Classical extension of quantum-correlated separable states

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Li and Luo [*Phys. Rev. A* **78** (2008), 024303] discovered a remarkable relation between discord and entanglement. It establishes that all separable states can be obtained via reduction of a classicaly-correlated state 'living' in a space of larger dimension. Starting from this result, we discuss here an *optimal classical extension* of separable states and explore this notion for low-dimensional systems. We find that the larger the dimension of the classical extension, the larger the discord in the original separable state. Further, we analyze separable states of maximum discord in $\mathbb{C}^2 \otimes \mathbb{C}^2$ and their associated classical extensions showing that, from the reduction of a classical state in $(\mathbb{C}^2 \otimes \mathbb{C}^3) \otimes \mathbb{C}^2$, one can obtain a separable state of maximum discord in $\mathbb{C}^2 \otimes \mathbb{C}^2$.

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I. INTRODUCTION

Entanglement and discord are known to be quantum resources for implementing information-computation protocols (ICP) with a higher efficiency than that attainable via classical resources (for a complete review see [15; 28] and references therein). The entanglement usefulness for such protocols has been extensively documented. As for discord's, one can cite, for instance, [3; 5; 6; 8; 13; 14; 19; 25; 26; 30], although some controversy arises regarding its *ICP*necessity [10; 12; 37]. It is clear, however, that entanglement and discord capture different features of the quantum world. Discord captures the fact that all classical states must be information-wise accessible to local observers. Thus, it is accepted that the dichotomy cassical/non-classical can be treated in similar fashion as that regarding discord/nodiscord. For a bipartite system one associates a Hilbert space $\mathcal{H}^{AB} = \mathcal{H}^A \otimes \mathcal{H}^B$. A system's state is represented by a positive semi-definite, hermitic operator of trace unity acting on \mathcal{H}^{AB} . If $\{\Pi_i^A\}$ and $\{\Pi_i^B\}$ are complete projective measurements over \mathcal{H}^A and \mathcal{H}^B , respectively, then [23; 28]

- If $\sigma^{AB} = \sum_i p_i \prod_i^A \otimes \rho_i^B$, the state is *classical-quantum* (CQ): there exists a basis in A for which the locally accessible information is maximal and, for an external observer, such information can be obtained without perturbing the composite system;
- If $\sigma^{AB} = \sum_{i,j} p_{ij} \Pi_i^A \otimes \Pi_j^B$, the state is *classical-classical* (CC): the locally accessible information is maximal for A and B, can be obtained without perturbing the composite system.

In analogous fashion, one defines quantum-classical (QC) states via interchange of A and B. We will generically speak of classical states when referring to any of these three sub-types. Moreover, we will speak of the set CC of classical-classical states, the set CQ (QC) of classical-quantum (quantum-classical) states, and the set S of separable states.

From the above definitions one easily ascertains that, even if the sets CC and CQ are included within the convex S, neither CC nor CQ (or QC) constitute a convex set by themselves. Precisely, this lack of convexity implies the existence of classical states that, via mixing amongst themselves, may give rise to non-classical states, endowed with discord [20]. This fact underlies the link between separability and classicality observed by Li and Luo in [20]: a bipartite state is separable iff it can be obtained as the reduction of a CS of larger dimension, respecting the original bipartition. This assertion is the source of the present investigation.

Herefrom, we speak of CS when referring to CQ states. Thus, given a bipartite state ρ^{ab} , with $\rho^a := \operatorname{tr}_b[\rho^{ab}]$ and $\rho^b := \operatorname{tr}_a[\rho^{ab}]$, we compute the discord [29]

$$\delta_a(\rho^{ab}) := I(\rho^{ab}) - C(\rho^{ab}), \qquad (1)$$

where

$$I(\rho^{ab}) := S(\rho^{a}) + S(\rho^{b}) - S(\rho^{ab}),$$
(2)

is the quantum mutual information of the bipartite state and

$$C(\rho^{ab}) := S(\rho^b) - \min_{\{M_i^a\}} S(\rho^b | \rho^a)$$
(3)

is the corresponding classical information for that state. $S(\cdot)$ is von Neumann's entropy (logarithms of basis 2) and $\{M_i^a\}$ a set of positive operators representing a generalized measurement over \mathcal{H}^a . $S(\rho^b|\rho^a) := S(\rho^{ab}) - S(\rho^a)$ is the conditional quantum entropy.

In Section II we shall introduce and adapt the Li-Luo's relation between separability and classicality to our present needs. We introduce in Sect. III the notion of *optimum classical extension* for separable states as that of smallest dimensionality. In Sect. IV we will show that, for low-dimensionality separable states ($\mathbb{C}^2 \otimes \mathbb{C}^2$), it is possible to find classical extensions that improve on the ones in [20]. Some explicit examples will be given. In Sect. V we discuss the existence of separable states with maximum discord in arbitrary dimensions and consider their relation with the notions of: (i) mutually unbiased basis and (ii) generalized measurements that are both symmetric and informationally complete. Some conclusions are drawn in Sect. VI.

II. SEPARABILITY VS. CLASSICALITY: LI-LUO'S RELATION

Monogamy is a fundamental feature of entanglement. Given a multipartite system, if two of its parties are maximally entangled, then they can not be entangled with a third party. Given a composite state σ^{AB} , with $\{A_i\}$ and $\{B_i\}$



Fig. 1 A separable state can always be obtained as the reduction of a classically correlated state embedded in a space of larger dimension. Li-Luo's extension algorithm provides the manner in which to determine the classical extension of any given separable state.

parts of A and B, respectively, a monogamous entanglement measure E is such that [18; 38]

$$E(A:B) \ge \sum_{i,j} E(A_i:B_j), \qquad (4)$$

where E(x : y) yields the entanglement between x and y, $E \ge 0$. It follows from (4) that, given σ^{AB} not entangled, none of its reductions will exhibit entanglement, i.e.,

$$E(A:B) = 0 \implies E(A_i:B_j) = 0 \quad \forall i,j.$$

$$\tag{5}$$

Reciprocally, an entangled state $\rho^{A_i B_j}$ can not be extended to a non-entangled one σ^{AB} . The vocable *extension* will be the subject of the precise definition 1 below.

In general, discord does not obey inequalities of the type (4) [2; 11; 31; 36]. Li and Luo showed that any bipartite separable state *can* be extended to a CC state in a space of larger dimension [20] (Fig. 1). They studied the 'separable \rightarrow classical-classical' extension. We, instead, are here interested in the separable \rightarrow classical-quantum extension. The following theorem explains just how to find the desired extension [20]:

Theorem 1. A bipartite state ρ^{ab} is separable in $\mathcal{H}^{ab} = \mathcal{H}^a \otimes \mathcal{H}^b$ iff there exists a CQ state σ^{Ab} in $\mathcal{H}^{Ab} = \mathcal{H}^A \otimes \mathcal{H}^b$, with $\mathcal{H}^A = \mathcal{H}^a \otimes \mathcal{H}^{\bar{a}}$ such that

$$\rho^{ab} = tr_{\bar{a}}[\sigma^{Ab}]. \tag{6}$$

Here, $\mathcal{H}^{\bar{a}}$ is an auxiliary Hilbert space for party a, while $tr_{\bar{a}}$ is the partial trace over $\mathcal{H}^{\bar{a}}$.

Proof. The demonstration is adapted from [20]. We start with an arbitrary separable state

$$\rho^{ab} = \sum_{k=1}^{K} p_k \rho_k^a \otimes \rho_k^b \,. \tag{7}$$

Each ρ_k^a can be expanded in its eigen-basis $\{|\alpha_{ku}\rangle\}$ so that (7) can be cast as

$$\rho^{ab} = \sum_{k} \sum_{u} p_k a_{ku} P^a_{ku} \otimes \rho^b_k \,, \tag{8}$$

where we define $P_{ku}^a := |\alpha_{ku}\rangle \langle \alpha_{ku}|$. Our extension demands consideration of an auxiliary system \bar{a} , defined in $\mathcal{H}^{\bar{a}} = \mathbb{C}^K$, such that $\{|k\rangle\}$, with k = 1, 2...K an orthonormal basis of \mathbb{C}^K . Then,

$$\left\{ \Pi_{ku}^{A} := \left| k \right\rangle \left\langle k \right| \otimes P_{ku}^{a} \right\},\tag{9}$$

is an orthogonal set of $\mathcal{H}^A := \mathcal{H}^{\bar{a}} \otimes \mathcal{H}^a$. Extension to a complete projective measurement in the extended space is feasible. Define the extended state (in $(\mathbb{C}^K \otimes \mathcal{H}^a) \otimes \mathcal{H}^b$)

$$\sigma^{Ab} := \sum_{k,u} p_k a_{ku} \Pi^A_{ku} \otimes \rho^b_k \,, \tag{10}$$

$$\operatorname{tr}_{\bar{a}}[\sigma^{Ab}] = \sum_{k,u} p_k a_{ku} P^a_{ku} \otimes \rho^b_{kv} = \rho^{ab} \,, \tag{11}$$

as we wished to show.

This classical-extension construction-process will be called, either *Li-Luo's extension* or *Li-Luo's algorithm* (LLA). Some observations are in order.

- Our extension depends on the separable decomposition of the original state (see (7)). The party one wishes to make classical is extended using an ancilla in \mathbb{C}^K , with K the number of terms in the decomposition. Luo *et al.* want instead a CC state which needs two ancillae (one per party) in \mathbb{C}^K .
- Extending party b does not change its classical nature when 'observed' from a (with a local measurement on a). The b-extension does not modify the classical-quantum character of the bipartite system. Conversely, assume the existence of a classical extension ω^{aB} in $\mathcal{H}^{aB} = \mathcal{H}^a \otimes \mathcal{H}^B$, with $\mathcal{H}^B := \mathcal{H}^b \otimes \mathcal{H}^{\bar{b}}$, compatible with a given separable state ρ^{ab} . In such a case, we can write

$$\omega^{aB} = \sum_{m,n} \gamma_{mn} \Pi^a_m \otimes \omega^B_n \,, \tag{12}$$

and tracing over the ancilla we obtain the classical state $\rho^{ab} = \sum_{m,n} \gamma_{mn} \Pi_m^a \otimes \omega_n^b$, with $\omega^b := \operatorname{tr}_{\bar{b}}[\omega^B]$. Thus, ρ^{ab} can not be an arbitrary separable state (it is classical).

• The LLA does not entangle the ancilla with the original system, that is, a with \bar{a} . Actually, from (9) and (10) it follows that

$$\sigma^{a\bar{a}} = \operatorname{tr}_{b}[\sigma^{Ab}] = \sum_{k} p_{k} \rho_{k}^{a} \otimes |k\rangle \langle k|, \qquad (13)$$

is the separable state from A. More general classical extensions (see Definition 1 in Sect. III) in which \bar{a} is entangled with a are possible. They would limit, though, the a-b correlation-capacity.

- The LLA is such that the final state does not exhibit any discord with respect to the ancilla: $\delta_{\bar{a}}(\bar{a}:\cdot) = 0$.
- Given a classical state, any reduction that preserves the bipartition gives rise to a separable state. Corollary: it is impossible to find a classical extension of an entangled state.

The statements above imply that LLA can not be unique, except for special separable states: those whose convex decomposition of product states is itself unique, which happens for pure states. Since separable pure states are product states, they are of no interest for us here.

A relevant question is whether one can find an *optimal* classical extension of a given separable state, where the vocable 'optimal' refers to some extremal criterion. One could define it, for instance, as being the classical extension of smallest dimension. We will tackle this issue with greater precision below and study the relation between optimality of the classical extension of separable states and their quantum correlations.

III. OPTIMAL EXTENSION FROM SEPARABLE STATE TO CLASSICAL STATE

Given a bipartite separable state ρ^{ab} in $\mathcal{H}^{ab} = \mathcal{H}^a \otimes \mathcal{H}^b$, it is always possible to find a decomposition of the form [9; 21; 39]

$$\rho^{ab} = \sum_{k=1}^{\ell} p_k \left| a_k \right\rangle \left\langle a_k \right| \otimes \left| b_k \right\rangle \left\langle b_k \right|, \tag{14}$$

where $\operatorname{rk}[\rho^{ab}] \leq \ell \leq (\operatorname{rk}[\rho^{ab}])^2$. Here, ℓ is the states's *cardinality* or *length* and represents the least number of product states needed for the purpose. Eq. (14) is the *optimum decomposition* of ρ^{ab} . For separable states in $\mathbb{C}^2 \otimes \mathbb{C}^2$, one can always find a decomposition of the type (14) with $\ell = \max \{\operatorname{rk}[\rho^{ab}], \operatorname{rk}[(\rho^{ab})^{Tb}]\} \leq 4$, where $(\rho^{ab})^{Tb}$ is the partial transpose of ρ^{ab} [33].

It is noteworthy that there are other possible decomposition schemes for bipartite states, even in the case of nonseparable states. Luo and Sun showed the equivalency of several non-broadcasting theorems using a particular form of bipartite decomposition [24].

Let us introduce some useful definitions:

Definition 1. Given the bipartite separable state ρ^{ab} in $\mathcal{H}^a \otimes \mathcal{H}^b$, we say that σ^{AB} in $\mathcal{H}^A \otimes \mathcal{H}^B$ is a classical extension of ρ^{ab} if

$$tr_{\bar{a},\bar{b}}[\sigma^{AB}] = \rho^{ab},\tag{15}$$

and σ^{AB} is classical. The partial trace is taken over $\mathcal{H}^{\bar{a}}$ and $\mathcal{H}^{\bar{b}}$, the extensions of ρ^{ab} , with $\mathcal{H}^{A} = \mathcal{H}^{a} \otimes \mathcal{H}^{\bar{a}}$ and $\mathcal{H}^{B} = \mathcal{H}^{b} \otimes \mathcal{H}^{\bar{b}}$.

Here, we could distinguish three possible extensions: from separable states to CC, CQ or QC states, respectively. As previously stated, we will be interested in CQ-extensions. Our following results, though, could be easily generalized to QC- or CC-extensions.

Definition 2. Given ρ^{ab} separable in $\mathcal{H}^a \otimes \mathcal{H}^b$, we say that σ^{AB} in $\mathcal{H}^A \otimes \mathcal{H}^B$ is the **optimal classical extension** of ρ^{ab} if: (a) σ^{AB} is a classical extension of ρ^{ab} ; and (b) for any other classical extension $\omega^{A'B'}$ in $\mathcal{H}^{A'} \otimes \mathcal{H}^{B'}$, $dim[\mathcal{H}^{A'} \otimes \mathcal{H}^{B'}] \geq dim[\mathcal{H}^A \otimes \mathcal{H}^B]$.

In general, the *best* Li-Luo's extension is that made from the optimum decomposition: then the ancilla is \mathbb{C}^{ℓ} , with ℓ the length of the state to be extended. However, our Definition 2 opens the door to possible extensions not foreseen by the LLA, since it makes no reference to any particular way of determining the extension. We may have, for instance, extensions that entangle a with \bar{a} . Alternatively, one may think of extensions that exhibit discord with respect to the ancilla (i.e., $\delta_{\bar{a}}(\bar{a}:\cdot) \neq 0$). None of them are contemplated in the LLA. Consequently, applying LLA to the optimum decomposition *does not guarantee* an optimal classical extension. Since we lack a closed formula for the optimum decomposition of arbitrary separable states, we can not find neither the best Li-Luo's extension for arbitrary states, nor even less the optimal classical extension. We show below, however, how to set dimensionality bounds to our extensions.

A. Bounds for optimal extension

Theorem 1 says something regarding the dimensionality of the optimal classical extension. Since $\operatorname{rk}[\rho^{ab}] \leq \ell \leq \operatorname{rk}[\rho^{ab}]^2$, using the optimum decomposition, Li-Luo's algorithm yields a classical extension for which the ancilla's dimension is $d_{\bar{a}}^{Luo} := \dim[\mathbb{C}^{\ell}] = \ell$, so that $\operatorname{rk}[\rho^{ab}] \leq d_{\bar{a}}^{Luo} \leq \operatorname{rk}[\rho^{ab}]^2$. The optimal classical extension might improve on Li-Luo's, in which case $d_{\bar{a}}^{opt} < d_{\bar{a}}^{Luo}$. Regarding our ancilla's dimension and with regards to bipartite separable states, the next proposition establishes a general lower bound.

Proposition 1. Let ρ^{ab} be separable in $\mathcal{H}^a \otimes \mathcal{H}^b$, with length ℓ , and consider the classical extension σ^{Ab} in $(\mathcal{H}^a \otimes \mathcal{H}^{\bar{a}}) \otimes \mathcal{H}^b$, as in Definition 1. Then, the ancilla's dimension obeys

$$d_{\bar{a}} \ge \lceil f(d_a, d_b, \ell) \rceil \tag{16}$$

where $d_x := \dim[\mathcal{H}^x]$ and $\lceil y \rceil = \min\{n \in \mathbb{Z} | y \leq n\}$. The function $f(d_a, d_b, \ell)$ is the only positive root of the quadratic polynomial $P_2(x) := c_2 x^2 + c_1 x + c_0$, with $c_2 := d_a^2$, $c_1 := d_a(d_b^2 - 1)$ and $c_0 := \ell(3 - 2d_a - 2d_b)$.

Proof. Let ℓ stand for the length of ρ^{ab} (see Eq. (14)), this separable state can be expressed via

$$\rho^{ab} = \sum_{k=1}^{\ell} p_k P_k^a \otimes P_k^b \,, \tag{17}$$

with $\{P_k^a\}_{1 \le k \le \ell}$ and $\{P_k^b\}_{1 \le k \le \ell}$ projector-sets of rank one in \mathcal{H}^a and \mathcal{H}^b , respectively. The number of independent real parameters needed for this state's determination is

$$\ell - 1 + \ell (2d_a + 2d_b - 4). \tag{18}$$

d	$d_{ar{a}}^{\min}$	$d^{Luo}_{\bar{a}}$
1	1	1
2^*	2	4
3	[2,8]	[9,81]
4	[3, 13]	[16, 256]

Tab. I Ancilla's dimension for the classical extension of a bipartite separable state ρ^{ab} with $d_a = d = d_b$ and maximum rank. 2nd. column: range of values allowed by Eq. (16). 3rd. column: Li-Luo's extension values from the optimum decomposition of ρ^{ab} . *For d = 2 we us the result from Sanpera et al. stating that for these states $\ell = 4$ [33].

This is obtained as follows. The set $\{p_k\}_{1 \le k \le \ell}$ with the condition $\sum_k p_k = 1$ is determined with $\ell - 1$ quantities. For each pure state P_k^a one needs $2d_a - 2$ real parameters. Similar for P_k^b . Additionally, given the classical state σ^{Ab} we can cast it as

$$\sigma^{Ab} = \sum_{m=1}^{d_A} q_m \Pi_m^A \otimes \rho_m^b \,, \tag{19}$$

with $\{\Pi_m^A\}$ a basis of rank one orthogonal projectors in \mathcal{H}^A , and $\{\rho_m^b\}$ a set of states in \mathcal{H}^b . The index *m* ranges between 1 and $d_A = d_a d_{\bar{a}}$. Accordingly, the set $\{q_m\}$ yields $d_A - 1$ independent real parameters. The set $\{\Pi_m^A\}$ yields $d_A(2d_A - 2)$ real parameters and we need to discount the $d_A(d_A - 1)$ restrictions imposed by the commutation rules $[\Pi_m^A, \Pi_n^A] = 0$, with m > n. Note that there are only $\frac{1}{2}d_A(d_A - 1)$ different commutation rules, but each complex equation $[\Pi_m^A, \Pi_n^A] = 0$ counts as two real constraints. In conclusion, $\{\Pi_m^A\}_{1 \le m \le d_A}$ has $d_A(d_A - 1)$ independent real parameters. Another way to see that $d_A(d_A - 1)$ is the correct amount of independent real parameters is to take $\{\Pi_m^A\}$ as the rows of a unitary matrix in $\mathbb{C}^{d_A \times d_A}$. Such a matrix has d_A^2 independent real parameters, but we must subtract d_A arbitrary independent phases, yielding the correct answer.

Also, each ρ_m^b is an arbitrary state of *b* that is cast as $\rho_m^b = \sum_s \beta_s^{(m)} \Pi_s^{b(m)}$ and is determined by $d_b - 1 + d_b(d_b - 1)$ independent real parameters. Finally, the state σ^{Ab} is determined by

$$d_A^2 + (d_b^2 - 1)d_A - 1 \tag{20}$$

real parameters. The CQ state σ^{Ab} requires a number of parameters greater or equal (Eq. (20)) to that for ρ^{ab} (Eq. (18)). One ends up with the above indicated bound for $d_{\bar{a}}$.

The following observations are in order.

- The minimum of our bound on $d_{\bar{a}}$ (16) is always smaller than ℓ . If $d_{\bar{a}}^{\min} := \lceil f(d_a, d_b, \ell) \rceil$ is the minimum of (16) for given d_a , d_b and ℓ , and $d_{\bar{a}}^{opt}$ is the unknown theoretical minimum for $d_{\bar{a}}$, then $d_{\bar{a}}^{\min} \le d_{\bar{a}}^{opt} \le \ell = d_{\bar{a}}^{Luo}$.
- $f(d_a, d_b, \ell)$ grows monotonously with ℓ , for all $\ell \ge 1$ and $d_a, d_b \ge 1$. Thus, the condition $\operatorname{rk}[\rho^{ab}] \le \ell \le \operatorname{rk}[\rho^{ab}]^2$ establishes both a minimum and a maximum to the bound of the proposition,

$$\left\lceil f(d_a, d_b, r_{ab}) \right\rceil \le d_{\bar{a}}^{\min} \le \left\lceil f(d_a, d_b, r_{ab}^2) \right\rceil,\tag{21}$$

with $r_{ab} := \operatorname{rk}[\rho^{ab}]$. For states of maximum rank i.e., $\operatorname{rk}[\rho^{ab}] = d_a d_b$, the bounds depend on the dimensions of the parties a and b. In particular, in the 2 qubits case one has $\ell = \max \{\operatorname{rk}[\rho^{ab}], \operatorname{rk}[(\rho^{ab})^{Tb}]\} \leq 4$. Thus, for extending 2 qubits separable states of maximum rank we find $d_{\bar{a}} \geq d_{\bar{a}}^{\min} = 2$.

- For full-rank states, $\lceil f(d_a, d_b, d_a d_b) \rceil$ and $\lceil f(d_a, d_b, d_a^2 d_b^2) \rceil$ are the limit-values for $d_{\bar{a}}^{\min}$. Values of $d_{\bar{a}}^{\min}$ are always smaller than those obtained via LLA (Tab. I).
- For systems of greater dimension, consider the case $d_a = d_b = d$ with full-rank states. From the asymptotic expansion of (16) we deduce that

$$4 \lesssim d_{\bar{a}}^{\min} \lesssim 2 \, d^{3/2} \, (d \to \infty) \,, \tag{22}$$

considering that $r_{ab} \leq \ell \leq r_{ab}^2$. For these states $d^2 \leq d_{\bar{a}}^{Luo} = \ell \leq d^4$.

The proposition establishes a lower bound to the ancilla's dimensionality in the extension from a separable state to a classical-quantum one. If we wished for an classical-classical optimal extension, we will deal with a state of the form σ^{AB} = Σ_{m,n} q_{mn}Π^A_m ⊗ Π^B_n. The number of real parameters of σ^{AB} is given by i) d_Ad_B - 1 for {p_{mn}}, ii) d_A(d_A - 1) for {Π^A_m}, and iii) d_B(d_B - 1) for {Π^B_n}. The bounds for d_ā and d_b are obtained in analogous fashion.

From these consideration it follows that, even if the optimal extension remains unknown, Li-Luo's classical extension, from the optimum decomposition of the separable state, yields a state that may differ from the one providing the best classical extension. We specialize to 2 qubits next and find more specific results.

IV. CLASSICAL EXTENSION OF SEPARABLE STATES IN $\mathbb{C}^2\otimes\mathbb{C}^2$

We investigate now possible classical extensions of two-qubits separable states, with emphasis on states of maximum discord.

A. Extensions in Li-Luo's scheme

In order to find states of maximum discord let us revisit the relation between discord and entanglement. We are interested in such states for a fixed rank of the density matrix. In [22], Luo compares the discord and the entanglement of formation for Werner states of two qubits. Moreover, in [32], the authors display such relation for randomly generated two-qubits states. Fig. 2 reproduces such relation, by numerically computing the discord for 3×10^6 states, and encounter those families that bound by below and by above the graph discord vs. entanglement. The family

$$\rho(\beta) := \frac{1}{2} \begin{pmatrix} \beta & 0 & 0 & \beta \\ 0 & 1 - \beta & 1 - \beta & 0 \\ 0 & 1 - \beta & 1 - \beta & 0 \\ \beta & 0 & 0 & \beta \end{pmatrix},$$
(23)

with $0 \leq \beta \leq 1$ gives a lower bound for any degree of entanglement. The states

$$\rho_{\alpha} := \frac{1}{2} \begin{pmatrix} \alpha & 0 & 0 & \alpha \\ 0 & 1 - \alpha & 0 & 0 \\ 0 & 0 & 1 - \alpha & 0 \\ \alpha & 0 & 0 & \alpha \end{pmatrix},$$
(24)

with $0 \le \alpha \le 1$, give an upper bound for states whose entanglement ranges between 0 and 0.620. For larger entanglement this limit is provided by Werner states (see Fig. 2)

$$\rho_{\xi} := (1 - \xi) \frac{\mathbb{1}}{4} + \xi |\psi\rangle \langle\psi| , \qquad (25)$$

with $-1/3 \leq \xi \leq 1$ and $|\psi\rangle := (|01\rangle - |10\rangle)/\sqrt{2}$. All these families are subsets of the so-called maximally mixed marginal states, for which an analytical discord-expression is known. The authors of [32] calculate the discord for the states ρ_{α} , finding

$$\delta_a(\alpha) = (1 - \alpha)\log(1 - \alpha) + \alpha\log(\alpha) + (1 + \alpha) - \frac{1 - \bar{\alpha}}{2}\log(1 - \bar{\alpha})\frac{1 + \bar{\alpha}}{2}\log(1 + \bar{\alpha}),$$
(26)

where $\bar{\alpha} := \max\{|\alpha|, |2\alpha - 1|\}$. These states' concurrence is $C(\alpha) = \max\{0, 2\alpha - 1\}$. The states α are separable for $\alpha \in (0, \frac{1}{2}]$. Of these separable ρ_{α} , the one of largest discord corresponds to $\alpha = \frac{1}{3}$. One has $\delta_a(\rho_{\alpha})|_{\alpha=\frac{1}{3}} = \frac{1}{3}$ (Fig. 3). Note that the optimization can be achieved in analytic fashion (Cf. Eq. (26)). Accordingly, the state

$$\rho_{\max}^{\ell=4} := \rho_{\alpha} \big|_{\alpha=\frac{1}{3}} = \frac{1}{6} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$
(27)



Fig. 2 Discord vs. Entanglement of formation for bipartite states in $\mathbb{C}^2 \otimes \mathbb{C}^2$. Dots correspond to 3×10^6 randomly generated states according to Haar's measure. We report results for 1×10^6 rank 2-states, 1×10^6 of rank 3, and 1×10^6 of rank 4. Green and blue curves correspond, respectively, to the families ρ_{α} and ρ_{β} .



Fig. 3 Discord and entanglement of formation for states of the family ρ_{α} .

is representative of maximum discord-separable states in $\mathbb{C}^2 \otimes \mathbb{C}^2$. We have $\operatorname{rk}[\rho_{\max}] = 3$ and $\operatorname{rk}[\rho_{\max}^{Tb}] = 4$, so one expects to find a separable decomposition of the type (14), with $\ell = 4$. Thus, $\rho_{\max}^{\ell=4}$ can be classically extended via LLA with $d_{\bar{a}}^{Luo} = 4$. On the other hand, it is possible to find classical states of smaller dimension whose separable reductions reaches a discord-amount close to the maximum. For instance, the state

$$\rho_{\max}^{\ell=3} := \rho_{\alpha} \big|_{\alpha=\frac{1}{2}} = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$
(28)

has a discord that equals 93% of the discord accrued to the state $\rho_{\max}^{\ell=4}$ and can be classically extended with $d_{\bar{a}}^{Luo} = 3$. Similarly, the state

$$\rho_{\max}^{\ell=2} := \frac{1}{2} (|0\rangle \langle 0| \otimes |0\rangle \langle 0| + |+\rangle \langle +| \otimes |1\rangle \langle 1|), \qquad (29)$$

that can be classically extended with $d_{\bar{a}}^{Luo} = 2$, exhibit a discord equal to 61 % of that of $\rho_{\max}^{\ell=4}$ (see Tab. II).

$\ell (= d^{Luo}_{\bar{a}})$	$\delta_a(a:b)$	
4	$\frac{1}{3} \approx 0.3333$	
3	$\left(\frac{3}{4}\right)\log\left(\frac{4}{3}\right) \approx 0.3113$	
2	$2 - (\frac{\sqrt{2}}{2}) \log(3 + 2\sqrt{2}) \approx 0.2018$	
1	0	

Tab. II Discord for maximally discording separable states in $\mathbb{C}^2 \otimes \mathbb{C}^2$ according to their length.

Separable decomposition of $\rho_{\max}^{\ell=3}$.

We continue with the issue of expressing, for different ranks, states of large discord. For $\ell = 3$ the maximum discord is 0.3113, a value reached by the state $\rho_{\max}^{\ell=3}$ of Eq. (28). It's easy to verify that

$$\rho_{\max}^{\ell=3} \cong \frac{1}{4} \left(P_0 \otimes P_0 + P_1 \otimes P_1 + P_+ \otimes P_+ + P_- \otimes P_- \right)$$
(30)

with $\{P_j\}_{j=0,1,+,-,r,l}$ the eigen-projectors of σ_z and σ_x , respectively. By ' \cong ' we indicate an equivalence up to unitary transformations. Eq. (30) is a possible separable decomposition, but it is not optimal. To find the separable optimum decomposition of a given bipartite state one proceeds as described in [33]. Denoting by

$$|\theta,\phi\rangle := \cos\left(\frac{\theta}{2}\right)|0\rangle + \exp(i\phi)\sin\left(\frac{\theta}{2}\right)|1\rangle ,$$
 (31)

an arbitrary pure state in \mathbb{C}^2 , we find that the set $\mathcal{W} = \{|0,0\rangle, |\frac{2\pi}{3}, 0\rangle, |\frac{2\pi}{3}, \pi\rangle\}$ defines the optimum decomposition

$$\rho_{\max}^{\ell=3} \cong \frac{1}{3} \sum_{i=1}^{3} W_k \otimes W_k \tag{32}$$

with $W_k = |w_k\rangle \langle w_k|$ and $|w_k\rangle \in \mathcal{W}$. We repeat things below for $\rho_{\max}^{\ell=4}$.

Separable decomposition of $\rho_{\max}^{\ell=4}$. It is easy to see that $\rho_{\max}^{\ell=4} \cong \rho_{\alpha}$, with $\alpha = \frac{1}{3}$, and that it can be decomposed as

$$\rho_{\max}^{\ell=4} \cong \frac{1}{6} \left(P_0 \otimes P_0 + P_1 \otimes P_1 + P_+ \otimes P_+ + P_- \otimes P_- + P_r \otimes P_r + P_l \otimes P_l \right) \,, \tag{33}$$

with $\{P_j\}_{j=0,1,+,-,r,l}$ the eigen-projectors of σ_z , σ_x and σ_y , respectively. We seek now for the optimum decomposition. For simplicity's sake, instead of $\rho_{\max}^{\ell=4}$ we consider

$$\tilde{\rho}_{\max} := \frac{1}{6} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} ,$$
(34)

obtained from $\rho_{\max}^{\ell=4}$ via a local (in b) unitary transformation, which does not change the discord. This transformation consists of a swap in b,

$$U_b := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{35}$$

such that $\tilde{\rho}_{\max} = U \rho_{\max}^{\ell=4} U^{\dagger}$, with $U := \mathbb{1}_a \otimes U_b$ and $\mathbb{1}_a$ the identity in a. Defining $\mathcal{Z} = \{ |0,0\rangle, |\theta^*, 0\rangle, |\theta^*, \frac{2\pi}{3}\rangle, |\theta^*, \frac{4\pi}{3}\rangle \}$, with $\theta^* = \arccos(-\frac{1}{3})$, the optimum decomposition of $\tilde{\rho}_{\max}$ is

$$\tilde{\rho}_{\max} = \frac{1}{4} \sum_{k=1}^{4} Z_k \otimes Z_k \,, \tag{36}$$



Fig. 4 So as to extend the 2 qubits, maximally discordant separable state $\rho_{\max}^{\ell=4}$, Li-Luo's algorithm employs an ancilla in \mathbb{C}^4 . In the optimal scheme, it is possible to find a compatible extension in \mathbb{C}^3 .

with $Z_k = |z_k\rangle \langle z_k|$ and $|z_k\rangle \in \mathcal{Z}$.

Note that all states exhibit the same overlap among themselves, i.e., that $|\langle \theta_k, \phi_k | \theta_{k'}, \phi_{k'} \rangle|^2 = c, \forall k \neq k' \ (c = 1/3)$. In terms of a parameterization of states on the Bloch sphere, where $r_k = (\sin(\theta_k) \cos(\phi_k), \sin(\theta_k) \sin(\phi_k), \cos(\theta_k))$ is the position-vector associated to $|\theta_k, \phi_k\rangle$, the angle between two different states is always $2\pi/3$. Summing up, the pure states in $\tilde{\rho}_{max}$ can be associated to the four vertices of the regular 3-simplex in a three-dimensional space (a tetrahedron). As shown by Eq. (36), both subsystems have the same pure states. Thus, the state of maximum discord for 2 qubits can be expressed as the equal-weights, convex combination of 4 symmetric product states given by 4 pure states that are maximally distinguishable. Given this states' symmetry in both qubits' spaces, any choice of projective measurement will yield the same discord.

B. Optimal classical extensions

As suggested by table I, it is possible to improve on the results of the LLA. Notice from Fig. 4 that it is possible to classically extend $\rho_{\max}^{\ell=4}$ with a qutrit, while the LLA needs 2 qubits. Similarly, we can extend $\rho_{\max}^{\ell=3}$ with 1 qubit, versus the 1 qutrit required by the LLA. These new extensions were numerically obtained via Monte Carlo so as to find the reductions in $\mathbb{C}^2 \otimes \mathbb{C}^2$ [of classical states in $\mathbb{C}^{d_A} \otimes \mathbb{C}^2$] of largest discord. One starts building up a classical state $\sigma_{Ab} = \sum_k p_k \Pi_k^A \otimes \rho_k^b$, with $\{\Pi_k^A\}_{1 \leq k \leq d_A}$ orthonormal projectors of \mathbb{C}^{d_A} . The family of orthonormal projectors is obtained as the columns of an arbitrary unitary matrix $U_A \in \mathbb{C}^{d_A \times d_A}$. The 4 states ρ_k^b are arbitrary in \mathbb{C}^2 and $\{p_k\}$ a probability distribution. Given the prevailing symmetry in the maximally discordant states, we choose $\rho_k^b = \rho_k^a = \operatorname{tr}_{\bar{a}} \Pi_k^A$ and $p_k = \frac{1}{d_A}$ for all k, so that the classical state becomes determined solely by U_A . This is the only element that varies in each algorithm's step, which considerably simplifies computations.

Fig. 5 displays our results. The maximally discordant separable state, with $\delta_a(a:b) = 0.3333$, is obtained as the reduction of a classical state with $d_A = 3$. For $d_A = 2$, the reductions' maximum discord is seen to be $\delta_a(a:b) = 0.3113$. The columns of the unitary matrix

$$U_{A}^{opt} = \begin{pmatrix} 0.5288 - 0.2428\,i & -0.0241 + 0.0541\,i & 0.2730 - 0.0396\,i & 0.5695 + 0.3689\,i & -0.1512 - 0.1230\,i & 0.2672 - 0.1097\,i \\ -0.0179 + 0.2237\,i & 0.1392 + 0.1287\,i & 0.1575 - 0.8817\,i & -0.2307 + 0.1243\,i & -0.1110 - 0.0388\,i & 0.1259 - 0.1150\,i \\ -0.0670 + 0.1750\,i & -0.0525 - 0.0246\,i & 0.0387 + 0.2783\,i & -0.2118 + 0.0457\,i & -0.4907 + 0.1406\,i & 0.1647 - 0.7403\,i \\ 0.4663 + 0.4930\,i & 0.0701 + 0.2679\,i & -0.0392 + 0.0417\,i & 0.1412 - 0.5644\,i & 0.2635 + 0.1158\,i & 0.1552 - 0.1193\,i \\ -0.2532 + 0.0657\,i & 0.8938 + 0.0569\,i & 0.0919 + 0.1655\,i & 0.1642 + 0.1537\,i & 0.1726 + 0.0124\,i & 0.0627 - 0.0954\,i \\ -0.2169 - 0.0076\,i & -0.2708 + 0.0706\,i & -0.0449 - 0.0414\,i & 0.0949 + 0.1610\,i & 0.6485 - 0.3928\,i & -0.0244 - 0.5103\,i \end{pmatrix}$$

determine, on the standard basis, the basis $\{\Pi_k^A\}_{1 \le k \le 6}$ of the classical state σ_{opt}^{Ab} such that $\operatorname{tr}_{\bar{a}}\sigma_{opt}^{Ab}$ exhibits maximum discord: $\delta_a(a:b) = 0.3333$. We are finding an extension in $\mathbb{C}^6 \otimes \mathbb{C}^2$ of $\rho_{\max}^{\ell=4}$, improving on the LLA. Why is this extension unattainable in $\mathbb{C}^6 \otimes \mathbb{C}^2$ via the Li-Luo's approach? It suffices to note that $\ell = 4$, so that the LLA demands an ancilla in \mathbb{C}^4 so as to classically extend things to $\rho_{\max}^{\ell=4}$. We conjecture that σ_{opt}^{Ab} is the optimal extension of $\rho_{\max}^{\ell=4}$.

Notice the following difference between Li-Luo's extension and the optimal one. In the later, the ancilla is correlated only with the set ab, but not individually with a or b, i.e., $I(\bar{a}:a) = 0$ and $I(\bar{a}:b) = 0$ but $I(\bar{a}:ab) = 0.585$. Instead, for Li-Luo's extension, one has $I(\bar{a}:a) = 1$, $I(\bar{a}:b) = 1$, and $I(\bar{a}:ab) = 1.585$.



Fig. 5 Search for the maximally discordant separable states of 2 qubits, obtained via reductions of classically correlated states using the Monte Carlo method. Each line corresponds to a different simulation-temperature. (a) Using classical states in $\mathbb{C}^4 \otimes \mathbb{C}^2$ one finds reductions whose maximum discord is $\delta_a(a:b) = 0.3113$. (b) Using classical states in $\mathbb{C}^6 \otimes \mathbb{C}^2$ one finds reductions with maximum discord $\delta_a(a:b) = 0.3333$.

V. MAXIMALLY DISCORDANT SEPARABLE STATES

The previous results in $\mathbb{C}^2 \otimes \mathbb{C}^2$ suggest that maximally discordant separable states (MDSS) posses a rank close to the maximum. We see next how some symmetries associated to the construction of maximally discordant separable states of 2 qubits can be generalized to spaces of greater dimension.

Eqs. (30) and (33) indicate that 2 qubits MDSS can be built by uniformly mixing states corresponding to different mutually unbiased bases (MUBs). Indeed, $\rho_{\max}^{\ell=3}$ is constructed mixing two MUBs (σ_z and σ_x in our example) and $\rho_{\max}^{\ell=4}$ is erected mixing the 3 possible MUBs. We look now for a possible generalization of these MDSS to arbitrary dimension.

For $d \times d$ -dimensional states, if $\{P_k^i\}_{1 \le k \le d+1}^{1 \le i \le d}$ is the set of projectors determining the d+1 MUBs of one of the parties, the state

$$\rho_{\max}^{d} := \frac{1}{d(d+1)} \sum_{k=1}^{d+1} \sum_{i=1}^{d} P_{k}^{i} \otimes P_{k}^{i} \,. \tag{38}$$

should be a plausible candidate of a maximally discordant state.

Another possible MDSS-generalization (Eq. (34)) to larger dimensions starts from noting that the projectors basis of rank 1 $\{Z_k\}_{1 \le k \le 4}$ of Eq. (36) constitutes a symmetric and informationally complete positive operator valued measure (SIC-POVM) in \mathbb{C}^2 . In fact, taking $E_k := Z_k/d$ and d = 2 one has

$$\sum_{k=1}^{d^2} E_k = 1,$$
(39)

and

$$tr(E_k E_{k'}) = \frac{1}{d^2(d+1)} , k \neq k'.$$
(40)

Equivalently,

$$\frac{1}{d} \sum_{k=1}^{d^2} Z_k = 1 , \qquad (41)$$

and

$$\operatorname{tr}(Z_k Z_{k'}) = \frac{1}{d+1}, k \neq k'.$$
 (42)

$$\tilde{\rho}_{\max}^{d} := \frac{1}{d^2} \sum_{k=1}^{d^2} Z_k \otimes Z_k \,. \tag{43}$$

The existence of SIC-POVMs in \mathbb{C}^d has not been demonstrated yet for arbitrary d, although it is proved for d prime or d a power of a prime. Our problem is equivalent to that of finding d^2 rays separated by equal angles in \mathbb{C}^d [16; 17], being intimately linked to the existence of d+1 mutually unbiased bases (MUBs) in \mathbb{C}^d and thus with the existence of complementary observables [1; 35]. Alternatively, our problem can be seen as that of embedding the simplex (d^2 -1)dimensional generated by d^2 pure states into the convex of quantum states in such a way that all pure states exhibit the same overlap [27]. This is the way in which we interpret the tetrahedron formed by the components of $\tilde{\rho}_{max}$ in Eq. (36). A SIC-POVM is that POVM that better approximates an orthonormal basis in the states-space [34]. It is interesting to note that recently some authors introduced a new measure of quantum correlations involved in the optimal acquisition of information over all the local MUBs [40].

A. Genuine quantum correlations

Recent works show that one can obtain states with finite discord by effecting local operations on states of null discord [10; 12]. Thus, one may view discord as a resource, *necessary*, but not sufficient, to attain genuine quantum correlations. A way of point out toward states with genuine quantum correlations is through their decomposition in product states of local bases [7]. If $\{A_m\}$ and $\{B_n\}$ are bases associated to Hermitic operators in \mathcal{H}^A and \mathcal{H}^B , respectively, the composite states σ^{AB} can be decomposed as

$$\sigma^{AB} := \sum_{m=1}^{d_A^2} \sum_{n=1}^{d_B^2} r_{mn} A_m \otimes B_n , \qquad (44)$$

with $d_A(d_B)$ the dimension of $\mathcal{H}^A(\mathcal{H}^B)$. The correlation matrix $R := (r_{mn})$ can be recast via decomposition in singular values. If $L_R := \operatorname{rk}[R]$ is its rank and s_l its singular values,

$$\sigma^{AB} := \sum_{l=1}^{L_R} s_l F_l \otimes G_l \,, \tag{45}$$

where F_l and G_l are the elements of A and B, respectively, in the new basis. If the states-components are pure, $L_R \leq (\dim[\mathcal{H}^{ab}])^2$ (Cf. Eq. (14)). If not (mixed states allowed) one has $L_R \leq d_{\min}^2$, where $d_{\min} := \min\{\dim[\mathcal{H}^a], \dim[\mathcal{H}^b]\}$ corresponds to that subsystem of smaller dimension. For classical states L_R is bound (by above) by the dimension of the subsystems, i.e., $L_R \leq d_{\min}$. There are states of finite discord with $L_R \leq d_{\min}$, but one can show that their discord can be created vial local operations, so that they do not constitute quantum resources [10; 12]. States with $L_R > d_{\min}$ have discord necessarily and their correlation matrix is not compatible with that pertaining to a classical state. Only these states are genuinely quantum (with respect to their correlations). Summing up, L_R is the signature of quantum-correlated states that can not be obtained from classical states via local operations.

For instance, if $\tilde{\rho}_{\max}$, Eq. (36) represents the decomposition (45), with $\{|\theta_l, \phi_l\rangle \langle \theta_l, \phi_l|\}_{1 \le l \le 4}$ the basis of hermitic operators both in \mathcal{H}^a and \mathcal{H}^b , and $s_l = \frac{1}{4} \forall l$. Here, the correlation matrix is of rank 4. Also, $d_{\min} = \dim[\mathbb{C}^2] = 2$. Thus, $L_R > d_{\min}$ and the correlations are indeed genuinely quantum. On the other hand, it is easy to see that for the state in Eq. 29 the correlation matrix is of rank 2. Discord-like correlations can here be locally created. As a corollary, for 2 qubits bipartite states, genuinely quantum states with discord are only those of $L_R > 2$. In Tab. II, only the states with $\ell > 2$ are relevant.

Note that, given our decomposition (43) of ρ_{\max}^d , since the $\{M_k\}$ are linearly independent, the number of terms automatically determines the rank of the correlation matrix. Here one has $\operatorname{rk}[R] = d^2 > d_{\min}$ [4], since $d_{\min} = \dim[\mathbb{C}^d] = d$. Thus, for these states the discord is not spurious in the sense discussed above. In other words, for any dimension, states that are separable and possess discord defined via Eq. (43) constitute genuine quantum resources.

VI. CONCLUSIONS

Summarizing our results:

- We have demonstrated in this work that the existence of genuine quantum correlations in separable states is related to the possibility of extending such states to classically correlated ones of larger dimension.
- We have introduced the notion of optimum classical extension of separable states and showed that the algorithm advanced by Li and Luo can be, in general, improved.
- We also found that the maximum degree of discord of a given separable state is linked to the dimensionality of its optimum classical extension.
- We demonstrated the existence of a lower bound for the dimension of such extension.
- For 2 qubits separable states we found different classical extensions for states of maximum discord. In particular, we showed that with one qutrit we can classically extend the 2 qubits state of maximum discord. On the basis of numerical simulations we conjectured that such a classical extension is the optimum one.
- Our results for low dimensionality systems induce hypothesis concerning the structure of separable states of maximum discord in arbitrary dimension that, in turn, suggest interesting links involving the notions of mutually unbiased basis and symmetric and informationally complete positive operator valued measures (SIC-POVMs).

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