similarly the set \mathcal{C}_B of B -classical states, which are the states with zero quantum discord when the subsystem B is measured. A state which is both A - and B -classical possesses an eigenbasis $\{|\alpha_i\rangle \otimes |\beta_j\rangle\}_{i=1, j=1}^{n_A, n_B}$ of product vectors. It is fully classical, in the sense that a quantum system in this state can be ‘simulated’ by a classical apparatus being in the state (i, j) with probability q_{ij} .

Let us point out that \mathcal{C}_A , \mathcal{C}_B and the set of classical states \mathcal{C} are not convex. Their convex hull is the set \mathcal{S} of separable states. A state σ_{sep} is separable if it admits a convex decomposition $\sigma_{\text{sep}} = \sum_m q_m |\phi_m\rangle\langle\phi_m| \otimes |\psi_m\rangle\langle\psi_m|$, where $\{|\phi_m\rangle\}$ and $\{|\psi_m\rangle\}$ are (not necessarily orthogonal) families of unit vectors in \mathcal{H}_A and \mathcal{H}_B and $q_m \geq 0$, $\sum_m q_m = 1$. For pure states, A -classical and B -classical, classical and separable states all coincide. Actually, according to (2) the pure A -classical (and, similarly, the pure B -classical) states are product states.

2.2. Distance measures of quantum correlations with the Bures distance

The GQD of a state ρ of AB has been defined in [14] as the square distance of ρ to the set \mathcal{C}_A of A -classical states

$$D_A^{(2)}(\rho) = d_2(\rho, \mathcal{C}_A)^2 = \min_{\sigma_{A\text{-cl}} \in \mathcal{C}_A} d_2(\rho, \sigma_{A\text{-cl}})^2, \quad (3)$$

where $d_2(\rho, \sigma) = (\text{tr}[(\rho - \sigma)^2])^{1/2}$ is the Hilbert–Schmidt distance. Instead of taking this distance, we use in this paper the Bures distance

$$d_B(\rho, \sigma) = \left[2(1 - \sqrt{F(\rho, \sigma)}) \right]^{\frac{1}{2}}, \quad (4)$$

where ρ and σ are two density matrices and $F(\rho, \sigma)$ is their fidelity [1, 18, 41]

$$F(\rho, \sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_1^2 = [\text{tr}([\sqrt{\sigma}\rho\sqrt{\sigma}]^{1/2})]^2. \quad (5)$$

It is known that (4) defines a Riemannian distance on the convex cone $\mathcal{E} \subset \text{Mat}(\mathbb{C}, N)$ of all density matrices of AB . Its metric is equal to the Fubini–Study metric for pure states and coincides (apart from a numerical factor) with the quantum Fisher information which plays an important role in quantum metrology [21]. Moreover, d_B satisfies the following properties [1, 41]: for any $\rho, \sigma, \rho_1, \rho_2, \sigma_1$ and $\sigma_2 \in \mathcal{E}$,

- (i) *joint convexity*: if $\eta_1, \eta_2 \geq 0$ and $\eta_1 + \eta_2 = 1$, then $d_B(\eta_1\rho_1 + \eta_2\rho_2, \eta_1\sigma_1 + \eta_2\sigma_2) \leq \eta_1 d_B(\rho_1, \sigma_1) + \eta_2 d_B(\rho_2, \sigma_2)$ and
- (ii) d_B is monotonous under the action of completely positive trace-preserving maps \mathcal{T} from $\text{Mat}(\mathbb{C}, N)$ into itself: for any such \mathcal{T} , $d_B(\mathcal{T}\rho, \mathcal{T}\sigma) \leq d_B(\rho, \sigma)$.

Property (ii) implies that d_B is invariant under unitary conjugations: if U is a unitary operator on \mathcal{H} , then $d_B(U\rho U^\dagger, U\sigma U^\dagger) = d_B(\rho, \sigma)$. Note that the Hilbert–Schmidt distance d_2 is also unitary invariant but fails to satisfy (ii) (a simple counter-example can be found in [42]). The monotonous Riemannian distances on \mathcal{E} have been classified by Petz [20]. The Bures distance can be used to bound from below and above the trace distance $d_1(\rho, \sigma) = \text{tr}(|\rho - \sigma|)$ as follows [1]:

$$d_B(\rho, \sigma)^2 \leq d_1(\rho, \sigma) \leq \left[1 - \left(1 - \frac{1}{2}d_B(\rho, \sigma)^2\right)^2\right]^{\frac{1}{2}}. \quad (6)$$

For good reviews on the Uhlmann fidelity and Bures distance, see the book of Nielsen and Chuang [1] and the nice introduction of the paper [43] devoted to the estimation of the Bures volume of \mathcal{E} .

We define the GQD as

$$D_A(\rho) = d_B(\rho, \mathcal{C}_A)^2 = 2(1 - \sqrt{F_A(\rho)}), \quad F_A(\rho) = \max_{\sigma_{A-\text{cl}} \in \mathcal{C}_A} F(\rho, \sigma_{A-\text{cl}}). \quad (7)$$

The unitary invariance of d_B and d_2 implies that D_A and $D_A^{(2)}$ are invariant under conjugations by local unitaries, $\rho \mapsto U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger$, since such transformations leave \mathcal{C}_A invariant. By property (ii), D_A is monotonous under local operations involving von Neumann measurements on A and generalized measurements on B .

By analogy with (7), one can define two other geometrical measures of quantum correlations: the square distance to the set of classical states \mathcal{C} and the geometric measure of entanglement

$$D(\rho) = d_B(\rho, \mathcal{C})^2 = 2(1 - \sqrt{F_C(\rho)}), \quad E(\rho) = d_B(\rho, \mathcal{S})^2 = 2(1 - \sqrt{F_S(\rho)}), \quad (8)$$

where $F_C(\rho)$ is the maximal fidelity between ρ and a classical state $\sigma_{\text{cl}} \in \mathcal{C}$ and $F_S(\rho)$ the maximal fidelity between ρ and a separable state $\sigma_{\text{sep}} \in \mathcal{S}$. The first measure D is a geometrical analogue of the measurement-induced disturbance (MID) [44], which has up to our knowledge not been studied so far (however, an analogue of the MID based on the relative entropy has been introduced in [27]). The second measure E satisfies all criteria of an entanglement measure [17] (in particular, it is monotonous under local operations and classical communication by the property (ii)) and has been studied in [17, 22, 25]. It is closely related to other entanglement measures [23, 24] defined via a convex roof construction thanks to the identity [22]

$$F_S(\rho) = \max_{\{p_m\}, \{|\Psi_m\rangle\}} \sum_m p_m F_S(|\Psi_m\rangle), \quad F_S(|\Psi_m\rangle) = \max_{\sigma_{\text{sep}} \in \mathcal{S}} F(|\Psi_m\rangle\langle\Psi_m|, \sigma_{\text{sep}}), \quad (9)$$

where the maximum is over all pure state decompositions $\rho = \sum_m p_m |\Psi_m\rangle\langle\Psi_m|$ of ρ (with $\|\Psi_m\|=1$ and $p_m \geq 0$, $\sum p_m = 1$). The measure E is a geometrical analogue of the entanglement of formation [45]. The latter is defined via a convex roof construction from the von Neumann entropy of the reduced state

$$E_{\text{EoF}}(\rho) = \min_{\{p_m\}, \{|\Psi_m\rangle\}} \sum_m p_m E_{\text{EoF}}(|\Psi_m\rangle), \quad (10)$$

$$E_{\text{EoF}}(|\Psi_m\rangle) = S(\text{tr}_A(|\Psi_m\rangle\langle\Psi_m|)) = S(\text{tr}_B(|\Psi_m\rangle\langle\Psi_m|)).$$

Since $\mathcal{C} \subset \mathcal{C}_A \subset \mathcal{S}$, the three distances are ordered as

$$E(\rho) \leq D_A(\rho) \leq D(\rho). \quad (11)$$

This ordering of quantum correlations is a nice feature of the geometric measures. In contrast, the entanglement of formation $E_{\text{EoF}}(\rho)$ can be larger or smaller than the quantum discord $\delta_A(\rho)$ [46, 47].

3. The Bures geometric quantum discord of pure states

We first restrict our attention to pure states, for which one can obtain a simple formula for D_A in terms of the Schmidt coefficients μ_i . We recall that any pure state $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ admits a Schmidt decomposition

$$|\Psi\rangle = \sum_{i=1}^n \sqrt{\mu_i} |\varphi_i\rangle \otimes |\chi_i\rangle, \quad (12)$$

where $n = \min\{n_A, n_B\}$ and $\{|\varphi_i\rangle\}_{i=1}^{n_A}$ (respectively $\{|\chi_j\rangle\}_{j=1}^{n_B}$) is an orthonormal basis of \mathcal{H}_A (\mathcal{H}_B). If the μ_i are non-degenerate, the decomposition (12) is unique, the μ_i and $|\varphi_i\rangle$ (respectively $|\chi_j\rangle$) being the eigenvalues and eigenvectors of the reduced state $(|\Psi\rangle\langle\Psi|)_A$ (respectively $(|\Psi\rangle\langle\Psi|)_B$). Note that $\mu_i \geq 0$ and $\sum_i \mu_i = \|\Psi\|^2 = 1$.

Theorem 1. *If $\rho_\Psi = |\Psi\rangle\langle\Psi|$ is a pure state, then*

$$D_A(\rho_\Psi) = D(\rho_\Psi) = E(\rho_\Psi) = 2(1 - \sqrt{\mu_{\max}}), \quad (13)$$

where μ_{\max} is the largest Schmidt eigenvalue μ_i . If this maximal eigenvalue is non-degenerate, the closest A -classical (respectively classical, separable) state to ρ_Ψ is the pure product state $\sigma = |\varphi_{\max}\rangle \otimes |\chi_{\max}\rangle\langle\varphi_{\max}\rangle \otimes \langle\chi_{\max}|$, where $|\varphi_{\max}\rangle$ and $|\chi_{\max}\rangle$ are the eigenvectors corresponding to μ_{\max} in the decomposition (12). If μ_{\max} is r -fold degenerate, say $\mu_{\max} = \mu_1 = \dots = \mu_r > \mu_{r+1}, \dots, \mu_n$, then infinitely many A -classical (respectively classical, separable) states σ minimize the distance $d_B(\rho_\Psi, \sigma)$. These closest states σ are convex combinations of the orthogonal pure product states $|\alpha_l\rangle \otimes |\beta_l\rangle\langle\alpha_l\rangle \otimes \langle\beta_l|$, $l = 1, \dots, r$, with $|\alpha_l\rangle = \sum_{i=1}^r u_{il} |\varphi_i\rangle$ and $|\beta_l\rangle = \sum_{i=1}^r u_{il}^* |\chi_i\rangle$, where $(u_{il})_{i,l=1}^r$ is an arbitrary $r \times r$ unitary matrix and $|\varphi_i\rangle$ and $|\chi_i\rangle$ are some eigenvectors in the decomposition (12).

The expression (13) of the geometric measure of entanglement $E(\rho_\Psi)$ is basically known in the literature [23, 24]. The closest separable states to pure and mixed states have been investigated in [22]. By inspection of (12) and (13), $D_A(\rho_\Psi) = 0$ if and only if $|\Psi\rangle$ is a product state, in agreement with the fact that A -classical pure states are product states (the same holds for the other quantum correlation measures D and E). Moreover, from the inequality $\mu_{\max} \geq 1/n$

(following from $\sum_{i=1}^n \mu_i = 1$) one deduces that $D_A(\rho_\Psi) \leq 2(1 - 1/\sqrt{n})$. The maximal value of D_A is reached when $\mu_i = 1/n$ for any i , that is, for the maximally entangled states (recall that such states are the pure states with reduced states $(\rho_\Psi)_A$ and $(\rho_\Psi)_B$ having a maximal entropy $S((\rho_\Psi)_A) = -\sum_{i=1}^n \mu_i \ln \mu_i = \ln(n)$). Note that when μ_{\max} is r -fold degenerate, the r vectors $|\alpha_i\rangle$ (respectively $|\beta_i\rangle$) are orthonormal eigenvectors of $[\rho_\Psi]_A$ (respectively $[\rho_\Psi]_B$) with eigenvalue μ_{\max} . One then obtains another Schmidt decomposition of $|\Psi\rangle$ by replacing in (12) the r eigenvectors $|\varphi_i\rangle$ and $|\chi_i\rangle$ with eigenvalue μ_{\max} by $|\alpha_i\rangle$ and $|\beta_i\rangle$.

Remarkably, the maximally entangled states are the pure states admitting the largest family of closest separable states (this family is a $(n^2 + n - 2)$ real-parameter submanifold of \mathcal{E}). For instance, in the case of two qubits (i.e. for $n_A = n_B = n = 2$), the Bell states $|\Phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ admit as closest separable states the classical states

$$\sigma_\pm = \sum_{l=0,1} q_l |\alpha_l\rangle\langle\alpha_l| \otimes |\beta_l\rangle\langle\beta_l|, \quad |\alpha_l\rangle = u_{0l}|0\rangle + u_{1l}|1\rangle, \quad |\beta_l\rangle = u_{0l}^*|0\rangle \pm u_{1l}^*|1\rangle \quad (14)$$

with $u_{0l}^*u_{0m} + u_{1l}^*u_{1m} = \delta_{ml}$ and $q_l \geq 0$, $q_0 + q_1 = 1$. Interestingly, typical decoherence processes such as pure phase dephasing transform ρ_{Φ^\pm} into one of its closest separable state $(|00\rangle\langle 00| + |11\rangle\langle 11|)/2$ at times $t \gg t_{\text{dec}}$, where t_{dec} is the decoherence time. Slower relaxation processes modifying the populations in the states $|00\rangle$ and $|11\rangle$ do not further increase the distance to the initial state ρ_{Φ^\pm} . The situation is different for a partially entangled state $|\Psi\rangle = \sqrt{\mu_0}|00\rangle + \sqrt{\mu_1}|11\rangle$ with $\mu_1 > \mu_0$: then the closest separable state is the pure state $|11\rangle$, but $|\Psi\rangle$ evolves asymptotically to a statistical mixture of $|00\rangle$ and $|11\rangle$ when the qubits are coupled e.g. to thermal baths at positive temperatures.

Proof. For a pure state ρ_Ψ , the fidelity reads $F(\rho_\Psi, \sigma_{A\text{-cl}}) = \langle\Psi|\sigma_{A\text{-cl}}|\Psi\rangle$. Replacing $\sigma_{A\text{-cl}}$ in (7) by the right-hand side of (2) we get

$$F_A(\rho_\Psi) = \max_{\{|\alpha_i\rangle\}, \{|\beta_j\rangle\}, \{q_{ij}\}} \left\{ \sum_{ij} q_{ij} |\langle\alpha_i \otimes \beta_j|\Psi\rangle|^2 \right\} = \max_{\|\alpha\|=\|\beta\|=1} |\langle\alpha \otimes \beta|\Psi\rangle|^2, \quad (15)$$

where we have used $\sum_{ij} q_{ij} = 1$. Thanks to the Cauchy–Schwarz inequality, for any normalized vectors $|\alpha\rangle \in \mathcal{H}_A$ and $|\beta\rangle \in \mathcal{H}_B$ one has

$$\begin{aligned} |\langle\alpha \otimes \beta|\Psi\rangle| &= \left| \sum_{i=1}^n \sqrt{\mu_i} \langle\alpha|\varphi_i\rangle \langle\beta|\chi_i\rangle \right| \\ &\leq \sum_{i=1}^n \sqrt{\mu_i} |\langle\alpha|\varphi_i\rangle \langle\beta|\chi_i\rangle| \leq \sqrt{\mu_{\max}} \sum_{i=1}^n |\langle\alpha|\varphi_i\rangle \langle\beta|\chi_i\rangle| \end{aligned} \quad (16)$$

$$\leq \sqrt{\mu_{\max}} \left[\sum_{i=1}^n |\langle\alpha|\varphi_i\rangle|^2 \right]^{1/2} \left[\sum_{i=1}^n |\langle\beta|\chi_i\rangle|^2 \right]^{1/2} \leq \sqrt{\mu_{\max}}. \quad (17)$$

Let us first assume that $\mu_1 = \mu_{\max} > \mu_2, \dots, \mu_n$. Then $|\langle\alpha \otimes \beta|\Psi\rangle| = \sqrt{\mu_{\max}}$ if and only if $|\alpha\rangle = |\varphi_1\rangle$ and $|\beta\rangle = |\chi_1\rangle$ up to irrelevant phase factors. Thus the maximal fidelity $F_A(\rho_\Psi)$ between ρ_Ψ and an A -classical state is simply given by the largest Schmidt eigenvalue μ_{\max} . Moreover, the maximum in the second member of equation (15) is reached when a single q_{ij} is non-vanishing, say $q_{ij} = \delta_{i1}\delta_{j1}$, and $|\alpha_1\rangle = |\varphi_1\rangle$, $|\beta_{11}\rangle = |\chi_1\rangle$. This means that the closest A -classical state to ρ_Ψ is the pure product state $|\varphi_1 \otimes \chi_1\rangle\langle\varphi_1 \otimes \chi_1|$. Since this is a classical state,

one has $F_C(\rho_\Psi) = F_A(\rho_\Psi) = \mu_{\max}$. One shows similarly that $F_S(\rho_\Psi) = \mu_{\max}$. Then (13) follows from the definitions (7) and (8) of D_A , D and E .

More generally, let $\mu_1 = \dots = \mu_r = \mu_{\max} > \mu_{r+1}, \dots, \mu_n$. We need to show that all inequalities in (16) and (17) are equalities for appropriately chosen normalized vectors $|\alpha\rangle$ and $|\beta\rangle$. The first inequality in (16) is an equality if and only if $\arg(\langle\alpha|\varphi_i\rangle\langle\beta|\chi_i\rangle) = \theta$ is independent of i . The second inequality in (16) is an equality if and only if $|\alpha\rangle$ belongs to $V_{\max} = \text{span}\{|\varphi_i\rangle\}_{i=1}^r$ or $|\beta\rangle$ belongs to $W_{\max} = \text{span}\{|\chi_i\rangle\}_{i=1}^r$. The Cauchy–Schwarz inequality in (17) is an equality if and only if $|\langle\alpha|\varphi_i\rangle| = \lambda|\langle\beta|\chi_i\rangle|$ for all i , with $\lambda \geq 0$. Finally, the last inequality in (17) is an equality if and only if both sums inside the square brackets are equal to unity, i.e. $|\alpha\rangle \in \text{span}\{|\varphi_i\rangle\}_{i=1}^n$ and $|\beta\rangle \in \text{span}\{|\chi_i\rangle\}_{i=1}^n$ (this holds trivially if $n_A = n_B = n$). Putting all conditions together, we obtain $|\alpha\rangle \in V_{\max}$, $|\beta\rangle \in W_{\max}$ and $\langle\beta|\chi_i\rangle = e^{i\theta}\langle\varphi_i|\alpha\rangle$ for $i = 1, \dots, r$. Therefore, from any orthonormal family $\{|\alpha_l\rangle\}_{l=1}^r$ of V_{\max} one can construct r orthogonal vectors $|\alpha_l \otimes \beta_l\rangle$ satisfying $|\langle\alpha_l \otimes \beta_l|\Psi\rangle| = \sqrt{\mu_{\max}}$ for all $l = 1, \dots, r$, with $\langle\beta_l|\chi_i\rangle = \langle\varphi_i|\alpha_l\rangle$. The probabilities $\{q_{ij}\}$ maximizing the sum inside the brackets in (15) are given by $q_{ij} = q_i$ if $i = j \leq r$ and zero otherwise, where $\{q_l\}_{l=1}^r$ is an arbitrary set of probabilities. The corresponding A -classical states with maximal fidelities $F(\rho_\Psi, \sigma)$ are the classical states $\sigma = \sum_{l=1}^r q_l |\alpha_l \otimes \beta_l\rangle\langle\alpha_l \otimes \beta_l|$. \square

The equality between the correlation measures D_A , D and E is a consequence of the fact that the closest states to ρ_Ψ are classical states. Such an equality is reminiscent from the equality between the entanglement of formation E_{EoF} and the quantum discord δ_A for pure states. Let us notice that it does *not* hold for the Hilbert–Schmidt distance, for which the closest A -classical state to a pure state is in general a mixed state. Actually, one infers from the expression

$$d_2(\rho_\Psi, \sigma_{A\text{-cl}})^2 = \text{tr}[(|\Psi\rangle\langle\Psi| - \sigma_{A\text{-cl}})^2] = 1 - 2F(\rho_\Psi, \sigma_{A\text{-cl}}) + \text{tr}(\sigma_{A\text{-cl}}^2) \quad (18)$$

that the closest A -classical state results from a competition between the maximization of the fidelity $F(\rho_\Psi, \sigma_{A\text{-cl}})$ and the minimization of the trace $\text{tr}(\sigma_{A\text{-cl}}^2)$, which is maximum for pure states. For instance, one can show [39] that the closest A -classical states to the Bell states $|\Phi^\pm\rangle$ for d_2 are mixed two-qubit states. The validity of theorem 1 is one of the major advantages of the Bures-GQD over the Hilbert–Schmidt-GQD.

4. The Bures geometric quantum discord of mixed states

4.1. Link with minimal error quantum state discrimination

The determination of $D_A(\rho)$ is much more involved for mixed states than for pure states. We show in this section that this problem is related to ambiguous QSD. As it has been recalled in the introduction, in ambiguous QSD a state ρ_i drawn from a known family $\{\rho_i\}_{i=1}^{n_A}$ with prior probabilities $\{\eta_i\}_{i=1}^{n_A}$ is sent to a receiver. The task of the latter is to determine which state he has received with a maximal probability of success. To do so, he performs a generalized measurement and concludes that the state is ρ_j when his measurement result is j . The generalized measurement is given by a family of positive operators $M_i \geq 0$ satisfying $\sum_i M_i = 1$ (POVM). The probability to find the result j is $P_{j|i} = \text{tr}(M_j \rho_i)$ if the system is in the state ρ_i . The maximal success probability of the receiver reads

$$P_S^{\text{opt}}(\{\rho_i, \eta_i\}) = \max_{\text{POVM } \{M_i\}} \sum_{i=1}^{n_A} \eta_i \text{tr}(M_i \rho_i). \quad (19)$$

Theorem 2. Let ρ be a state of the bipartite system AB with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and let $\alpha = \{|\alpha_i\rangle\}_{i=1}^{n_A}$ be a fixed orthonormal basis of \mathcal{H}_A . Consider the subset $\mathcal{C}_A(\alpha) \subset \mathcal{C}_A$ of all A -classical states $\sigma_{A\text{-cl}}$ such that α is an eigenbasis of $\text{tr}_B(\sigma_{A\text{-cl}})$ (i.e. $\mathcal{C}_A(\alpha)$ is the set of all states $\sigma_{A\text{-cl}}$ of the form (1), for arbitrary probabilities q_i and states $\sigma_{B|i}$ on \mathcal{H}_B). Then the maximal fidelity $F(\rho, \mathcal{C}_A(\alpha)) = \max_{\sigma_{A\text{-cl}} \in \mathcal{C}_A(\alpha)} F(\rho, \sigma_{A\text{-cl}})$ of ρ to this subset is equal to

$$F(\rho, \mathcal{C}_A(\alpha)) = P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) \equiv \max_{\{\Pi_i\}} \sum_{i=1}^{n_A} \eta_i \text{tr}(\Pi_i \rho_i), \quad (20)$$

where $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\})$ is the maximal success probability over all von Neumann measurements given by orthogonal projectors Π_i of rank n_B (that is, self-adjoint operators on \mathcal{H} satisfying $\Pi_i \Pi_j = \delta_{ij} \Pi_i$ and $\dim(\Pi_i \mathcal{H}) = n_B$), and

$$\eta_i = \langle \alpha_i | \rho_A | \alpha_i \rangle, \quad \rho_i = \eta_i^{-1} \sqrt{\rho} | \alpha_i \rangle \langle \alpha_i | \otimes 1 \sqrt{\rho} \quad (21)$$

(if $\eta_i = 0$ then ρ_i is not defined but does not contribute to the sum in (20)).

This theorem will be proven in section 4.2. Note that the ρ_i are quantum states of AB if $\eta_i > 0$, because the right-hand side of the last identity in (21) is a non-negative operator and η_i is chosen such that $\text{tr}(\rho_i) = 1$. Moreover, $\{\eta_i\}_{i=1}^{n_A}$ is a set of probabilities (since $\eta_i \geq 0$ and $\sum_i \eta_i = \text{tr}(\rho) = 1$) and $\{\rho_i, \eta_i\}_{i=1}^{n_A}$ defines a convex decomposition of ρ , i.e. $\rho = \sum_i \eta_i \rho_i$.

Let us assume that ρ is invertible. Then the application of a result by Eldar [48] shows that the POVM maximizing the success probability $P_S(\{\rho_i, \eta_i\})$ in (19) is a von Neumann measurement with projectors Π_i of rank n_B , i.e.

$$F(\rho, \mathcal{C}_A(\alpha)) = P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) = P_S^{\text{opt}}(\{\rho_i, \eta_i\}), \quad \rho > 0. \quad (22)$$

In fact, one may first notice that all matrices ρ_i have rank $r_i = n_B$ (for indeed, ρ_i has the same rank as $\eta_i \rho^{-1/2} \rho_i = |\alpha_i\rangle \langle \alpha_i| \otimes 1 \sqrt{\rho}$ and the latter matrix has rank n_B). Next, we argue that the ρ_i are linearly independent, in the sense that their eigenvectors $|\xi_{ij}\rangle$ form a linearly independent family $\{|\xi_{ij}\rangle\}_{i=1, \dots, n_A}^{j=1, \dots, n_B}$ of vectors in \mathcal{H} . Actually, a necessary and sufficient condition for $|\xi_{ij}\rangle$ to be an eigenvector of ρ_i with eigenvalue $\lambda_{ij} > 0$ is $|\xi_{ij}\rangle = (\lambda_{ij} \eta_i)^{-1} \sqrt{\rho} |\alpha_i\rangle \otimes |\zeta_{ij}\rangle$, $|\zeta_{ij}\rangle \in \mathcal{H}_B$ being an eigenvector of $R_i = \langle \alpha_i | \rho | \alpha_i \rangle$ with eigenvalue $\lambda_{ij} \eta_i > 0$. For any i , the Hermitian invertible matrix R_i admits an orthonormal eigenbasis $\{|\zeta_{ij}\rangle\}_{j=1}^{n_B}$. Thanks to the invertibility of $\sqrt{\rho}$, $\{|\xi_{ij}\rangle\}_{i=1, \dots, n_A}^{j=1, \dots, n_B}$ is a basis of \mathcal{H} and thus the states ρ_i are linearly independent. It is shown in [48] that for such a family of linearly independent states the second equality in (22) holds true.

The following result on the Bures-GQD of mixed states is a direct consequence of theorem 2.

Theorem 3. For any state ρ of the bipartite system AB , the fidelity to the closest A -classical state is given by

$$F_A(\rho) = \max_{\{\alpha_i\}} \max_{\{\Pi_i\}} \sum_{i=1}^{n_A} \text{tr}[\Pi_i \sqrt{\rho} |\alpha_i\rangle \langle \alpha_i| \otimes 1 \sqrt{\rho}], \quad (23)$$

where the maxima are over all orthonormal basis $\{|\alpha_i\rangle\}$ of \mathcal{H}_A and all orthogonal families $\{\Pi_i\}_{i=1}^{n_A}$ of projectors of $\mathcal{H}_A \otimes \mathcal{H}_B$ with rank n_B . Hence, using the notation of theorem 2,

$$F_A(\rho) = \max_{\{\alpha_i\}} P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}). \quad (24)$$

If $\rho > 0$ then one can replace $P_S^{\text{opt v.N.}}$ in (24) by the maximal success probability (19) over all POVMs.

It is noteworthy to observe that the basis vectors $|\alpha_i\rangle$ can be recovered from the states ρ_i and probabilities η_i by forming the square-root measurement operators $M_i = \eta_i \rho^{-1/2} \rho_i \rho^{-1/2}$, with $\rho = \sum_i \eta_i \rho_i$ (we assume here $\rho > 0$). Actually, such measurement operators are equal to the rank- n_B projectors $M_i = |\alpha_i\rangle\langle\alpha_i| \otimes 1$. By bounding from below $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\})$ by the success probability corresponding to $\Pi_i = M_i$, we obtain

$$F_A(\rho) \geq \max_{\{|\alpha_i\rangle\}} \sum_{i=1}^{n_A} \text{tr}_B [\langle\alpha_i| \sqrt{\rho} |\alpha_i\rangle^2]. \quad (25)$$

The square-root measurement plays an important role in the discrimination of almost orthogonal states [49, 50] and of ensembles of states with certain symmetries [32, 33].

To illustrate our result, let us study the ambiguous QSD task for some specific states ρ .

- (i) If ρ is an A -classical state, i.e. if it admits the decomposition (1), then the basis $\{|\alpha_i\rangle\}$ maximizing the optimal success probability in (24) coincides with the basis appearing in this decomposition. With this choice, one obtains $\eta_i = q_i$ and $\rho_i = |\alpha_i\rangle\langle\alpha_i| \otimes \sigma_{B|i}$ for all i such that $q_i > 0$. The states ρ_i are orthogonal and can thus be perfectly discriminated by von Neumann measurements, so that $F_A(\rho) = P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) = 1$. Reciprocally, if $F_A(\rho) = 1$ then $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) = 1$ for some basis $\{|\alpha_i\rangle\}$ of \mathcal{H}_A and the corresponding ρ_i must be orthogonal, that is, $\rho_i = \Pi_i \rho_i \Pi_i$ for some orthogonal family $\{\Pi_i\}$ of projectors with rank n_B . Hence $\rho = \sum_i \eta_i \rho_i = \sum_i \eta_i \Pi_i \rho_i \Pi_i$, $\sqrt{\rho} = \sum_i \Pi_i \sqrt{\rho} \Pi_i$ and (21) entails $\eta_i \rho_i = \eta_i \Pi_i \rho_i \Pi_i = \sqrt{\rho} |\alpha_i\rangle\langle\alpha_i| \otimes 1 \sqrt{\rho} = \sqrt{\rho} \Pi_i |\alpha_i\rangle\langle\alpha_i| \otimes 1 \Pi_i \sqrt{\rho}$, implying $\Pi_i = |\alpha_i\rangle\langle\alpha_i| \otimes 1$ if ρ is invertible. Thus ρ is A -classical (this was of course to be expected since $D_A(\rho) = 0$ if and only if ρ is A -classical, see section 2). Therefore, we can interpret our result (24) as follows: *the non-zero-discord states ρ are such that the states (21) are non-orthogonal and thus cannot be perfectly discriminated for any orthonormal basis $\{|\alpha_i\rangle\}$ of \mathcal{H}_A .*
- (ii) If $\rho = \rho_\Psi$ is a pure state, then all ρ_i with $\eta_i > 0$ are identical and equal to ρ_Ψ , so that $P_S^{\text{opt}} = P_S^{\text{opt v.N.}} = \sup_{\{\Pi_i\}} \sum_i \eta_i \langle\Psi|\Pi_i|\Psi\rangle = \eta_{\max}$. One gets back the result $F_A(\rho_\Psi) = \mu_{\max}$ of section 3 by optimization over the basis $\{|\alpha_i\rangle\}$.
- (iii) Let us determine the states ρ having the highest possible GQD, i.e. the smallest possible fidelity $F_A(\rho)$.

Proposition. *If $n_A \leq n_B$, the smallest fidelity $F_A(\rho)$ for all states ρ of AB is equal to $1/n_A$. If $rn_A \leq n_B < (r+1)n_A$ with $r = 1, 2, \dots$, the states ρ with $F_A(\rho) = 1/n_A$ are any convex combinations of the r maximally entangled pure states $|\Psi_k\rangle = n_A^{-1/2} \sum_{i=1}^{n_A} |\phi_i^{(k)}\rangle \otimes |\psi_i^{(k)}\rangle$, $k = 1, \dots, r$, with $\langle\phi_i^{(k)}|\phi_j^{(k)}\rangle = \delta_{ij}$ and $\langle\psi_i^{(k)}|\psi_j^{(l)}\rangle = \delta_{kl}\delta_{ij}$.*

We deduce from this result that the GQD $D_A(\rho)$ varies between 0 and $2 - 2/\sqrt{n_A}$ when $n_A \leq n_B$. By virtue of theorem 1, the proposition, and the inequality $E(\rho) \leq D_A(\rho)$, the geometric measure of entanglement $E(\rho)$ also varies between these two values. This means that *the most distant states from the set of A -classical states \mathcal{C}_A are also the most distant from the set of separable states \mathcal{S} .* If $n_A \leq n_B < 2n_A$, these most distant states are always maximally entangled pure states.

Proof. The success probability $P_S^{\text{opt v.N.}}$ must be clearly larger than the highest prior probability $\eta_{\max} = \max_i \{\eta_i\}$. (A receiver would obtain $P_S = \eta_{\max}$ by simply guessing that his state is $\rho_{i_{\max}}$,

with $\eta_{i_{\max}} = \eta_{\max}$; a better strategy is of course to perform the von Neumann measurement $\{\Pi_i\}$ such that $\Pi_{i_{\max}}$ projects on a n_B -dimensional subspace containing the range of $\rho_{i_{\max}}$; this range has a dimension $\leq n_B$ by a similar argument as in the discussion following theorem 2.) In view of (24) and by using $\eta_{\max} \geq 1/n_A$ (since $\sum_i \eta_i = 1$) we get

$$F_A(\rho) \geq \frac{1}{n_A} \quad (26)$$

for any mixed state ρ .

When $n_A \leq n_B$ the bound (26) is optimum, the value $1/n_A$ being reached for the maximally entangled pure states, see section 3. Thus $1/n_A$ is the smallest possible fidelity. Let ρ be a state having such a fidelity $F_A(\rho) = 1/n_A$. According to (24) and since it has been argued before that $P_S^{\text{opt.v.N.}} \geq \eta_{\max} \geq 1/n_A$, $F_A(\rho) = 1/n_A$ implies that $P_S^{\text{opt.v.N.}}(\{\rho_i, \eta_i\}) = 1/n_A$ whatever the orthonormal basis $\{|\alpha_i\rangle\}$. It is intuitively clear that this can only happen if the receiver gets a collection of identical states ρ_i with equal prior probabilities $\eta_i = 1/n_A$. A rigorous proof of this fact is given in the appendix. From (21) and $\rho = \sum \eta_i \rho_i$ we then obtain $\langle \alpha_i | \rho_A | \alpha_i \rangle = 1/n_A$ and $\rho_i = \rho$ for any $i = 1, \dots, n_A$ and any orthonormal basis $\{|\alpha_i\rangle\}$. The first equality implies $\rho_A = 1/n_A$. By replacing the spectral decomposition $\rho = \sum_k p_k |\Psi_k\rangle \langle \Psi_k|$ into (21), the second equality yields $\text{tr}_B(|\Psi_k\rangle \langle \Psi_l|) = n_A^{-1} \delta_{kl}$ for all k, l with $p_k p_l \neq 0$. Taking advantage of this identity for $k = l$, one finds that the eigenvectors $|\Psi_k\rangle$ of ρ with positive eigenvalues p_k have all their Schmidt eigenvalues equal to $1/n_A$, that is, their Schmidt decompositions read $|\Psi_k\rangle = n_A^{-1/2} \sum_{i=1}^{n_A} |\phi_i^{(k)}\rangle \otimes |\psi_i^{(k)}\rangle$. Moreover, $\text{tr}_B(|\Psi_k\rangle \langle \Psi_l|) = 0$ is equivalent to $\mathcal{V}_B^{(k)} \perp \mathcal{V}_B^{(l)}$ with $\mathcal{V}_B^{(k)} = \text{span}\{|\psi_i^{(k)}\rangle\}_{i=1}^{n_A} \subset \mathcal{H}_B$. If $n_B < (r+1)n_A$ then at most r subspaces $\mathcal{V}_B^{(k)}$ may be pairwise orthogonal. Thus at most r eigenvalues p_k are non-zero. \square

Let us now discuss the case $n_A > n_B$. In that case the smallest value of the maximal fidelity $F_S(\rho)$ to a separable state is equal to $1/n_B$ and $F_S(\rho) = 1/n_B$ when ρ is a pure maximally entangled state. This is a consequence of (9) and of the bound $F_S(\rho_\Psi) \geq 1/n_B$ for pure states ρ_Ψ (see section 3). As a result, the geometric measure of entanglement $E(\rho)$ varies between 0 and $2 - 2/\sqrt{n}$ with $n = \min\{n_A, n_B\}$, in both cases $n_A \leq n_B$ and $n_B > n_A$. We could not establish a similar result for the GQD $D_A(\rho)$. When $n_A > n_B$, the bound (26) is still correct but it is not optimal, i.e. there are no states ρ with fidelities $F_A(\rho)$ equal to $1/n_A$. Indeed, following the same lines as in the proof above, one shows that if $F_A(\rho) = 1/n_A$ then the eigenvectors $|\Psi_k\rangle$ of ρ with non-zero eigenvalues must have maximally mixed marginals $[\rho_{\Psi_k}]_A = 1/n_A$. But this is impossible since $\text{rank}([\rho_{\Psi_k}]_A) \leq n_B$ by (12). According to the results of section 3, pure states ρ_Ψ have fidelities $F_A(\rho_\Psi) \geq 1/n_B$, so one may expect that states close enough to pure states have fidelities close to $1/n_B$ or larger. This can be shown rigorously by invoking the bound

$$F_A(\rho) \geq \frac{\|\rho\|}{n_B} + \frac{1 - \|\rho\|}{n_A} \frac{n_B - \delta_\rho}{n_B}, \quad (27)$$

where $\|\rho\|$ is the norm of ρ and $\delta_\rho = 0$ if $\text{rank}(\rho) \leq n_B$ and 1 otherwise. This bound can be established as follows. Let us write $\rho = p|\Psi\rangle \langle \Psi| + (1-p)\rho'$ where $|\Psi\rangle$ is the eigenvector of ρ with maximal eigenvalue $p = \|\rho\|$ and the density matrix ρ' has support on $[\mathbb{C}|\Psi\rangle]^\perp$. Choosing an orthonormal family $\{\Pi_i\}$ of projectors of rank n_B satisfying $\Pi_1|\Psi_1\rangle = |\Psi_1\rangle$, we get from (24)

$$F_A(\rho) \geq \sum_i \eta_i \text{tr}(\Pi_i \rho_i) = p \langle \alpha_1 | \text{tr}_B(|\Psi\rangle \langle \Psi|) | \alpha_1 \rangle + (1-p) \sum_i \eta'_i \text{tr}(\Pi_i \rho'_i) \quad (28)$$

with $\eta'_i \rho'_i = \sqrt{\rho'} |\alpha_i\rangle \langle \alpha_i| \otimes 1 \sqrt{\rho'}$ and $\eta'_i = \langle \alpha_i | \rho'_A | \alpha_i \rangle$. Let us fix the orthonormal basis $\{|\alpha_i\rangle\}$ such that $|\alpha_1\rangle$ is the eigenvector with maximal eigenvalue μ_{\max} in the Schmidt decomposition (12) of $|\Psi\rangle$. This leads to the maximal possible value $p\mu_{\max}$ of the first term in the right-hand side of (28). We now bound the sum in this right-hand side by its i_m th term $\eta'_{\max} \text{tr}(\Pi_{i_m} \rho'_{i_m})$, where i_m is the index i such that η'_i is maximum, i.e. $\eta'_{i_m} = \eta'_{\max}$. If $i_m > 1$, one can find orthogonal projectors Π_1 and Π_{i_m} such that $|\Psi\rangle \in \Pi_1 \mathcal{H}$ and $\rho'_{i_m} \mathcal{H} \subset \Pi_{i_m} \mathcal{H} \subset [\mathbb{C}|\Psi\rangle]^\perp$ (recall that the ρ'_i have ranks $\leq n_B$). If $i_m = 1$, we choose $\Pi_1 = |\Psi\rangle \langle \Psi| + \Pi'_1$ where Π'_1 is the spectral projector of ρ'_1 associated to the $(n_B - 1)$ highest eigenvalues $q'_1 \geq q'_2 \geq \dots \geq q'_{n_B-1}$. In all cases, $\text{tr}(\Pi_{i_m} \rho'_{i_m}) \geq 1 - q'_{n_B}$. If $\text{rank}(\rho) \leq n_B$ then $q'_{n_B} = 0$, otherwise we bound q'_{n_B} by $1/n_B$ (since $\sum_{j=1}^{n_B} q'_j = 1$). Collecting the above results and using the inequalities $\mu_{\max} \geq 1/n_B$ and $\eta'_{\max} \geq 1/n_A$ (since $\sum_{i=1}^{n_A} \eta'_i = 1$), one gets (27). Note that this bound is stronger than (26) only for states ρ satisfying $\|\rho\| \geq (1 + n_A - n_B)^{-1}$ or $\text{rank}(\rho) \leq n_B$. In summary, we can only conclude from the analysis above that when $n_A > n_B$ the smallest possible fidelity $\min_{\rho \in \mathcal{E}} F_A(\rho)$ lies in the interval $(1/n_A, 1/n_B]$.

4.2. Derivation of the variational formula (23)

To prove theorems 2 and 3, we start by evaluating the trace norm in (5) by means of the formula $\|T\|_1 = \max_U |\text{tr}(UT)|$, the maximum being over all unitary operators on \mathcal{H} . Using also (2), one gets

$$\begin{aligned} \sqrt{F(\rho, \sigma_{A\text{-cl}})} &= \max_U |\text{tr}(U \sqrt{\rho} \sqrt{\sigma_{A\text{-cl}}})| \\ &= \max_U \left| \sum_{i,j} \sqrt{q_{ij}} \text{tr}(U \sqrt{\rho} |\alpha_i\rangle \langle \alpha_i| \otimes |\beta_{j|i}\rangle \langle \beta_{j|i}|) \right| \\ &= \max_{\{|\Phi_{ij}\rangle\}} \left| \sum_{i,j} \sqrt{q_{ij}} \langle \Phi_{ij} | \sqrt{\rho} |\alpha_i \otimes \beta_{j|i}\rangle \right| \\ &= \max_{\{|\Phi_{ij}\rangle\}} \sum_{i,j} \sqrt{q_{ij}} |\langle \Phi_{ij} | \sqrt{\rho} |\alpha_i \otimes \beta_{j|i}\rangle|. \end{aligned} \quad (29)$$

In the third line we have replaced the maximum over unitaries U by a maximum over all orthonormal basis $\{|\Phi_{ij}\rangle\}$ of \mathcal{H} (with $|\Phi_{ij}\rangle = U^\dagger |\alpha_i \otimes \beta_{j|i}\rangle$). The last equality in (29) can be explained as follows. The expression in the last line is clearly larger than that of the third line; since for any i and j one can choose the phase factors of the vectors $|\Phi_{ij}\rangle$ in such a way that $\langle \Phi_{ij} | \sqrt{\rho} |\alpha_i \otimes \beta_{j|i}\rangle \geq 0$, the two expressions are in fact equal.

One has to maximize the last member of (29) over all families of i -dependent orthonormal basis $\{|\beta_{j|i}\rangle\}$ of \mathcal{H}_B and all set of probabilities $\{q_{ij}\}$. The maximum over the probabilities q_{ij} is easy to evaluate by using the Cauchy–Schwarz inequality and $\sum_{i,j} q_{ij} = 1$. It is reached for

$$q_{ij} = \frac{|\langle \Phi_{ij} | \sqrt{\rho} |\alpha_i \otimes \beta_{j|i}\rangle|^2}{\sum_{i,j} |\langle \Phi_{ij} | \sqrt{\rho} |\alpha_i \otimes \beta_{j|i}\rangle|^2}. \quad (30)$$

We thus obtain

$$F(\rho, \mathcal{C}_A(\alpha)) = \max_{\{|\beta_{j|i}\rangle\}} \max_{\{q_{ij}\}} F(\rho, \sigma_{A\text{-cl}}) = \max_{\{|\beta_{j|i}\rangle\}} \max_{\{|\Phi_{ij}\rangle\}} \sum_{i,j} |\langle \psi_{j|i} | \beta_{j|i}\rangle|^2, \quad (31)$$

where we have set $|\psi_{j|i}\rangle = \langle \alpha_i | \sqrt{\rho} | \Phi_{ij} \rangle \in \mathcal{H}_B$. We proceed to evaluate the maximum over $\{|\beta_{j|i}\rangle\}$ and $\{|\Phi_{ij}\rangle\}$. Let us fix i and consider the orthogonal family of projectors of \mathcal{H} of rank n_B defined by

$$\Pi_i = \sum_j |\Phi_{ij}\rangle \langle \Phi_{ij}|. \quad (32)$$

By the Cauchy–Schwarz inequality, for any fixed i one has

$$\max_{\{|\beta_{j|i}\rangle\}} \sum_j |\langle \psi_{j|i} | \beta_{j|i} \rangle|^2 \leq \sum_j \|\psi_{j|i}\|^2 = \text{tr}[\Pi_i \sqrt{\rho} |\alpha_i\rangle \langle \alpha_i| \otimes 1 \sqrt{\rho}]. \quad (33)$$

Note that (33) is an inequality if the vectors $|\psi_{j|i}\rangle$ are orthogonal for different j 's. We now show that this is the case provided that the $|\Phi_{ij}\rangle$ are chosen appropriately. In fact, let us take an arbitrary orthonormal basis $\{|\Phi_{ij}\rangle\}$ of \mathcal{H} and consider the Hermitian $n_B \times n_B$ matrix $S^{(i)}$ with coefficients given by the scalar products $S_{jk}^{(i)} = \langle \psi_{j|i} | \psi_{k|i} \rangle$. One can find a unitary matrix $V^{(i)}$ such that $\tilde{S}^{(i)} = (V^{(i)})^\dagger S^{(i)} V^{(i)}$ is diagonal and has non-zero diagonal elements in the first r_i rows, where r_i is the rank of $S^{(i)}$. Let $|\tilde{\Phi}_{ij}\rangle = \sum_{l=1}^{n_B} V_{lj}^{(i)} |\Phi_{il}\rangle$. Then $\{|\tilde{\Phi}_{ij}\rangle\}$ is an orthonormal basis of \mathcal{H} and $\sum_j |\tilde{\Phi}_{ij}\rangle \langle \tilde{\Phi}_{ij}| = \Pi_i$. Moreover, the vectors $|\tilde{\psi}_{j|i}\rangle = \langle \alpha_i | \sqrt{\rho} | \tilde{\Phi}_{ij} \rangle = \sum_{l=1}^{n_B} V_{lj}^{(i)} |\psi_{l|i}\rangle$ form an orthogonal set $\{|\tilde{\psi}_{j|i}\rangle\}_{j=1}^{r_i}$ and vanish for $j > r_i$. Therefore, for any fixed orthogonal family $\{\Pi_i\}_{i=1}^{n_A}$ of projectors of rank n_B , there exists an orthonormal basis $\{|\Phi_{ij}\rangle\}$ of \mathcal{H} such that (32) holds and the inequality in (33) is an equality. Substituting this equality into (31), one finds

$$F(\rho, \mathcal{C}_A(\alpha)) = \max_{\{\Pi_i\}} \sum_{i,j} \|\tilde{\psi}_{j|i}\|^2 = \max_{\{\Pi_i\}} \sum_i \text{tr}[\Pi_i \sqrt{\rho} |\alpha_i\rangle \langle \alpha_i| \otimes 1 \sqrt{\rho}], \quad (34)$$

which yields the result (20). The formula (23) is obtained by maximization over the basis $\{|\alpha_i\rangle\}$. \square

4.3. Closest A -classical states

The proof of the previous subsection also gives an algorithm to find the closest A -classical states to a given mixed state ρ . To this end, one must find the orthonormal basis $\{|\alpha_i^{\text{opt}}\rangle\}$ of \mathcal{H}_A maximizing $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\})$ in (24) and the optimal von Neumann measurement $\{\Pi_i^{\text{opt}}\}$ yielding the minimal error in the discrimination of the ensemble $\{\rho_i^{\text{opt}}, \eta_i^{\text{opt}}\}$ associated to $\{|\alpha_i^{\text{opt}}\rangle\}$ in equation (21).

Theorem 4. *The closest A -classical states to ρ are*

$$\sigma_\rho = \frac{1}{F_A(\rho)} \sum_{i=1}^{n_A} |\alpha_i^{\text{opt}}\rangle \langle \alpha_i^{\text{opt}}| \otimes \langle \alpha_i^{\text{opt}} | \sqrt{\rho} \Pi_i^{\text{opt}} \sqrt{\rho} | \alpha_i^{\text{opt}} \rangle, \quad (35)$$

where $\{|\alpha_i^{\text{opt}}\rangle\}_{i=1}^{n_A}$ and $\{\Pi_i^{\text{opt}}\}_{i=1}^{n_A}$ are such that $F_A(\rho) = \sum_i \text{tr}[\Pi_i^{\text{opt}} \sqrt{\rho} |\alpha_i^{\text{opt}}\rangle \langle \alpha_i^{\text{opt}}| \otimes 1 \sqrt{\rho}]$ (see equation (23)).

Proof. This follows directly from the proof of the previous subsection. Actually, by using the expression (30) of the optimal probabilities q_{ij} and the fact that the Cauchy–Schwarz

inequality (33) is an equality if and only if $|\beta_{j|i}\rangle = |\psi_{j|i}\rangle / \|\psi_{j|i}\|$ when $\|\psi_{j|i}\| \neq 0$, we conclude that the closest A -classical states to ρ are given by (1) with $|\alpha_i\rangle = |\alpha_i^{\text{opt}}\rangle$ and

$$q_i \sigma_{B|i} = \sum_{j=1}^{n_B} q_{ij} |\beta_{j|i}\rangle \langle \beta_{j|i}| = \frac{\sum_{j=1}^{n_B} |\tilde{\psi}_{j|i}\rangle \langle \tilde{\psi}_{j|i}|}{\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} \|\tilde{\psi}_{j|i}\|^2}. \quad (36)$$

The denominator is equal to $F_A(\rho)$, see (34). The numerator is the same as the second factor in the right-hand side of (35). For indeed, by construction $|\tilde{\psi}_{j|i}\rangle = \langle \alpha_i^{\text{opt}} | \sqrt{\rho} | \tilde{\Phi}_{ij}\rangle$ and $\sum_j |\tilde{\Phi}_{ij}\rangle \langle \tilde{\Phi}_{ij}| = \Pi_i^{\text{opt}}$. □

Let us stress that the optimal measurement $\{\Pi_i^{\text{opt}}\}$ and basis $\{|\alpha_i^{\text{opt}}\rangle\}$ may not be unique, so that ρ may have several closest A -classical states σ_ρ . This is the case for instance when ρ is a pure state with a degenerate maximal Schmidt eigenvalue, as we have seen in theorem 1. If $\sigma_\rho = \sum q_i |\alpha_i^{\text{opt}}\rangle \langle \alpha_i^{\text{opt}}| \otimes \sigma_{B|i}$ and $\sigma'_\rho = \sum q'_i |\alpha_i^{\text{opt}}\rangle \langle \alpha_i^{\text{opt}}| \otimes \sigma'_{B|i}$ are two closest A -classical states to ρ with the same basis $\{|\alpha_i^{\text{opt}}\rangle\}$ then so are all convex combinations $\sigma_\rho(\eta) = \eta \sigma_\rho + (1 - \eta) \sigma'_\rho$ with $0 \leq \eta \leq 1$. This fact is a direct consequence of the convexity of the Bures distance (property (i) in section 2), given that $\sigma_\rho(\eta) \in \mathcal{C}_A$. As a result, states ρ having more than one closest A -classical state will generally admit a continuous family of such states.

5. Conclusions

We have established in this paper a link between ambiguous QSD and the problem of finding the minimal Bures distance of a state ρ of a bipartite system AB to a state with vanishing quantum discord. More precisely, the maximal fidelity between ρ and an A -classical (i.e. zero discord) state coincides with the maximal success probability in discriminating the n_A states ρ_i^{opt} with prior probabilities η_i^{opt} given by equation (21), n_A being the space dimension of subsystem A (theorem 3). These states and probabilities depend upon an optimal orthonormal basis $\{|\alpha_i^{\text{opt}}\rangle\}$ of A . The closest A -classical states to ρ are, in turn, given in terms of this optimal basis and of the optimal von Neumann measurements in the discrimination of $\{\rho_i^{\text{opt}}, \eta_i^{\text{opt}}\}$ (theorem 4). Finally, we have shown that when $n_A \leq n_B$, the ‘most quantum’ states characterized by the highest possible distance to the set of A -classical states are the maximally entangled pure states, or convex combinations of such states with reduced B -states having supports on orthogonal subspaces. These states are also the most distant from the set of separable states.

As stated in the introduction, the QSD task can be solved for $n_A = 2$ states. Thus the aforementioned results provide a method to find the geometric discord D_A and the closest A -classical states for bipartite systems composed of a qubit A and a subsystem B with arbitrary space dimension $n_B \geq 2$. In particular, explicit formulae can be derived for two qubits in states with maximally mixed marginals and for $(n_B + 1)$ -qubits in the DQC1 algorithm [39]. For subsystems A with higher space dimensions $n_A > 2$, several open issues deserve further studies. Firstly, it would be desirable to characterize the ‘most quantum’ states when $n_A > n_B$. Secondly, it is not excluded that the specific QSD task associated to the minimal Bures distance admits an explicit solution. Thirdly, the relation of D_A with the geometric measure of entanglement in tripartite systems should be investigated; in particular, there may exist some inequality analogous to the monogamy relation [15] between the quantum discord and the entanglement of formation.

Let us emphasize that our results may shed new light on dissipative dynamical processes involving decoherence, i.e. evolutions toward classical states. In fact, our analysis may allow in some cases to determine the geodesic segment linking a given state ρ_0 with a non-zero discord to its closest A -classical state σ_{ρ_0} . Such a piece of geodesic is contained in the set of all states ρ having the same closest A -classical state $\sigma_\rho = \sigma_{\rho_0}$ as ρ_0 . It would be of interest to compare in specific physical examples these Bures geodesics with the actual paths followed by the density matrix during the dynamical evolution.

Acknowledgments

We are grateful to Maria de los Angeles Gallego for revising the derivation of equation (23) and for providing us some notes about the calculation of the geometric discord for Werner states. DS thanks Aldo Delgado for interesting discussions. We acknowledge financial support from the French project no. ANR-09-BLAN-0098-01, the Chilean Fondecyt project no. 100039 and the project Conicyt-PIA anillo no. ACT-1112 ‘Red de Análisis estocástico y aplicaciones’.

Appendix. Necessary and sufficient condition for the optimal success probability to be equal to the inverse number of states

Let $\{\rho_i\}_{i=1}^{n_A}$ be a family of n_A states on \mathcal{H} with prior probabilities η_i , where $n_A = N/n_B$ is a divisor of $\dim(\mathcal{H}) = N$. We assume that the ρ_i have ranks $\text{rank}(\rho_i) \leq n_B$ for any i . Let $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\})$ be the optimal success probability in discriminating the states ρ_i , defined by equation (20). We prove in this appendix that $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) = 1/n_A$ if and only if $\eta_i = 1/n_A$ for any i and all states ρ_i are identical.

The conditions $\eta_i = 1/n_A$ and $\rho_i = \rho$ are clearly sufficient to have $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) = 1/n_A$ (a measurement cannot distinguish the identical states ρ_i and thus cannot do better than a random choice with equal probabilities). We need to show that they are also necessary conditions. Let us assume $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) = 1/n_A$. The equality $\eta_i = 1/n_A$ for all i is obvious from the bounds $P_S^{\text{opt v.N.}}(\{\rho_i, \eta_i\}) \geq \eta_{\max} \equiv \max_i \{\eta_i\}$ and $\eta_{\max} \geq 1/n_A$ (see section 4.1). Therefore, according to our hypothesis, any orthogonal family $\{\Pi_i\}_{i=1}^{n_B}$ of projectors of rank n_B satisfies $\sum_i \text{tr}(\Pi_i \rho_i) = n_A P_S(\{\rho_i, \eta_i\}) \leq 1$. We now argue that the states ρ_i have ranges contained in a common subspace \mathcal{V} . In fact, let \mathcal{V} be the n_B -dimensional subspace of \mathcal{H} spanned by the eigenvectors of ρ_1 associated to the n_B highest eigenvalues (including degeneracies), and let us denote by Π_1 the projector onto \mathcal{V} . Then $\rho_1 \mathcal{H} \subset \mathcal{V}$ (since we have assumed $\text{rank}(\rho_1) \leq n_B$) and thus $\rho_1 = \Pi_1 \rho_1$. Thanks to the inequality above, $1 \geq \sum_i \text{tr}(\Pi_i \rho_i) \geq \text{tr}(\Pi_1 \rho_1) = 1$. It follows that $\text{tr}(\Pi_2 \rho_2) = 0$ for any projector Π_2 of rank n_B orthogonal to Π_1 . Hence ρ_2 , and similarly all ρ_i , $i = 3, \dots, n_A$, have ranges contained in \mathcal{V} . This proves the aforementioned claim.

In order to show that all the states ρ_i are identical, we further introduce, for each $1 \leq k \leq n_B$, some n_B -dimensional subspace $\mathcal{V}^{(k)}$ containing the eigenvectors associated to the k highest eigenvalues $\lambda_1 \geq \dots \geq \lambda_k$ of ρ_1 , the other eigenvectors being orthogonal to $\mathcal{V}^{(k)}$ (then $\mathcal{V}^{(n_B)} = \mathcal{V}$). We also choose a n_B -dimensional subspace $\mathcal{W}^{(k)} \subset \mathcal{H}$ orthogonal to $\mathcal{V}^{(k)}$ such that $\mathcal{W}^{(k)} \oplus \mathcal{V}^{(k)} \supset \mathcal{V}$. Let $\{\Pi_i^{(k)}\}_{i=1}^{n_A}$ be an orthogonal family of projectors of rank n_B such that $\Pi_1^{(k)}$ and $\Pi_2^{(k)}$ are the projectors onto $\mathcal{V}^{(k)}$ and $\mathcal{W}^{(k)}$, respectively. Then

$$1 \geq \sum_i \text{tr}(\Pi_i^{(k)} \rho_i) = \text{tr}(\Pi_1^{(k)} \rho_1) + \text{tr}[(1 - \Pi_1^{(k)}) \rho_2] = 1 + \lambda_1 + \dots + \lambda_k - \text{tr}(\Pi_1^{(k)} \rho_2), \quad (\text{A.1})$$

where we used $\sum_i \Pi_i^{(k)} = 1$ and $\rho_i \mathcal{H} \subset \mathcal{W}^{(k)} \oplus \mathcal{V}^{(k)}$ in the first equality. By virtue of the min-max theorem, $\text{tr}(\Pi_1^{(k)} \rho_2)$ is smaller than the sum of the k highest eigenvalues of ρ_2 (including degeneracies). By (A.1), this sum is larger than the sum $\lambda_1 + \dots + \lambda_k$ of the k highest eigenvalues of ρ_1 . By exchanging the roles of ρ_1 and ρ_2 , we obtain the reverse equality. Since moreover k is arbitrary between 1 and n_B , it follows that ρ_1 and ρ_2 have identical eigenvalues. By using (A.1) again, $\text{tr}(\Pi_1^{(k)} \rho_2)$ is equal to the sum of the k highest eigenvalues of ρ_2 . Hence the k corresponding eigenvectors of ρ_2 are contained in the k -dimensional subspace $\mathcal{V}^{(k)} \cap \mathcal{V}$. Since k is arbitrary, this proves that ρ_1 and ρ_2 have identical eigenspaces. Therefore $\rho_1 = \rho_2$. Repeating the same argument for the other states ρ_i , $i \geq 3$, we obtain $\rho_1 = \dots = \rho_{n_A}$.

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