Quantum discord for general two-qubit states: Analytical progress

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We present a reliable algorithm to evaluate quantum discord for general two-qubit states, amending and extending an approach recently put forward for the subclass of X states. A closed expression for the discord of arbitrary states of two qubits cannot be obtained, as the optimization problem for the conditional entropy requires the solution to a pair of transcendental equations in the state parameters. We apply our algorithm to run a numerical comparison between quantum discord and an alternative, computable measure of nonclassical correlations, namely, the geometric discord. We identify the extremally nonclassically correlated two-qubit states according to the (normalized) geometric discord, at a fixed value of the conventional quantum discord. The latter cannot exceed the square root of the former for systems of two qubits.

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I. INTRODUCTION

It is as well theoretically proven as experimentally tested that the exploitation of entangled states improves our ability to manage information in several ways [1]. The development of quantum information theory is definitely due to this fundamental result [2]. However, it has recently been discovered that even multipartite separable states can play a relevant role in performing better-than-classical communication and information protocols [3–5]. In general, then, the usefulness of a particular state of a quantum system for such tasks can be traced back to the presence of internal correlations among parts of the system, that is, to the knowledge that an observer Alice, probing a subsystem A, gains about the state of another subsystem B, controlled by another observer Bob, and vice versa.

The quantitative and qualitative evaluation of such correlations and the proper discrimination of their nature—classical versus quantum—stand as open problems. Several quantifiers of nonclassicality of correlations have been introduced in the literature [6–15] (not to be confused with the nonclassicality of quantum optical states [16]), but there are still neither clear criteria of faithfulness or *bona fide*–ness for them nor a well-established hierarchy of reliability. Despite that, they are heavily used in current research [17–30]. The most popular one by far is the *quantum discord* [6,7], a measure of nonclassical correlations that goes beyond entanglement and whose definition has an immediate interpretation in information theory: discord equals the difference of the total correlations between two subsystems A and B before and after a local measurement process is performed on one of them. The quantum discord admits at least three other operational interpretations, in contexts ranging from thermodynamics to communication protocols, such as quantum state merging [21]. The evaluation of quantum discord is a hard task from a computational point of view, implying an optimization of the conditional entropy between Alice and Bob, $\mathcal{S}(A|B)$, over all local (generalized) measurements on one party, which is often obtainable by numerical methods only. A closed analytical solution is known in the case of arbitrary two-mode Gaussian states [20], under the restriction of Gaussian local measurements. Narrowing our overview to two-qubit states, an analytical expression of discord has been derived, in particular, for the subclass of so-called X states [24–27], and a successful attempt to generalize this procedure has not been advanced yet (to the best of our knowledge), apart from an upper bound quantity for the discord defined in [26].

The difficulty in calculating quantum discord motivated the introduction of alternative measures of nonclassical correlations. In particular, the *geometric discord* [13] is one such a measure, which quantifies the amount of nonclassical correlations of a state in terms of its minimal distance from the set of genuinely classical states. The geometric discord involves a simpler optimization and is easily computable analytically for general two-qubit states. However, its relationship with the original quantum discord is not entirely clear at the present stage.

In this work, we present an algorithm to calculate quantum discord for general two-qubit states. First, we obtain an explicit and simplified expression for the conditional entropy, exploiting the Bloch representation of the density matrix; second, we employ new variables that allow us to set the optimization conditions in a closed form. Finally, we associate them with constraints over the eigenvalues of the statistical ensemble obtained after the measurement process. Our approach qualifies as the most efficient and reliable way to evaluate quantum discord for arbitrary states of two qubits [31].

Exploiting our algorithm, we perform a detailed numerical exploration of the Hilbert space of two-qubit states to compare the quantum discord and geometric discord as quantifiers of nonclassical correlations. We shed light on the relationship between these two quantities by identifying the states that extremize geometric discord at a fixed quantum discord (and vice versa). We are motivated by the aim of establishing a reliable hierarchy of nonclassical states based on physically and mathematically consistent criteria. We find that, interestingly, the quantum discord of a two-qubit state can never exceed the square root of its (normalized) geometric discord. In analogy with the study of maximal entanglement [32], we find that the notion of maximal nonclassical correlations is measure dependent: therefore, the feasibility in a specific experimental realization will determine which, among the various classes of

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maximally quantumly correlated states, are the most suitable ones to be employed for applications.

The paper is organized as follows. Section II provides an introduction to quantum discord and geometric discord (hereafter denoted $\mathcal{D}$ and D_G, respectively), presenting definitions, main properties, and a summary of the results obtained in the literature. In Sec. III, we pursue an analytical approach to the calculation of quantum discord for general two-qubit states, eventually recasting the optimization problem into a system of two transcendental equations, whose solution specifies the local measurement that minimizes the conditional entropy. Section IV concerns the comparison between quantum discord and geometric discord by using the results of the previous sections; we identify the classes of states with maximal and minimal geometric discord at a fixed quantum discord. Finally, Sec. V recalls the main results of our work and suggests further issues worthy of investigation.

II. BASIC DEFINITIONS

A. Quantum discord

One of the lessons we can apprehend from quantum mechanics is that the measurement process disturbs the state in which a physical system is set. This differs from what happens in the classical scenario, hence it is possible to conclude that the disturbance induced by a measurement on a state is a good evidence of its "quantumness." Now, let us suppose we have a bipartite system in a certain state and make a measurement on one of its subsystems. We can analyze the nature of the internal correlations of the system in such a state by studying in which way they are affected by the measurement. Information theory provides the tools to accomplish this task.

As a starting point, let us consider the case of information stored in two classical probability distributions. The quantity expressing the total amount of correlations between two random variables X and Y, assuming values $\{x_i\},\{y_j\}$ with probability $\{p_i\},\{q_j\}$, is the *mutual information* $\mathcal{I}$, defined as

$$\mathcal{I}(X:Y)=\mathcal{H}(X)+\mathcal{H}(Y)-\mathcal{H}(X,Y), \tag{1}$$

where $\mathcal{H}(X)=-\sum_i p_i\log_2 p_i$ is the Shannon entropy associated with the random variable X; consequently, $\mathcal{H}(Y)=-\sum_j q_j\log_2 q_j$ is the entropy for Y, while $\mathcal{H}(X,Y)$ is the joint entropy of X and Y. Following Bayesian rules, we can retrieve equivalent formulations, $\mathcal{I}(X:Y)=\mathcal{I}(Y:X)=\mathcal{J}(X:Y)=\mathcal{J}(Y:X)$, where

$$\mathcal{J}(X:Y)=\mathcal{H}(X)-\mathcal{H}(X|Y), \tag{2}$$

$$\mathcal{J}(Y:X)=\mathcal{H}(Y)-\mathcal{H}(Y|X). \tag{3}$$

Here the conditional entropy is straightforwardly defined as $\mathcal{H}(X|Y)=\mathcal{H}(X,Y)-\mathcal{H}(Y)$ and represents how much uncertainty (ignorance) we have on X given the value of Y [and vice versa for $\mathcal{H}(Y|X)$].

In the quantum scenario, we consider a bipartite system AB described by a density matrix $\rho\equiv\rho_{AB}$, and subsystems A,B with marginal density matrices ρ_A,ρ_B. The mutual information can be used once more to quantify the total correlations between A and B. The quantum analog of expression (1) straightforwardly reads

$$\mathcal{I}(A:B)=\mathcal{S}(A)+\mathcal{S}(B)-\mathcal{S}(A,B), \tag{4}$$

where $\mathcal{S}(A)=-\mathrm{Tr}[\rho_A\log_2\rho_A]$ is the von Neumann entropy of subsystem A, and equivalently, $\mathcal{S}(B)=-\mathrm{Tr}[\rho_B\log_2\rho_B]$, $\mathcal{S}(A,B)=-\mathrm{Tr}[\rho\log_2\rho]$. In contrast, if we try to define a quantum version of $\mathcal{J}$, we have

$$\mathcal{J}(A:B)=\mathcal{S}(A)-\mathcal{S}(A|B), \tag{5}$$

which is an "ambiguous" quantity [6,7], since the conditional quantum entropy $\mathcal{S}(A|B)$ is clearly dependent on which observable we have measured on B. Using the same notation as in [25], we recall that a von Neumann measurement (henceforth, just measurement) on B projects the system into a statistical ensemble $\{p_k,\rho_k\}$, such that

$$\rho\to\rho_k=\frac{(I_A\otimes P_{Bk})\rho(I_A\otimes P_{Bk})}{p_k}, \tag{6}$$

where

$$p_k=\mathrm{Tr}[\rho(I_A\otimes P_{Bk})],\quad P_{Bk}=V\Pi_k V^\dagger,\qquad \Pi_k=|k\rangle\langle k|,\quad k=0,1,\quad V\in SU(2). \tag{7}$$

We stress that in this case study, the use of generalized positive-operator-valued measurements is not required, since it was proven in [23] that for two-qubit states the optimal measurement for the conditional entropy is always a projective one. We can say that the amount of truly classical correlations is expressed by the mutual information obtained by adopting the least disturbing measurement [7]:

$$\mathcal{C}(A:B)=\max_{\{P_{Bk}\}}\mathcal{J}(A:B)=\mathcal{S}(A)-\min_{\{P_{Bk}\}}\sum_k p_k\mathcal{S}(A|B_{\{P_{Bk}\}}). \tag{8}$$

Consequently, the amount of genuinely quantum correlations, called *quantum discord*, is given by [6]

$$\mathcal{D}(A:B)=\mathcal{I}(A:B)-\mathcal{C}(A:B)=\mathcal{S}(B)-\mathcal{S}(A,B)+\min_{\{P_{Bk}\}}\sum_k p_k\mathcal{S}(A|B_{\{P_{Bk}\}}). \tag{9}$$

We note that quantum discord is not symmetric:

$$\mathcal{S}(A)-\mathcal{S}(A|B)\neq\mathcal{S}(B)-\mathcal{S}(B|A); \tag{10}$$

performing the measurement on Alice's subsystem rather than on Bob's is perfectly legitimate, but it returns, in general, a different value of discord. See, e.g., [14] and [22] for a discussion of the implications of it. It is immediate to verify that not only entangled states, but almost all separable states have a nonvanishing quantum discord [19], that is, are affected by the measurement process, thus exhibiting some pretty quantum properties. In the case of pure bipartite states, the discord reduces to the marginal entropy of one of the two subsystems and, therefore, to the canonical measure of entanglement. Quantum discord for two-qubit states is normalized to1.

B. Geometric discord

Recently, it has been argued that the experienced difficulty of calculating quantum discord can be coped with, for a general two-qubit state, by the introduction of its geometrized version, hereafter just called *geometric discord* [13]. Let us suppose, to be coherent with Sec. II A, that we have a bipartite system AB and make a measurement on B. As we have remarked, almost all (entangled or separable) states are disturbed by the measurement; however, there is a subclass of states that is invariant and presents zero discord. It is the class of the so-called *classical-quantum* states [4], whose elements have a density matrix of the form

$$\rho = \sum_i p_i \rho_{Ai} \otimes |i\rangle\langle i|, \tag{11}$$

where p_i is a probability distribution, ρ_{Ai} is the marginal density matrix of A, and $\{|i\rangle\}$ is an orthonormal vector set. A classical-quantum state is not affected by a measurement on B in any case.

Letting Ω be the set of classical-quantum two-qubit states, and χ be a generic element in this set, the geometric discord D_G is defined as the distance between the state ρ and the closest classical-quantum state. In the original definition [13], the (squared) Hilbert-Schmidt distance is adopted. Recalling that $||A||_2^2 = \mathrm{Tr}[AA^T]$ is the square of the Hilbert-Schmidt norm of a matrix A, the geometric discord has been introduced as

$$D_G(\rho) = \min_{\chi\in\Omega} ||\rho - \chi||_2^2. \tag{12}$$

It is possible to obtain an explicit closed expression of D_G for two-qubit states. First, one needs to express the 4×4 density matrix of a two-qubit state in the so-called Bloch basis [33]:

$$\rho = \frac{1}{4}\sum_{i,j=0}^{3} R_{ij}\sigma_i \otimes \sigma_j = \frac{1}{4}\Bigg(I_{4\times4} + \sum_{i=1}^{3} x_i\sigma_i \otimes I_{2\times2} + \sum_{j=1}^{3} y_j I_{2\times2} \otimes \sigma_j + \sum_{i,j=1}^{3} t_{ij}\sigma_i \otimes \sigma_j\Bigg), \tag{13}$$

where $R_{ij} = \mathrm{Tr}[\rho(\sigma_i \otimes \sigma_j)]$, $\sigma_0 = I_{2\times2}$, σ_i $(i = 1,2,3)$ are the Pauli matrices, $\vec{x} = \{x_i\}, \vec{y} = \{y_i\}$ are the three-dimensional Bloch vectors associated with subsystems A, B, and t_{ij} denote the elements in the correlation matrix T. Then, it is shown in [13] that the geometric discord is given by

$$D_G(\rho) = \frac{1}{4}\left(\left|\left|\vec{y}\vec{y}^T\right|\right|_2 + ||T||_2^2 - k\right), \tag{14}$$

with k being the largest eigenvalue of the matrix $\vec{y}\vec{y}^T + T^T T$ (in case of measurement on Alice, one needs to replace $\vec{y}$ with $\vec{x}$ and $T^T T$ with TT^T). An alternative formulation for the geometric discord has been provided in [30]. It is easy to see that D_G is not normalized to 1: its maximum value is $1/2$ for two-qubit states, so it is natural to consider $2D_G$ a proper measure for a comparison with the quantum discord $\mathcal{D}$.

III. QUANTUM DISCORD FOR TWO-QUBIT STATES

A. General setting

Even though quantum discord has an apparently simple definition [6], the practice reveals that its explicit evaluation is hard to accomplish. In this paper we restrict our attention to two-qubit states. An analytical algorithm has been proposed for the subclass of states with maximally mixed marginals (described by five real parameters) in [24]. Also, an extension to states spanned by seven real parameters, called X states because of the peculiar form of their density matrix (with vanishing elements outside the leading diagonal and the antidiagonal), has been introduced in [25] and amended in [27]. Here, we attempt to generalize the procedure to the entire class of two-qubit states.

First, we consider that by performing local unitary transformations we can recast the density matrix for an arbitrary two-qubit state, Eq. (13), in the Bloch normal form [24,33],

$$\rho = \frac{1}{4}\Bigg(I_{4\times4} + \sum_i a_i\sigma_i \otimes I_{2\times2} + \sum_i b_i I_{2\times2} \otimes \sigma_i + \sum_i c_i\sigma_i \otimes \sigma_i\Bigg), \tag{15}$$

which is a density matrix completely defined by nine real parameters arranged in three three-dimensional column vectors, $\vec{a} = \{a_i\}$, $\vec{b} = \{b_i\}$, and $\vec{c} = \{c_i\}$. This follows from the fact that local unitary operations $\rho' = (U_A \otimes U_B)\rho(U_A \otimes U_B)^\dagger$ correspond to left and right multiplication of the Bloch matrix R with orthogonal matrices [33],

$$R' = \begin{pmatrix} 1 & 0 \\ 0 & O_A^T \end{pmatrix} R \begin{pmatrix} 1 & 0 \\ 0 & O_B \end{pmatrix}, \tag{16}$$

with $O_{A,B} \in SO(3)$. It is then straightforward to obtain the normal form of Eq. (15): one needs to calculate the singular value decomposition of the lower diagonal $3 \otimes 3$ block T in R, $T = O_A C O_B^T$, divide O_A and O_B by their respective determinants (to make sure they both have determinant $+1$), and then apply Eq. (16). The density matrix is correspondingly transformed into the normal form of Eq. (15), where the c_i are identified with the elements of the diagonal matrix C, that is, the singular values of T. Every two-qubit state can be then transformed in its simplified normal form by means of local unitaries (which preserve entanglement and correlations in general, by definition), so we can restrict our analysis to density matrices of this type without incurring any loss of generality.

Now we move to calculate the quantum discord $\mathcal{D}$, Eq. (10), for generic states in normal form. The marginal entropy $\mathcal{S}(B)$ and the global entropy $\mathcal{S}(A,B)$ are trivial to obtain. The main issue regards the optimization involved in the conditional entropy.

B. Conditional entropy

First, we have to write the conditional entropy in an explicit form, adopting, for simplicity, the notation in [25]. We remarked that a measurement sends state ρ into an ensemble

$\{p_k,\rho_k\}$ as expressed in Eq. (6). The entropy of the ensemble can be written as

$$\tilde{\mathcal{S}} = \sum_k p_k \mathcal{S}(A|B_{\{P_{Bk}\}}) = \sum_k p_k \mathcal{S}(\rho_k) = p_0 S_0 + p_1 S_1, \tag{17}$$

where S_0, S_1 are the entropies associated with ρ_0, ρ_1. The measurement is defined by the quantity P_{Bk} and is consequently parametrized by the elements of the unitary matrix V, which we can write in the basis of the Pauli matrices as

$$V = v_0 I_{2\times 2} + \vec{v}\cdot\vec{\sigma} = \begin{pmatrix} v_0 + v_3 & v_1 - i v_2 \\ v_1 + i v_2 & v_0 - v_3 \end{pmatrix}. \tag{18}$$

We notice that the real vector $\{v_0,\vec{v}\} = \{v_i\}$ has norm 1. Therefore, it is possible to rearrange the four parameters in three variables only, for example, in this way:

$$h = v_0 v_1 + v_2 v_3, \quad j = v_1 v_3 - v_0 v_2, \quad k = v_0^2 + v_3^2. \tag{19}$$

Setting the vectors $\vec{X} = \{2j,2h,2k-1\}$ and $\vec{m}_\pm = \{m_{i\pm}\} = \{a_i \pm c_i X_i\}$, we have that, after a straightforward calculation, the conditional entropy takes the following expression:

$$\begin{aligned}\tilde{\mathcal{S}} = -\frac{1}{4}\Bigg\{&(1-\vec{b}\cdot\vec{X})\Bigg[\left(1-\frac{|\vec{m}_-|}{1-\vec{b}\cdot\vec{X}}\right)\log_2\left(1-\frac{|\vec{m}_-|}{1-\vec{b}\cdot\vec{X}}\right)\\ &+\left(1+\frac{|\vec{m}_-|}{1-\vec{b}\cdot\vec{X}}\right)\log_2\left(1+\frac{|\vec{m}_-|}{1-\vec{b}\cdot\vec{X}}\right)\Bigg]\\ &+(1+\vec{b}\cdot\vec{X})\Bigg[\left(1-\frac{|\vec{m}_+|}{1+\vec{b}\cdot\vec{X}}\right)\log_2\left(1-\frac{|\vec{m}_+|}{1+\vec{b}\cdot\vec{X}}\right)\\ &+\left(1+\frac{|\vec{m}_+|}{1+\vec{b}\cdot\vec{X}}\right)\log_2\left(1+\frac{|\vec{m}_+|}{1+\vec{b}\cdot\vec{X}}\right)\Bigg]\Bigg\}.\end{aligned} \tag{20}$$

This result is consistent with the formula provided in the Appendix of [26], but here we have reached a simpler expression by exploiting the normal form of the density matrix, Eq. (15). However, we must remark that in this picture we can operate with local unitaries on it, obtaining a new state ρ (albeit with the same entropies and discord) described by the simplified normal form presented in Eq. (15); we then perform a projective measurement on subsystem B, obtaining an ensemble whose conditional entropy is plotted in Fig. 1.

One sees that there are no further apparent symmetries for the conditional entropy. Therefore the analysis so far, while not being conclusive, allows us just to refine the problem by safely letting the optimization of the conditional entropy be restricted to the interval $\theta \in [0,\pi/2)$. To determine the minimum of $\tilde{\mathcal{S}}$, we need to calculate its derivatives with respect to θ and ϕ. The dependence on these variables involves logarithms of nonlinear quantities, so we cannot expect to solve the problem analytically in any case, whatever ingenious variables we might choose. However, we can seek to write the two constraints in a compact and elegant form. Let us impose

$$p = \vec{b}\cdot\vec{X}, \quad r_+ = |\vec{m}_+|, \quad r_- = |\vec{m}_-|. \tag{26}$$

After a bit of algebra, we obtain

$$\begin{aligned}\tilde{\mathcal{S}} = -\tfrac{1}{4}\{&(1-p-r_-)\log_2[1-p-r_-] + (1-p+r_-)\\ &\times\log_2[1-p+r_-] + (1+p+r_+)\log_2[1+p+r_+]\\ &+(1+p-r_+)\log_2[1+p-r_+] - 4 + 2(-(1-p)\\ &\times\log_2[1-p] - (1+p)\log_2[1+p])\}.\end{aligned} \tag{27}$$

there is still an amount of redundancy [26]. A projective measurement on a two-qubit state can be characterized by two independent variables only, identifiable as the angles θ and ϕ, which parametrize a generic single-qubit pure state as $|\psi\rangle = \cos\theta|0\rangle + e^{i\phi}\sin\theta|1\rangle$, and the Bloch sphere of coordinates $\{x,y,z\}$ in this way:

$$x = 2j = 2\cos\theta\sin\theta\cos\phi, \quad y = 2h = 2\cos\theta\sin\theta\sin\phi, \quad z = 2k-1 = 2\cos^2\theta - 1. \tag{21}$$

It is immediate to verify that the following constraint holds:

$$k^2 + h^2 + j^2 = k. \tag{22}$$

The algorithm originally designed for X states in [25] is flawed just in not considering the mutual dependence of h,j,k, proving to be reliable only for a more restricted class of states identified in [27].

The above mapping enables us to reparameterize the conditional entropy, Eq. (20), as a function of the azimuthal and polar angles θ,ϕ; we can then write $\tilde{\mathcal{S}}(h,j,k) = \tilde{\mathcal{S}}(\theta,\phi)$ and perform the optimization of $\tilde{\mathcal{S}}$ over these two independent variables.

C. Optimization

Inspired by [25], we look for symmetries in the expression of the conditional entropy. We notice immediately the invariance under the transformation $\theta \to \theta \pm \pi$, which, however, can be englobed by the one

$$k \to 1-k, \quad h \to -h, \quad j \to -j, \tag{23}$$

which corresponds to

$$\theta \to \theta \pm \pi/2. \tag{24}$$

We can appreciate this with an example. Let us pick a random state, such as

$$\begin{pmatrix} 0.437 & 0.126+0.197i & 0.0271-0.0258i & -0.274+0.0997i \\ 0.126-0.197i & 0.154 & -0.0115-0.0187i & -0.0315+0.170i \\ 0.0271+0.0258i & -0.0115+0.0187i & 0.0370 & 0.00219-0.0367i \\ -0.274-0.0997i & -0.0315-0.170i & 0.00219+0.0367i & 0.372 \end{pmatrix}; \tag{25}$$

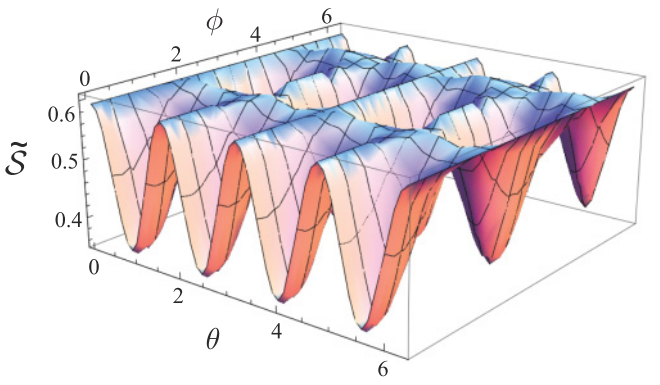

FIG. 1. (Color online) Example of conditional entropy $\tilde{\mathcal{S}}$ for a random two-qubit state [Eq. (25)]. The angles θ and ϕ parametrize the measurement: we can appreciate the symmetry properties of $\tilde{\mathcal{S}}$ with respect to such variables, expressed by the invariance $\tilde{\mathcal{S}}(\theta,\phi) = \tilde{\mathcal{S}}(\theta \pm \pi/2,\phi)$. All quantities plotted are dimensionless.

Now we set the partial derivatives to 0:

$$\frac{\partial\tilde{\mathcal{S}}}{\partial\theta} = \frac{\partial\tilde{\mathcal{S}}}{\partial p}\frac{\partial p}{\partial\theta} + \frac{\partial\tilde{\mathcal{S}}}{\partial r_+}\frac{\partial r_+}{\partial\theta} + \frac{\partial\tilde{\mathcal{S}}}{\partial r_-}\frac{\partial r_-}{\partial\theta} = 0;$$
$$\frac{\partial\tilde{\mathcal{S}}}{\partial\phi} = \frac{\partial\tilde{\mathcal{S}}}{\partial p}\frac{\partial p}{\partial\phi} + \frac{\partial\tilde{\mathcal{S}}}{\partial r_+}\frac{\partial r_+}{\partial\phi} + \frac{\partial\tilde{\mathcal{S}}}{\partial r_-}\frac{\partial r_-}{\partial\phi} = 0.$$

Defining the quantities

$$\alpha = \det\begin{pmatrix} \frac{\partial p}{\partial\theta} & \frac{\partial p}{\partial\phi} \\ \frac{\partial r_+}{\partial\theta} & \frac{\partial r_+}{\partial\phi} \end{pmatrix} \quad \beta = \det\begin{pmatrix} \frac{\partial p}{\partial\theta} & \frac{\partial p}{\partial\phi} \\ \frac{\partial r_-}{\partial\theta} & \frac{\partial r_-}{\partial\phi} \end{pmatrix}$$
$$\gamma = \det\begin{pmatrix} \frac{\partial r_+}{\partial\theta} & \frac{\partial r_+}{\partial\phi} \\ \frac{\partial r_-}{\partial\theta} & \frac{\partial r_-}{\partial\phi} \end{pmatrix}, \tag{28}$$

after some manipulations, we can write the stationarity conditions in the following form:

$$\frac{1}{4}\log_2\left[\frac{1+p-r_+}{1+p+r_+}\right] + \frac{1}{2}\log_2\left[\frac{(1+p)(1-p-r_-)}{(1-p)(1+p-r_+)}\right]\frac{\beta}{\alpha+\beta+\gamma} = 0;$$
$$\frac{1}{4}\log_2\left[\frac{1-p-r_-}{1-p+r_-}\right] - \frac{1}{2}\log_2\left[\frac{(1+p)(1-p-r_-)}{(1-p)(1+p-r_+)}\right]\frac{\alpha}{\alpha+\beta+\gamma} = 0. \tag{29}$$

We see immediately that this system can be further simplified to

$$\frac{\log_2\left[\frac{1+p-r_+}{1+p+r_+}\right]}{\beta} + \frac{\log_2\left[\frac{1-p-r_-}{1-p+r_-}\right]}{\alpha} = 0;$$
$$\frac{1}{4}\log_2\left[\frac{1-p-r_-}{1-p+r_-}\right] - \frac{1}{2}\log_2\left[\frac{(1+p)(1-p-r_-)}{(1-p)(1+p-r_+)}\right]\frac{\alpha}{\alpha+\beta+\gamma} = 0. \tag{30}$$

We can still express these equations as relations among the eigenvalues of the ensemble $\{p_k,\rho_k\}$. Calling λ_0^+,λ_0^- the eigenvalues of ρ_0 and λ_1^+,λ_1^- the eigenvalues of ρ_1, we have

$$\lambda_0^\pm = \tfrac{1}{2}\left(1 \pm \tfrac{r_-}{1-p}\right), \quad \lambda_1^\pm = \frac{1}{2}\left(1 \pm \frac{r_+}{1+p}\right), \tag{31}$$

After some straightforward algebra, one can show that the vanishing of the derivatives of $\tilde{\mathcal{S}}$ occurs when the following constraints are satisfied:

$$\lambda_0^- = \frac{\left(\frac{\lambda_1^+}{\lambda_1^-}\right)^{\frac{\alpha}{\beta}}}{1+\left(\frac{\lambda_1^+}{\lambda_1^-}\right)^{\frac{\alpha}{\beta}}}; \quad \lambda_1^- = \lambda_0^-\left(\frac{\lambda_0^+}{\lambda_0^-}\right)^{\frac{\alpha+\beta+\gamma}{2\alpha}}. \tag{32}$$

These two transcendental equations can be solved numerically. They represent the most compact formulation to date for the problem of calculating the quantum discord of arbitrary two-qubit states. Let us call s_i the solutions obtained, corresponding to values $\{\theta_i,\phi_i\}$. To establish if they represent minima of $\tilde{\mathcal{S}}$, we adopt the conventional method and evaluate the signature of the Hessian matrix H at points $\{\theta_i,\phi_i\}$, and, in the case of $\det H = 0$, we study the sign of the functions $\delta_i = \tilde{\mathcal{S}}(\theta,\phi) - \tilde{\mathcal{S}}(\theta_i,\phi_i)$. Naming $\{\theta_{mj},\phi_{mj}\}$ the angles such that H is positive definite or $\delta_i > 0$, we clearly have that the absolute minimum of the conditional entropy is defined as

$$\min_{\{P_{Bk}\}}\sum_k p_k\mathcal{S}(A|B_{\{P_{Bk}\}}) = \min_{\{\theta_{mj},\phi_{mj}\}}\tilde{\mathcal{S}}(\theta_{mj},\phi_{mj}).$$

The quantum discord for generic two-qubit states of the form Eq. (15) finally reads

$$\mathcal{D}(A:B) = \mathcal{S}(B) - \mathcal{S}(A,B) + \min_{\{\theta_{mj},\phi_{mj}\}}\tilde{\mathcal{S}}(\theta_{mj},\phi_{mj}). \tag{33}$$

IV. COMPARISON BETWEEN QUANTUM DISCORD AND GEOMETRIC DISCORD

We can use our results to compare the quantum discord $\mathcal{D}$ [6] with the geometric discord D_G [13] for general two-qubit states [34]. We have generated up to 10^6 random general two-qubit states. After transforming each of them into the normal form of Eq. (15), we have calculated their quantum discord $\mathcal{D}$, as numerically obtained from the algorithm in Sec. III, and their normalized geometric discord $2D_G$. The latter admits the following explicit analytic expression for states ρ in normal form, derived from Eq. (14):

$$D_G(\rho) = \frac{1}{4}\left(\left|\left|\vec{b}\vec{b}^T\right|\right|_2 + \left|\left|\vec{c}\vec{c}^T\right|\right|_2 - \tilde{k}\right), \tag{34}$$

where $\tilde{k}$ is the largest eigenvalue of the matrix $\vec{b}\vec{b}^T + \vec{c}\vec{c}^T$.

The results are shown in Fig. 2. We notice that physical states of two qubits fill up a two-dimensional area in the space of the two nonclassicality measures, meaning that the two impose inequivalent orderings on the set of mixed two-qubit quantum states; this is reminiscent of the case of entanglement measures (see, e.g., [32]), and a similar feature has been reported concerning the comparison between discord and other nonclassicality indicators [14]. Nevertheless, at a fixed quantum discord, the geometric discord admits exact lower and upper bounds (and vice versa). We have identified them numerically.

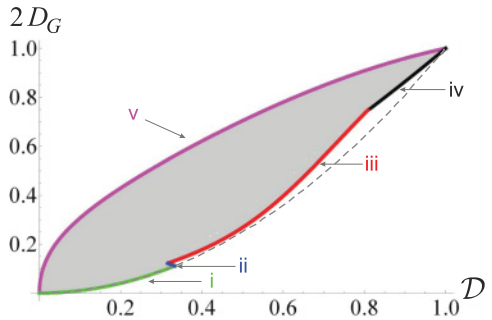

FIG. 2. (Color online) Comparison between normalized geometric discord $2D_G$ and quantum discord $\mathcal{D}$ for 10^6 randomly generated general two-qubit states. The dashed line is obtained by taking the equality sign in Ineq. (35). Refer to the text for details on the other boundary curves. All quantities plotted are dimensionless.

First, we have observed that the following hierarchical relationship holds for arbitrary two-qubit states:

$$2D_G \geqslant \mathcal{D}^2. \tag{35}$$

In other words, the quantum discord for any two-qubit state can never exceed its (normalized) distance from the set of classical-quantum states. The corresponding boundary curve is plotted as the dashed (gray) line in Fig. 2. However, we see that such a bound is tight only in the region $0 \leqslant \mathcal{D} \leqslant 1/3$, in which it coincides with what we refer to as branch i (see below), while it is not attainable for higher degrees of nonclassical correlations. The actual, tight lower bound in the whole $\{\mathcal{D}, 2D_G\}$ plane accommodates states with minimal geometric discord at a fixed quantum discord or, equivalently maximal quantum discord at a fixed geometric discord: such extremal states are constituted by the union of four families, which sit on branches i–iv in Fig. 2.

(i) (Green online) This branch is filled by so-called α states [28],

$$\rho_\alpha = \begin{pmatrix} \frac{\alpha}{2} & 0 & 0 & \frac{\alpha}{2} \\ 0 & \frac{1-\alpha}{2} & 0 & 0 \\ 0 & 0 & \frac{1-\alpha}{2} & 0 \\ \frac{\alpha}{2} & 0 & 0 & \frac{\alpha}{2} \end{pmatrix}, \quad 0 \leqslant \alpha \leqslant 1/3, \tag{36}$$

for which $\mathcal{D}(\rho_\alpha) = \alpha$ and $2D_G(\rho_\alpha) = \alpha^2$, thus saturating the inequality (35).

(ii) (Blue online) This small branch is filled by a subclass of the two-parameter family

$$\rho_r = \begin{pmatrix} (1-a)/2 & 0 & 0 & r/2 \\ 0 & a & 0 & 0 \\ 0 & 0 & 0 & 0 \\ r/2 & 0 & 0 & (1-a)/2 \end{pmatrix},$$
$$\frac{1}{3} \leqslant a \leqslant \frac{5}{14}, \quad \sqrt{4a - 3a^2 - 1}, \tag{37}$$

with $r \in [\sqrt{4a - 3a^2 - 1}, \frac{1-a}{3}]$ given by the solution to $\frac{2r \tanh^{-1}(\sqrt{a^2+r^2})}{\sqrt{a^2+r^2}} + \ln(-a - r + 1) - \ln(-a + r + 1) + 2\tanh^{-1}(r) = 0$. The geometric discord of these states is simply $2D_G(\rho_r) = a^2$, while their quantum discord is calculated in [28]. We highlight the presence of the "pimple" at the joint between branch i and branch ii, a recurring feature in the profile of extremal states involving quantum discord [14,28,29].

(iii) (Red online) This branch accommodates asymmetric X states of the form

$$\rho_g = \begin{pmatrix} a & 0 & 0 & \sqrt{a - a^2 - ac} \\ 0 & c & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sqrt{a - a^2 - ac} & 0 & 0 & 1 - a - c \end{pmatrix},$$
$$a = \frac{1 - 2c + 2c^2 - g}{2c}, \quad 0 \leqslant g \leqslant 1, \tag{38}$$

with

$$c \in \left[\frac{1 - \sqrt{g}}{2}, \frac{1}{2} - \begin{cases} \frac{1}{2}\sqrt{2g-1}, & g > \frac{1}{2}; \\ 0, & \text{otherwise;} \end{cases} \right],$$

solution to $8(1-2c)c^2 \tanh^{-1}[\sqrt{8(c-1)c - 2g + 3}] - 4c^2\sqrt{8(c-1)c - 2g + 3}\tanh^{-1}(1-2c) + 2\sqrt{8(c-c^2) - 2g + 3}(2c^2 + g - 1)\tanh^{-1}(\frac{3c - 2c^2 + g - 1}{c}) = 0$. For these states, $2D_G(\rho_g) = g$ and $\mathcal{D}(\rho_g) = \frac{1}{\ln 4}\{-\ln[-4c(a + c - 1)] - 2\sqrt{4c(a + c - 1) + 1}\tanh^{-1}[\sqrt{4c(a + c - 1) + 1}] - 2\ln(1 - a) + 4a\tanh^{-1}(1 - 2a) + 2\ln(2 - 2c) - 4c\tanh^{-1}(1 - 2c)\}$.

(iv) (Black online) The top-right-most branch accommodates just pure states $\rho_p = |\psi\rangle_{AB}\langle\psi|$, for which the discord equals the marginal von Neumann entropy, $\mathcal{D}(\rho_p) = \mathcal{S}(\rho_A) = -p\log_2 p - (1-p)\log_2(1-p)$, and the geometric discord equals the marginal linear entropy, $2D_G(\rho_p) = 2(1 - \mathrm{Tr}\rho_A^2) = 4\det\rho_A = 4p(1-p)$, where we have denoted the eigenvalues of the reduced density matrix ρ_A by $\{p, 1-p\}$.

In contrast, the upper boundary (v) in Fig. 2, despite being single-branched, is more involved and we are unable to provide a tractable parametrization of the states that saturate it. They can be sought among symmetric X states of full rank, but with the two biggest eigenvalues dominating the other two. The extremal curve has been obtained as the result of extensive numerical optimization, in which the parameter space has been finely sliced in discrete intervals of nearly constant discord, and for each interval the data point corresponding to the random state with the maximum geometric discord has been selected. Joining all such extremal states we have obtained the smooth (magenta online) line in Fig. 2.

The two measures $\mathcal{D}$ and $2D_G$ correctly coincide in classical-quantum states, Eq. (11), where both vanish, and in maximally entangled Bell states, where both reach unity.

V. CONCLUSIONS

We have presented a reliable and effective algorithm for evaluation of the quantum discord $\mathcal{D}$ of general two-qubit states. We have simplified the optimization involved in calculating the conditional entropy, by removing the redundant degrees of freedom that can be set to 0 by means of local unitaries in the first place and by properly taking into account the symmetries of the problem. The optimization problem for the conditional entropy, and equivalently for the discord, is recast into a compact form that implies an elegant relationship

among the eigenvalues of the ensemble obtained after the local measurement process on one qubit. The derived transcendental constraints are is amenable to direct numerical solution.

We have then compared quantum discord with an alternative but affine quantity, the geometric discord D_G, identifying the classes of states with extremal values of geometric discord at a fixed quantum discord. For a fixed geometric discord, maximal quantum discord is attained by different families of states, depending on the degree of nonclassical correlations, encompassing pure as well as mixed symmetric and nonsymmetric states. In general, the hierarchical bound $\mathcal{D} \leqslant \sqrt{2D_G}$ holds for all two-qubit states.

We hope that our results will provide further insight into the fascinating but still not well-understood paradigm of nonclassical correlations beyond entanglement in composite quantum systems. The methods presented here can be generalized to higher dimensional and continuous variable systems.

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