Interplay between computable measures of entanglement and other quantum correlations

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Interplay between computable measures of entanglement and other quantum correlations

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Composite quantum systems can be in generic states characterized not only by entanglement but also by more general quantum correlations. The interplay between these two signatures of nonclassicality is still not completely understood. In this work we investigate this issue, focusing on computable and observable measures of such correlations: entanglement is quantified by the negativity $\mathcal{N}$, while general quantum correlations are measured by the (normalized) geometric quantum discord D_G. For two-qubit systems, we find that the geometric discord reduces to the squared negativity on pure states, while the relationship $D_G \geqslant \mathcal{N}^2$ holds for arbitrary mixed states. The latter result is rigorously extended to pure, Werner, and isotropic states of two-qudit systems for arbitrary d, and numerical evidence of its validity for arbitrary states of a qubit and a qutrit is provided as well. Our results establish an interesting hierarchy, which we conjecture to be universal, between two relevant and experimentally friendly nonclassicality indicators. This ties in with the intuition that general quantum correlations should at least contain and in general exceed entanglement on mixed states of composite quantum systems.

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I. INTRODUCTION

The distinction between quantum and classical correlations in the state of a multipartite physical system is a fundamental problem with far-reaching implications [1,2]. Correlations can be regarded as genuinely classical if they are essentially revealed by classical information theory tools as analogs of correlations between random variables. On the other hand, entangled states have been traditionally considered to be the only quantum-correlated class of states [3], but this statement has recently proven to be misleading. Several features of separable (i.e., unentangled) states are incompatible with a purely classical description. To mention a few, an ensemble of separable nonorthogonal states cannot be discriminated perfectly [4], general separable states may have off-diagonal coherences in any product basis [5], or, more practically, a measurement process on part of a composite system in a separable state may (and in general does) induce disturbance on the state of the complementary subsystems [6]. These are some genuine signatures of nonclassicality of correlations in the considered states but without any entanglement.

Renewed attention toward the properties and the usefulness of such general quantum correlations in separable (and entangled) states has been triggered by the observation that, in mixed-state models of quantum computation (e.g., the so-called DQC1), such general quantum correlations may be at the root of a speedup compared to the classical scenario, despite the presence of zero or nearly vanishing entanglement [7,8]. In general, it still remains an open issue whether such general quantum correlations are just related to the statistical properties of a state or if they represent truly some stronger, physical correlations of quantum nature that reduce to the entanglement in some cases and go beyond it in general [9].

It is clear that on pure bipartite states of arbitrary quantum systems, entanglement and quantum correlations are just synonyms. Both of them collapse onto the notion of a lack of information about the system under scrutiny when only a subsystem is probed. Quantitatively, this implies that any meaningful measure of entanglement or general quantum correlations should just reduce to some monotonic function of the marginal entropy of each reduced subsystem when applied to pure bipartite states. The question becomes significantly more interesting for mixed bipartite states. One would expect to find, in general, an amount of quantum correlations that is no less than some valid entanglement monotone. In this paper we prove such an intuition to hold true for a particular choice of quantifiers of entanglement and quantum correlations on arbitrary two-qubit states and on a relevant subclass of two-qudit states.

We recall that, in the last decade, a zoo of entanglement measures (say $\mathcal{E}$, the amount of entanglement they aim to quantify) has been introduced [10], and in a more recent drift several measures have been proposed as well to evaluate the degree of general quantum correlations (say $\mathcal{Q}$) in composite systems [1,2,6,11–15]. It seems reasonable to expect that

$$\mathcal{Q} \geqslant \mathcal{E} \tag{1}$$

should hold for a *bona fide* chosen pair of quantifiers (see also [16]). However, this claim turns out to be not mathematically fulfilled in some canonical cases. Selecting, for instance, two well-established entropic quantifiers such as the “entanglement of formation” [17] as an entanglement monotone and the “quantum discord” [1,2] as a measure of quantum correlations, one finds that the latter can be greater as well as smaller than the former depending on the states, and no clear hierarchy can be established, even in the simple cases of two-qubit systems [18] or two-mode Gaussian states [19]. An interesting study has recently succeeded in describing entanglement, classical, and quantum correlations under a unified geometric picture [13] by quantifying each type of correlations in terms of the smallest distance (according to the relative entropy) from the corresponding set of states without that type of correlations. For example, the amount of entanglement in a state ρ is given by the relative entropic distance between ρ and its closest separable state, and it is called relative

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entropy of entanglement [20]. In this context, our expectation holds: the relative entropy of entanglement $\mathcal{E}_R$ is automatically smaller in general than the so-called relative entropy of quantumness $\mathcal{Q}_R$ [12], which in turn quantifies the minimum relative entropic distance from the set of purely classically correlated states (a null-measure subset of the convex set of separable states [21]). The latter measure $\mathcal{Q}_R$ has been recently interpreted operationally within an "activation" framework that recognizes the value of general quantum correlations as resources to generate entanglement with an ancillary system [15] (see also [22,23]). Such a protocol is sufficiently general to let one define, in a natural way, quantumness measures $\mathcal{Q}_E$ associated with any proper entanglement monotone $\mathcal{E}$. In this way the question of the validity of Eq. (1) becomes especially meaningful given the natural compatibility of the involved quantifiers [16]. However, there is a nontrivial optimization step required for the calculation of each $\mathcal{Q}_E$ that hinders the explicit computability of the desired resources.

In this paper, we choose *computable* measures for entanglement and general quantum correlations. In the case of entanglement, we adopt the squared "negativity" $\mathcal{N}^2$ [24], which is a measure of abstract algebraic origin quantifying how much a bipartite state fails to satisfy the positivity of partial transpose (PPT) criterion for separability introduced by Peres and Horodecki [25]. In the case of quantum correlations, we pick the "geometric quantum discord" D_G [14], which measures (as suggested by the name) the minimum distance of a state from the set of classically correlated states, in terms of the squared Hilbert-Schmidt norm. Both measures are taken to be normalized between 0 and 1. Despite the very different origin and nature of these two measures, we prove that Eq. (1) holds, namely $D_G \geqslant \mathcal{N}^2$, for arbitrary mixed states of two qubits.

We remark that both measures play key roles in the quantum correlation scenario, especially for their observability and usefulness in quantum information applications. In fact, the negativity is a popular entanglement measure, operationally related to the entanglement cost under PPT-preserving operations [26] and amenable to experimental estimation via quantitative entanglement witnesses (which provide measurable lower bounds to $\mathcal{N}$) [27]. On the other hand, the geometric discord, operationally interpreted in [28], also admits a tight lower bound Q [29] (which is by itself a faithful, observable quantifier of general quantum correlations), whose detection, which does not require complete state tomography, currently constitutes the optimal pathway to reveal and quantitatively estimate nonclassical correlations in quantum algorithms such as DQC1 mixed-state quantum computation [8]. In this respect, we show specifically that the chain $D_G \geqslant Q \geqslant \mathcal{N}^2$ holds in general two-qubit states (where the leftmost inequality is analytical [29] and the rightmost one is corroborated by numerical simulations).

Furthermore, we prove that the inequality $D_G \geqslant \mathcal{N}^2$ extends to arbitrary pure, Werner [3], and isotropic states [30] of two qudits for any higher dimension d. We further provide numerical evidence that supports the validity of the inequality also in generic states of $2 \otimes 3$ systems. We then conjecture that $D_G \geqslant \mathcal{N}^2$ should hold for arbitrary mixed states of a $d \otimes d'$ bipartite system. Our results demonstrate an interesting hierarchy between two apparently unrelated quantifiers of nonclassicality, both of which have closed formulas (and experimentally friendly detection schemes) available on the classes of states considered here.

The fact that the geometric discord stands as a sharp upper bound on a computable measure of entanglement such as the (squared) negativity is a worthwhile issue to impose a rigorous ordering of resources for all those applications where the performance of a quantum information and communication primitive relies on the amount and the nature of nonclassical correlations between the involved parties [31].

This paper is organized as follows. Section II recalls the definitions of negativity and geometric discord. In Sec. III we compare the two measures on arbitrary states of two qubits. In Sec. IV we extend our analysis to higher-dimensional systems. We summarize our results and discuss future perspectives in Sec. V.

II. MEASURES OF ENTANGLEMENT AND QUANTUM CORRELATIONS

A. Negativity

According to the PPT criterion [25], if a state $\rho_{AB} \equiv \rho$ of a bipartite quantum system is separable, then the partially transposed matrix ρ^{t_A} is still a valid density operator, namely, it is positive semidefinite. In general, ρ^{t_A} is defined as the result of the transposition performed on only one (A in this case) of the two subsystems in some given basis. Even though the resulting ρ^{t_A} does depend on the choice of the transposed subsystem and on the transposition basis, the statement $\rho^{t_A} \geqslant 0$ is invariant under such choices [25]. For $2 \otimes 2$ and $2 \otimes 3$ mixed states [25], for arbitrary $d \otimes d'$ pure states, and for all Gaussian states of $1 \otimes n$ mode continuous variable systems [32], the PPT criterion is a necessary and sufficient condition for separability, and at the same time, its failure reliably marks the presence of entanglement. In all the other cases, there exist states that can be entangled with a positive partial transpose: they are so-called bound entangled states, whose entanglement cannot be distilled by means of local operations and classical communications (LOCC) [33].

On a quantitative level, the negativity of the partial transpose, or, simply, "negativity," $\mathcal{N}(\rho)$ [24,34] can be adopted as a valid, computable measure of (distillable) entanglement for arbitrary bipartite systems. The negativity of a quantum state ρ of a bipartite $d \otimes d$ system can be defined as

$$\mathcal{N}(\rho) = \frac{1}{d-1}(\|\rho^{t_A}\|_1 - 1)\,, \tag{2}$$

where

$$\|M\|_1 = \mathrm{Tr}|M| = \sum_i |m_i| \tag{3}$$

stands for the 1-norm, or trace norm, of the matrix M with eigenvalues $\{m_i\}$. The quantity $\mathcal{N}(\rho)$ is proportional to the modulus of the sum of the negative eigenvalues of ρ^{t_A}, quantifying the extent to which the partial transpose fails to be positive.

The negativity $\mathcal{N}$ is in general an easily computable entanglement measure, and it has been proven to be (along with its square $\mathcal{N}^2$) convex and monotone under LOCC [24].

The squared negativity $\mathcal{N}^2$ satisfies a monogamy inequality on the sharing of entanglement for multiqubit systems [35].

B. Geometric quantum discord

The "geometric quantum discord" D_G has been recently introduced as a simple geometrical quantifier of general nonclassical correlations in bipartite quantum states [14]. Let us suppose to have a bipartite system AB in a state ρ and to perform a local measurement on the subsystem B. Almost all (entangled or separable) states will be subject to some disturbance due to such a measurement [21]. However, there is a subclass of states that is left unperturbed by at least one measurement: it is the class of the so-called "classical-quantum" states [5], whose representatives have a density matrix of this form:

$$\rho = \sum_i p_i \rho_{Ai} \otimes |i\rangle\langle i|, \tag{4}$$

where p_i is a probability distribution, ρ_{Ai} is the marginal density matrix of A, and $\{|i\rangle\}$ is an orthonormal vector set. Letting Ω be the set of classical-quantum states and χ be a generic element of 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 [14], the (unnormalized) squared Hilbert-Schmidt distance is adopted. We employ here a normalized version of the geometric quantum discord for arbitrary mixed states ρ of a $d \otimes d$ quantum system,

$$D_G(\rho) = \frac{d}{d-1} \min_{\chi \in \Omega} \|\rho - \chi\|_2^2, \tag{5}$$

where

$$\|M\|_2 = \sqrt{\mathrm{Tr}(MM^\dagger)} = \sqrt{\sum_i m_i^2} \tag{6}$$

stands for the 2-norm, or Hilbert-Schmidt norm, of the matrix M with eigenvalues $\{m_i\}$. The quantity $D_G(\rho)$ in Eq. (5) is normalized between 0 (on classical-quantum states) and 1 (on maximally entangled states $\rho = |\psi\rangle\langle\psi|$, $|\psi\rangle = d^{-1/2}\sum_{j=0}^{d-1} |j\rangle|j\rangle$).

The geometric discord can be reinterpreted as the minimal disturbance, again measured according to the squared Hilbert-Schmidt distance, induced by any projective measurement Π^B on subsystem B [28],

$$D_G(\rho) = \frac{d}{d-1} \min_{\Pi^B} \|\rho - \Pi^B(\rho)\|_2^2 .$$

We notice that the geometric discord is not symmetric under a swap of the two parties, $A \leftrightarrow B$.

The minimization involved in the definition of the geometric quantum discord can be solved exactly for arbitrary two-qubit states [14] and pure two-qudit states [28,36], leading to computable formulas, as detailed in the following sections. In the remainder of the paper, we will compare entanglement, quantified by $\mathcal{N}^2$, and quantum correlations, quantified by D_G. The latter will be shown to majorize the former. We observe that picking the square of the negativity as the entanglement measure is unconventional yet necessary in this case: we want to make a mathematically consistent comparison of the measures, both acting quadratically on the eigenvalues of the involved matrices [compare Eqs. (2) and (5)].

III. GEOMETRIC DISCORD VERSUS NEGATIVITY IN TWO-QUBIT SYSTEMS

The main result of this section is the following.

Theorem 1. For every general two-qubit state ρ, the geometric quantum discord is always greater than or equal to the squared negativity,

$$D_G(\rho) \geqslant \mathcal{N}^2(\rho) . \tag{7}$$

Let us review the formulas needed to evaluate the two chosen measures for generic two-qubit states.

The geometric discord D_G admits an explicit closed expression for two-qubit states [14]. First, one needs to express the 4×4 density matrix ρ of a two-qubit state in the so-called Bloch basis (or R picture) [37]:

$$\begin{aligned}\rho &= \frac{1}{4}\sum_{i,j=0}^{3} R_{ij}\sigma_i \otimes \sigma_j \\ &= \frac{1}{4}\left(\mathbb{I}_4 + \sum_{i=1}^{3} x_i\sigma_i \otimes \mathbb{I}_2 + \sum_{j=1}^{3} y_j \mathbb{I}_2 \otimes \sigma_j + \sum_{i,j=1}^{3} t_{ij}\sigma_i \otimes \sigma_j\right),\end{aligned} \tag{8}$$

where $R_{ij} = \mathrm{Tr}[\rho(\sigma_i \otimes \sigma_j)]$, $\sigma_0 = \mathbb{I}_2$ and σ_i $(i = 1,2,3)$ are the Pauli matrices, $\vec{x} = \{x_i\}$ and $\vec{y} = \{y_i\}$ are the three-dimensional Bloch column vectors associated with subsystems A and B, and t_{ij} denote the elements of the correlation matrix T. Then, following [14], the normalized geometric discord D_G, Eq. (5), takes the form

$$D_G(\rho) = \tfrac{1}{2}\big(\|\vec{y}\|^2 + \|T\|_2^2 - k\big), \tag{9}$$

with k being the largest eigenvalue of the matrix $\vec{y}\vec{y}^t + T^tT$. The expression in Eq. (9) can be also recast as the solution to a variational problem [28]; namely, for two qubits,

$$D_G(\rho) = 2\big[\mathrm{Tr}(C^tC) - \max_A \mathrm{Tr}(AC^tCA^t)\big] , \tag{10}$$

where $C = R/2$ and the maximum is taken over all 2×4 isometries $A = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix}1 & \vec{a}\\ 1 & -\vec{a}\end{smallmatrix}\right)$, with $\vec{a}$ being a three-dimensional unit vector.

Concerning the negativity $\mathcal{N}$, Eq. (2), it is known that a two-qubit state ρ is separable if and only if $\rho^{t_A} \geqslant 0$ [25], and for entangled two-qubit states ρ, at most one eigenvalue of the partial transpose ρ^{t_A} can be negative [37]. Denoting by $\{\lambda_i\}$ the eigenvalues of ρ^{t_A} in decreasing order, for two-qubit entangled states we have $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant 0 \geqslant \lambda_4$, and the negativity of ρ takes the form [24]

$$\mathcal{N}(\rho) = \|\rho^{t_A}\|_1 - 1 = 2|\lambda_4| , \tag{11}$$

while for separable states ($\lambda_4 \geqslant 0$) one has $\mathcal{N}(\rho) = 0$.

We first compare entanglement and quantum correlations in the simple instance of pure two-qubit states $\rho^p = |\psi\rangle\langle\psi|$. Up to local unitary operations (which leave correlations invariant), a two-qubit pure state can be written in its Schmidt decomposition, corresponding to a density matrix of the form

$$\rho^p = \begin{pmatrix} \frac{1}{2}(\sqrt{1-\mathcal{N}^2}+1) & 0 & 0 & \frac{\mathcal{N}}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{\mathcal{N}}{2} & 0 & 0 & \frac{1}{2}(1-\sqrt{1-\mathcal{N}^2}) \end{pmatrix}. \tag{12}$$

It is straightforward to show that in this case,

$$D_G(\rho^p) = \mathcal{N}^2(\rho^p) \equiv S_L(\rho_A^p), \tag{13}$$

where $S_L(\rho_A^p) = 4\mathrm{Det}(\rho_A^p)$ denotes the marginal linear entropy of one subsystem in its reduced state. As expected, entanglement and quantum correlations correctly coincide for pure two-qubit states, and specifically, the two chosen measures (geometric discord and squared negativity) collapse onto the very same quantifier of local lack of purity.

For general two-qubit mixed states, our intuition dictates that the amount of quantum correlations should exceed entanglement. This is formalized in Theorem 1, which we are now ready to prove.

Proof. We focus on the case of entangled states, as Eq. (7) trivially holds when ρ is separable.

First, we look at the original formulation of geometric discord in [14]: the closest classical-quantum state $\bar{\chi}$ that achieves the minimum of the Hilbert-Schmidt norm $||\rho-\chi||_2^2$ is such that $\mathrm{Tr}[\rho\bar{\chi}] = \mathrm{Tr}[\bar{\chi}^2]$. Thus, we can rewrite Eq. (5) as

$$\begin{aligned} D_G &= 2\min_{\chi\in\Omega}\|\rho-\chi\|_2^2 = 2(\mathrm{Tr}[\rho^2]-\mathrm{Tr}[\bar{\chi}^2]) \\ &= 2(\mathrm{Tr}[\rho^{t_A\,2}]-\mathrm{Tr}[\bar{\chi}^2]). \end{aligned} \tag{14}$$

Then, denoting (as before) by $\lambda = \{\lambda_i\}$ the vector of eigenvalues of ρ^{t_A} in decreasing order ($\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant 0 \geqslant \lambda_4$) and similarly denoting by $\varsigma = \{\varsigma_i\}$ the vector of eigenvalues of $\bar{\chi}$ ($\varsigma_1 \geqslant \varsigma_2 \geqslant \varsigma_3 \geqslant \varsigma_4 \geqslant 0$), recalling that the Hilbert-Schmidt norm is invariant under partial transposition [38], we obtain $\sum_{i=1}^4 \varsigma_i^2 = \mathrm{Tr}[\rho^{t_A}\bar{\chi}]$. We can further exploit the Hoffman-Wielandt theorem [39], which implies that

$$\|\rho^{t_A}-\bar{\chi}\|_2^2 \geqslant \sum_{i=1}^4 |\lambda_i-\varsigma_i|^2 = \sum_{i=1}^3 |\lambda_i-\varsigma_i|^2 + (|\lambda_4|+\varsigma_4)^2. \tag{15}$$

Thus, from (14) and (15) we have

$$\sum_{i=1}^4 \varsigma_i^2 = \sum_{i=1}^4 \lambda_i\varsigma_i. \tag{16}$$

Now, let us consider the function

$$f(\lambda,\varsigma) = \sum_{i=1}^3 \lambda_i|\lambda_i-\varsigma_i| - |\lambda_4|(|\lambda_4|-\varsigma_4); \tag{17}$$

it is easy to see that, performing an optimization by the Lagrange multipliers method, the minimum of f remaining fixed $|\lambda_4|$ and ς_4 (say f') is reached when $\lambda_1 = \lambda_2 = \lambda_3 = \frac{(1+|\lambda_4|)}{3}$ and $\varsigma_1 = \varsigma_2 = \varsigma_3 = \frac{1-\varsigma_4}{3}$. Hence, we have

$$\begin{aligned} f'(|\lambda_4|,\chi_4) = (1+|\lambda_4|)\left(\frac{1+|\lambda_4|}{3} - \frac{1-\varsigma_4}{3}\right) \\ - |\lambda_4|(|\lambda_4|-\varsigma_4). \end{aligned}$$

Furthermore, optimizing over ς_4, we obtain f'', which is the minimum of f at fixed $|\lambda_4|$ (i.e., at fixed negativity):

$$f''(|\lambda_4|) = \frac{1+|\lambda_4|}{3} - |\lambda_4| \geqslant 0. \tag{18}$$

Finally, the last inequality implies $\sum_{i=1}^3 \lambda_i|\lambda_i-\varsigma_i| \geqslant |\lambda_4|(|\lambda_4|-\varsigma_4)$, i.e.,

$$\sum_{i=1}^3 \lambda_i|\lambda_i-\varsigma_i| + |\lambda_4|(|\lambda_4|+\varsigma_4) \geqslant 2|\lambda_4|^2,$$

and thanks to Eq. (16) this yields

$$\sum_{i=1}^4 |\lambda_i-\varsigma_i|^2 \geqslant 2|\lambda_4|^2, \tag{19}$$

which is equivalent to Eq. (7), thus demonstrating the claim. This concludes the proof of Theorem 1 for all two-qubit mixed states. ■

To illustrate the comparison between geometric discord and squared negativity, we plot in Fig. 1(a) the physical region filled with 10^5 randomly generated two-qubit states in the space D_G versus $\mathcal{N}^2$. Along with the lower bound (red online) emerging from Theorem 1, saturated by pure states [Eq. (12)] for which $D_G = \mathcal{N}^2$, we notice the existence of an upper bound as well on D_G at fixed negativity. This shows that the quantum correlations in excess of entanglement or, in general, beyond entanglement are somehow constrained. Two-qubit states saturating the upper bound (green online) can be sought within the class of rank-2 X-shaped density matrices of the form

$$\rho^X = \begin{pmatrix} a & 0 & 0 & \sqrt{ad} \\ 0 & b & \sqrt{bc} & 0 \\ 0 & \sqrt{bc} & c & 0 \\ \sqrt{ad} & 0 & 0 & d \end{pmatrix}, \tag{20}$$

where $d=1-a-b-c$ and $b=[2-2a-2c+2(-1+6a-7a^2+6c-18ac-7c^2+4\sqrt{2}\sqrt{ac(-1+2a+2c)^2})^{\frac{1}{2}}]/4$, with a and c varying in the parameter range $0 \leqslant a,c \leqslant 1/2$, $-1+6a-7a^2+6c-18ac-7c^2+4\sqrt{2}\sqrt{ac}|2a+2c-1| \geqslant 0$. The remaining optimization of D_G at fixed $\mathcal{N}^2$ can be efficiently done numerically.

In the limiting case of separable two-qubit states, $\mathcal{N}(\rho^{\mathrm{sep}}) = 0$, the maximum value of the (normalized) geometric discord can be analytically found to be [40]

$$D_G(\rho_{\mathrm{opt}}^{\mathrm{sep}}) = \tfrac{1}{4}. \tag{21}$$

This is achieved by imposing the edge of separability, $\lambda_4 = 0$, that corresponds to $ad = bc$ in Eq. (20). The maximum D_G

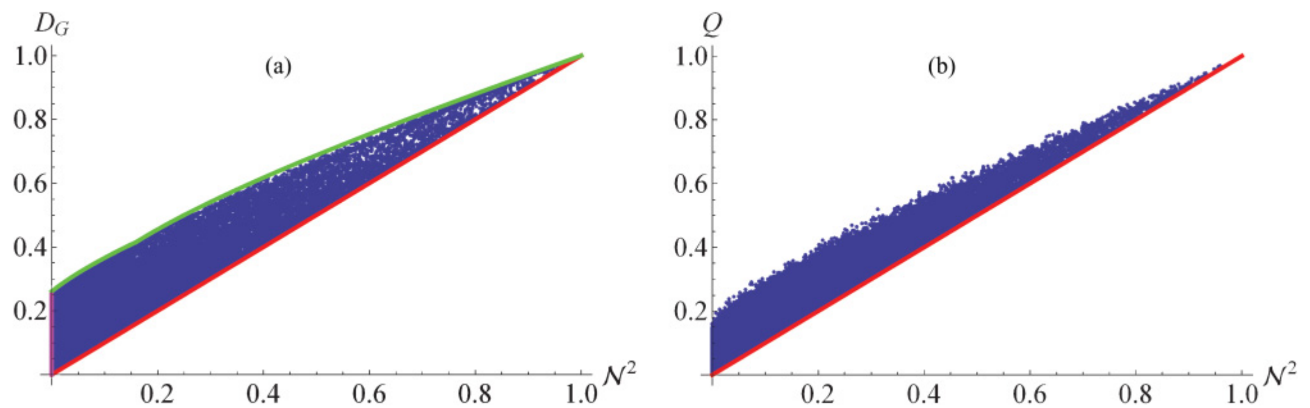

FIG. 1. (Color online) (a) Geometric quantum discord D_G and (b) its observable lower bound Q vs squared negativity $\mathcal{N}^2$ for 10^5 randomly generated states of two qubits. The lower boundary (red online) in both plots accommodates pure states. In (a), the upper boundary (green online) can be saturated by a subclass of rank-2 states of the form of Eq. (20), while the side (magenta online) vertical line at $\mathcal{N}^2 = 0$ is filled by separable states with nonzero quantum correlations, which reach up to the value $D_G = 1/4$ on states of the form of Eq. (22). All the quantities plotted are dimensionless.

is then reached, e.g., for $a = c = \frac{1}{8}(2 + \sqrt{2})$. Notice that the corresponding state $\rho^{\rm sep}_{\rm opt}$,

$$\rho^{\rm sep}_{\rm opt} = \begin{pmatrix} \frac{1}{8}(2+\sqrt{2}) & 0 & 0 & \frac{1}{4\sqrt{2}} \\ 0 & \frac{1}{8}(2-\sqrt{2}) & \frac{1}{4\sqrt{2}} & 0 \\ 0 & \frac{1}{4\sqrt{2}} & \frac{1}{8}(2+\sqrt{2}) & 0 \\ \frac{1}{4\sqrt{2}} & 0 & 0 & \frac{1}{8}(2-\sqrt{2}) \end{pmatrix}, \tag{22}$$

upon swapping the subsystems A and B, becomes of the classical-quantum form of Eq. (4), i.e., a state with zero D_G. This suggests that the maximum geometric discord for general two-qubit separable states is obtained on an extremally asymmetric state [the marginal state $\rho^{\rm sep}_{{\rm opt}\,A}$ is maximally mixed, while the marginal state of subsystem B is quasipure, ${\rm Tr}(\rho^{\rm sep\,2}_{{\rm opt}\,B}) = 3/4$] that displays no signature of quantum correlations at all if subsystem A rather than B is probed by local measurements. The example in Eq. (22) is just one of an entire class of two-qubit states that enjoy the same property [23].

The full allowed range $0 \leqslant D_G \leqslant 1/4$ for the geometric discord of separable states [vertical magenta line in Fig. 1(a)] can be spanned, for instance, by mixtures of the form $\rho^{\rm sep}_p = p\rho^{\rm sep}_{\rm opt} + (1-p)I/4$, with $0 \leqslant p \leqslant 1$, for which $D_G(\rho^{\rm sep}_p) = p^2/4$.

We can refine the hierarchy proven in this section by taking into account the observable measure of quantum correlations Q introduced in [29]. In particular, for arbitrary two-qubit states this quantity takes the form of a state-independent function of the density matrix elements given by

$$Q = \tfrac{2}{3}\left({\rm Tr}[S] - \sqrt{6{\rm Tr}[S^2] - 2({\rm Tr}[S])^2}\right), \tag{23}$$

where $S = \frac{1}{4}(\vec{y}\vec{y}^t + T^t T)$. We have shown in [29] how to recast Q in terms of observables that can be measured experimentally via simple quantum circuits. We also proved that Q is a tight lower bound to the geometric discord, i.e., $D_G \geqslant Q$, where the inequality is saturated for pure states and $Q = 0 \iff D_G = 0$. In Fig. 1 we plot Q versus the squared negativity: numerics confirm that this quantity is still an upper bound to $\mathcal{N}^2$. Therefore, the following hierarchical ordering is satisfied for all two-qubit states: $D_G \geqslant Q \geqslant \mathcal{N}^2$, while all the quantifiers become equal for pure states.

IV. GEOMETRIC DISCORD VERSUS NEGATIVITY IN HIGHER-DIMENSIONAL SYSTEMS

Here we provide extensions of the results of the previous section to $d \otimes d$ and $d \otimes d'$ systems.

A. Pure $d \otimes d$ states

We first generalize Theorem 1 to arbitrary pure states of two qudits. Namely, we prove the following.

Theorem 2. For every pure two-qudit state $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$, the geometric quantum discord is always greater than or equal to the squared negativity,

$$D_G(\psi) \geqslant \mathcal{N}^2(\psi). \tag{24}$$

Proof. Any pure state $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ can be written without loss of generality in the Schmidt decomposition:

$$|\psi\rangle = \sum_{j=0}^{d-1} \sqrt{\alpha_j}|j\rangle|j\rangle\,, \tag{25}$$

where the Schmidt coefficients are probability amplitudes, $\sum_j \alpha_j = 1$.

The geometric discord [Eq. (5)] can be computed in this case following Luo and Fu [28,36]. The closest classical state to $|\psi\rangle$, entering the definition [Eq. (5)], turns out to be the completely uncorrelated state $\rho^{\otimes} = \rho_A \otimes \rho_B$ obtained as the tensor product of the marginal states $\rho_A = {\rm Tr}_B(|\psi\rangle\langle\psi|)$ and $\rho_B = {\rm Tr}_A(|\psi\rangle\langle\psi|)$. This implies

$$D_G(\psi) = \frac{d}{d-1}\left(1 - \sum_i \alpha_i^2\right) = \frac{2d}{d-1}\sum_{j>i}\alpha_i\alpha_j\,. \tag{26}$$

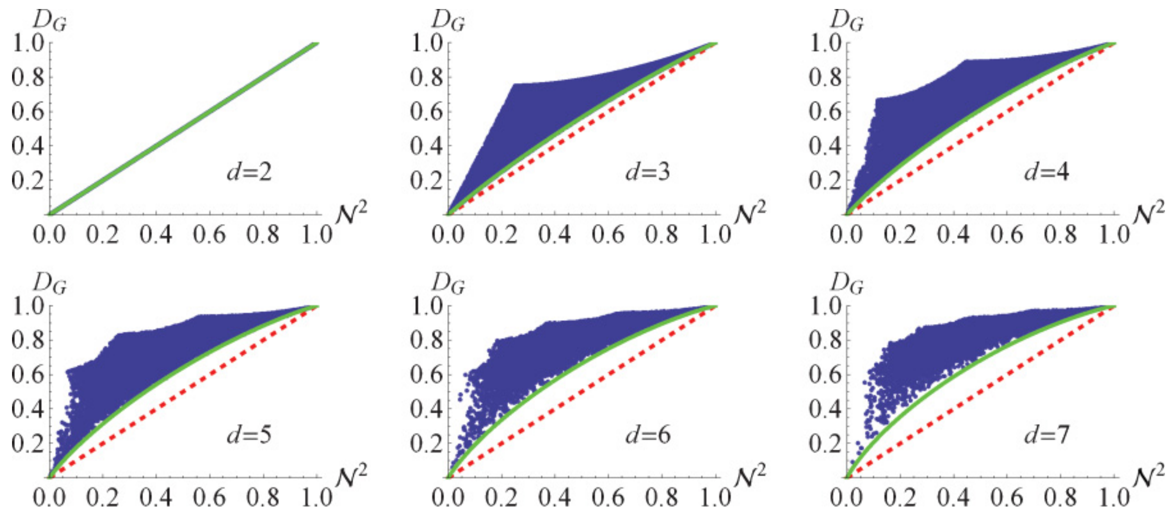

FIG. 2. (Color online) Geometric quantum discord vs squared negativity for 3×10^4 (per panel) randomly generated pure states of two qudits with $d = 2, \ldots, 7$. The two measures coincide for $d = 2$ (pure two-qubit states). In general, the dashed red line $D_G = \mathcal{N}^2$ is not attainable for intermediate values of both measures, while a tighter lower bound (solid green line) on D_G exists at fixed negativity, given by Eq. (31). Such a bound is saturated by states with Schmidt decomposition as in Eq. (30). The upper bound on D_G at fixed negativity is more structured. Notice that these plots can be also interpreted as the span of the pair of entanglement measures τ_2 [42] vs $\mathcal{N}^2$ [24] for two-qudit pure states. All the quantities plotted are dimensionless.

Meanwhile, the negativity [Eq. (2)] is given by [24]

$$\mathcal{N}(\psi) = \frac{1}{d-1}\left[\left(\sum_i \sqrt{\alpha_i}\right)^2 - \sum_i \alpha_i\right] = \frac{1}{d-1}\left[\left(\sum_i \sqrt{\alpha_i}\right)^2 - 1\right]. \tag{27}$$

We know from [41] that the following inequality holds:

$$4\sum_{j>i} \alpha_i\alpha_j \geqslant \frac{2}{d(d-1)}\left[\left(\sum_i \sqrt{\alpha_i}\right)^2 - 1\right]^2; \tag{28}$$

therefore we obtain

$$2\frac{d}{d-1}\sum_{j>i} \alpha_i\alpha_j \geqslant \frac{1}{(d-1)^2}\left[\left(\sum_i \sqrt{\alpha_i}\right)^2 - 1\right]^2. \tag{29}$$

The left side is the normalized geometric discord, while the right side is the normalized squared negativity. ∎

We have already seen that for $d = 2$, the two measures D_G and $\mathcal{N}^2$ indeed coincide on pure states. However, for any $d > 2$, the geometric discord is in general strictly larger than the negativity. This seems to go against the expectation that quantum correlations should reduce to entanglement on pure states. In fact, D_G does reduce to an entanglement measure on general two-qudit pure states, but such a measure is in general different from the squared negativity for $d \geqslant 3$. The pure-state entanglement monotone that takes the very same expression as in Eq. (26) is a particular coefficient τ_2 of the characteristic polynomial of the nontrivial block of the Gram matrix of pure two-qudit states (see [42] for details). Such a measure has not been studied for mixed states, and it is an interesting (yet technically challenging) open problem to see whether the hierarchy $D_G \geqslant \tau_2$ holds for general two-qudit mixed states beyond $d = 2$.

Coming back to our measures of choice in this work, geometric discord and squared negativity, we can visualize their interplay on pure two-qudit states with increasing d. We have generated a large ensemble of two-qudit states up to $d = 7$ with random Schmidt coefficients. At fixed negativity, the geometric discord displays both upper and lower bounds. The upper bounds are multibranched, with an increasing number of nodes appearing with increasing d. The lower bounds are regular curves lying in general strictly above the bisectrix for any $d > 2$, with $D_G = \mathcal{N}^2$ occurring only at the extremal points where both vanish (on factorized states) or both reach the maximum (on maximally entangled states). We find that, for any d, the pure two-qudit states that achieve the minimum geometric discord at fixed negativity (solid green curve in Fig. 2) have a peculiar distribution of Schmidt coefficients:

$$\alpha_0 = \sin^2\theta\,, \qquad \alpha_i = \frac{\cos^2\theta}{d-1} \;\; \forall\, i = 1, \ldots, d-1\,, \tag{30}$$

with $\arccos\sqrt{(d-1)/d} \leqslant \theta \leqslant \pi/2$. Since this is true for every pure state in the special case $d = 2$, this is a further proof that on two-qubit pure states D_G equals $\mathcal{N}^2$, as observed in the previous section. In general, the lower bound on D_G at fixed $\mathcal{N}$ as saturated by the states of Eq. (30) is given by

$$\begin{aligned} D_G^{\text{low}}(\mathcal{N}) = {} & [2(d-R-1) + (d-2)(d-1)\mathcal{N}] \\ & \times \{2[(d-1)^2 + R] - (d-2)(d-1)\mathcal{N}\} \\ & \times [(d-1)^2 d^2]^{-1}\,, \end{aligned} \tag{31}$$

with $R = \sqrt{(d-1)^2(1-\mathcal{N})[1+(d-1)\mathcal{N}]}$.

B. Werner and isotropic $d \otimes d$ states

The ordering relationship between geometric discord and squared negativity can be further extended rigorously to two special classes of *mixed* $d \otimes d$ highly symmetric states, namely, the Werner states [3] and the isotropic states [30]. We recall that for both families of states the PPT criterion is necessary and sufficient for separability [43].

The Werner states in arbitrary d dimension take the form [3]

$$\rho_w = \frac{d+k}{d^3-d}\mathbb{I}_d + \frac{-dk-1}{d^3-d}|\Phi\rangle\langle\Phi|, \tag{32}$$

where $|\Phi\rangle = \sum_{i,j=0}^{d-1}(|ij\rangle + |ji\rangle)$ and $k \in [-1,1]$ with $0 < k \leqslant 1$ for entangled states. The geometric discord calculated in [28] and then normalized is

$$D_G(\rho_w) = \frac{(dk+1)^2}{(d+1)^2}, \tag{33}$$

while after simple algebra we obtain the following expression for the (normalized) negativity:

$$\mathcal{N}(\rho_w) = \max\{0,k\}. \tag{34}$$

The isotropic states can be instead defined as [30]

$$\rho_i = \frac{1-p}{d^2-1}\mathbb{I}_d + \frac{d^2p-1}{d^2-1}|\Psi\rangle\langle\Psi|, \tag{35}$$

where $|\Psi\rangle = \frac{1}{\sqrt{d}}\sum_{i=0}^{d-1}|ii\rangle$ and $p \in [0,1]$, with the states being entangled for $p > 1/d$. In such a case the (normalized) geometric discord [28] is

$$D_G(\rho_i) = \frac{(d^2p-1)^2}{(d^2-1)^2}, \tag{36}$$

and the negativity is given by [44]

$$\mathcal{N}(\rho_i) = \max\left\{0, \frac{dp-1}{d-1}\right\}. \tag{37}$$

Interestingly, for both classes of states (in the nontrivial region of parameters where they are entangled) some straightforward algebra shows that the simple relationship

$$D_G(\rho_{w,i}) = \left[\frac{1+d\,\mathcal{N}(\rho_{w,i})}{1+d}\right]^2 \geqslant \mathcal{N}^2(\rho_{w,i}) \tag{38}$$

holds, thus establishing once again the desired hierarchy.

We notice a radical difference between quantum correlations of Werner and isotropic states in the region in which they are separable. Namely, for Werner states the quantum correlations measured by the geometric discord can grow, approaching the maximum (which is 1 in normalized units) even without entanglement, with increasing dimension d, so that $\lim_{d\to\infty} D_G(\rho_w) = k^2$ in the full range $k \in [-1,1]$, half of which contains separable states. Therefore Werner states with

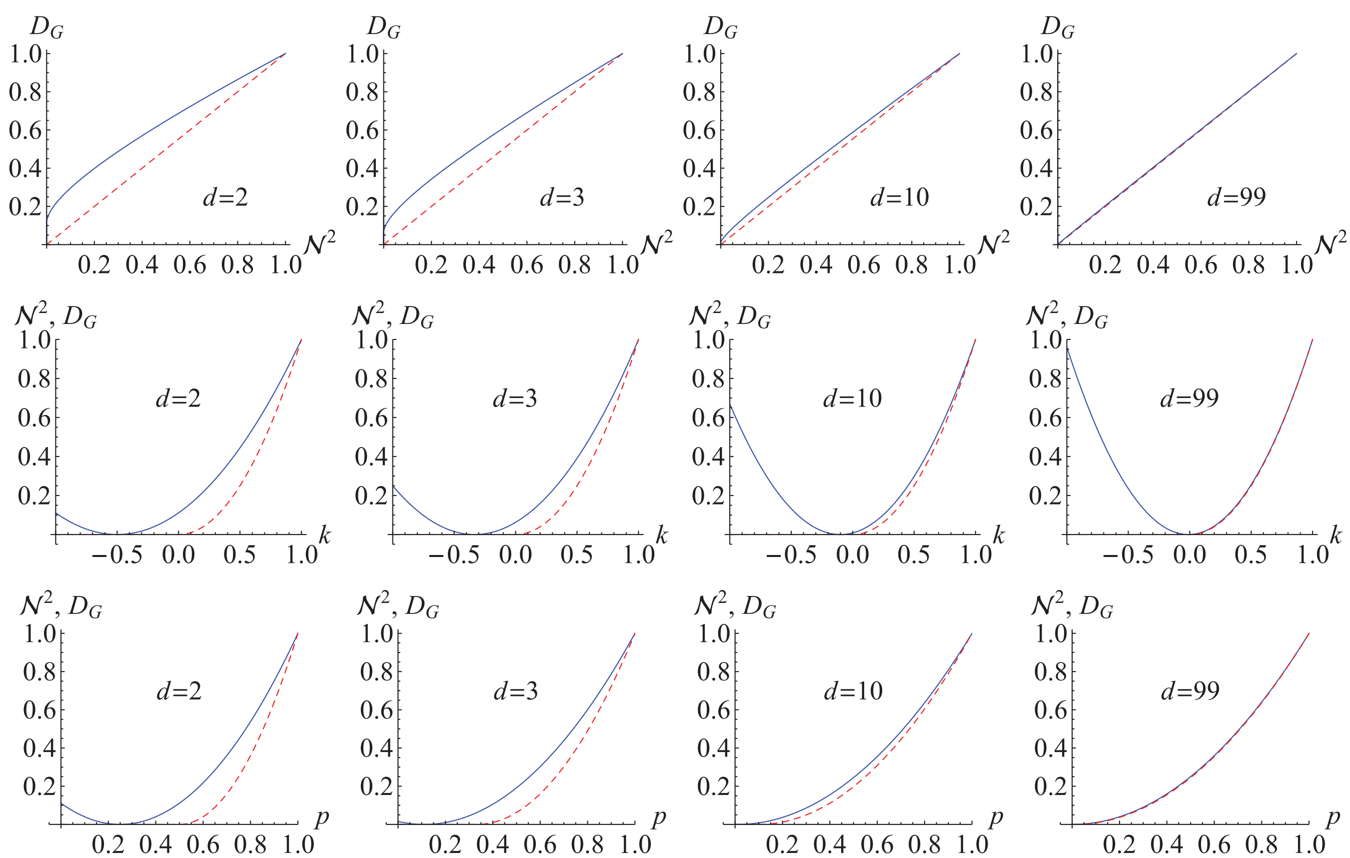

FIG. 3. (Color online) (top) Geometric quantum discord vs squared negativity (solid blue line) [Eq. (38)] for $d \otimes d$ Werner states with dimensions $d = 2,3,10,99$ (from left to right); the dashed red line of the equation $D_G = \mathcal{N}^2$ is just a guide to the eye. The corresponding plots for isotropic states are identical, apart from the extra vertical branch at $\mathcal{N} = 0$ that is absent in those cases. (middle) D_G (solid blue line) and $\mathcal{N}^2$ (red dashed line) for $d \otimes d$ Werner states (32) plotted as a function of the parameter $k \in [-1,1]$. (bottom) D_G (solid blue line) and $\mathcal{N}^2$ (red dashed line) for $d \otimes d$ isotropic states (35) plotted as a function of the parameter $p \in [0,1]$. All the quantities plotted are dimensionless.

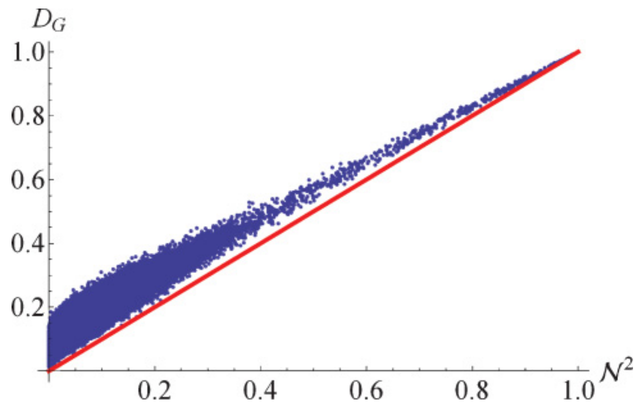

FIG. 4. (Color online) Geometric discord vs squared negativity for 2×10^5 mixed states of $2 \otimes 3$ systems, randomly generated by using the MATHEMATICA package available in [47]. All the quantities plotted are dimensionless.

high dimension and $k \to -1$ are examples of highly mixed, completely separable states whose quantum correlations are asymptotically as big as those of pure maximally entangled states, as predicted in [15] (see also [45]). On the other hand, for isotropic states, with increasing d the separability region ($0 \leqslant p \leqslant 1/d$) just shrinks to zero, meaning that in such a case the geometric discord just converges to the squared negativity in the full parameter range, with no significant signatures of quantum correlations exhibited in absence of entanglement. Note that the two families of states are instead completely equivalent in the limiting case $d = 2$ (upon identifying $k = 2p - 1$). The interplay between D_G and $\mathcal{N}^2$ for Werner and isotropic states of varying dimension is illustrated in Fig. 3.

C. Generic $d \otimes d'$ states

Encouraged by the previous results, we now wish to test the validity of the inequality $D_G \geqslant \mathcal{N}^2$ for generic mixed states of arbitrary $d \otimes d'$ dimensional systems. Specifically, we run a numerical exploration of the D_G versus $\mathcal{N}^2$ plane for randomly generated mixed states of $2 \otimes 3$ systems. In this case, the geometric discord can be computed according to the prescription of Ref. [46], while the negativity still captures all entanglement potentially present in the states [25]. Remarkably, based on extensive numerical evidence (see Fig. 4), we find that the hierarchy between geometric discord and squared negativity holds as well for arbitrary states of a qubit and a qutrit. This finding, in addition to the results of the previous sections, motivates us to conjecture that $D_G \geqslant \mathcal{N}^2$ might be a universal ordering relationship for arbitrary $d \otimes d'$ dimensional systems. A general proof of this statement would be very valuable, and an interesting, related open question concerns investigating the role of bound entanglement in higher dimensions and its interplay (not captured by the negativity) with geometric measures of quantum correlations.

V. CONCLUDING REMARKS

We have presented a qualitative and quantitative study of entanglement and general quantum correlations for arbitrary two-qubit states and for relevant instances of higher-dimensional states.

First, we identified a computable measure of entanglement, the squared negativity $\mathcal{N}^2$ [24], and proved that it is always majorized by a compatible measure of quantum correlations, the geometric discord D_G [14], in the case of generic two-qubit states. The inequality is saturated for pure states. We also provided numerical evidence that the squared negativity is still majorized by a tight lower bound Q to the geometric discord, recently proposed as an observable measure of quantum correlations [29]. Thus, the chain $D_G \geqslant Q \geqslant \mathcal{N}^2$ holds for two-qubit states.

Then, we explored the pattern of the plane D_G versus $\mathcal{N}^2$, identifying the classes of two-qubit states with maximal geometric discord at fixed negativity. In particular, the bound is reached by a family of X states given in Eq. (20). Remarkably, for separable states the upper bound accommodates a fully asymmetric state, i.e., a state becoming a zero-discord classical-quantum state upon swapping of the subsystems.

Finally, we extended our analysis to arbitrary $d \otimes d'$ systems. For two-qudit pure states, we found that the hierarchy between geometric discord and squared negativity still holds rigorously. We characterized the states with minimal D_G at fixed $\mathcal{N}^2$: they present an elegant parametrization of the distribution of their Schmidt coefficients, allowing us to express analytically the lower bound in the D_G versus $\mathcal{N}^2$ plane for any d, as in Eq. (31). In the mixed-state case, the inequality is still valid for Werner and isotropic $d \otimes d$ states, for which D_G is a simple function of the negativity for each dimension d. We further provided numerical evidence supporting the validity of the hierarchy between geometric discord and squared negativity for general mixed states of $2 \otimes 3$ systems. In all the instances analyzed in this paper, D_G and $\mathcal{N}$ were computable in closed form and were always found to obey the ordering relationship $D_G \geqslant \mathcal{N}^2$. We thus conjecture its validity on arbitrary bipartite states of any dimension, leaving open at the present the task of providing a rigorous general proof (or a counterexample) to our claim.

Our results agree with the intuitive prediction that general quantum correlations should be somehow related to entanglement and definitely incorporate it [16]. Geometric discord [14] (or its lower bound Q [29]) and negativity [24] are two computable, observable, and experimentally friendly measures of quantum correlations whose interplay, explored in this paper, is important for getting a quantitative grip on the performance of several quantum information protocols, ranging from quantum computation to quantum metrology and state discrimination [31]. Understanding the nature of nonclassical correlations and their role in determining advantages over fully classical scenarios is a central issue in quantum information processing and communication [9]. On a more fundamental level, our findings suggest that nonclassical correlations measured by geometric discord could be regarded as a more general feature that somehow incorporates entanglement and state mixedness, following the intuition advanced in [15]. Encouraging preliminary evidence that the geometric discord (the lower bound Q) can be employed to characterize the dynamics of quantum correlations in open systems and possibly other relevant features of open systems themselves (e.g., non-Markovianity [48]) has been recently presented in [29]. In this respect, the ordering relations we found suggest that entanglement and general quantum correlations as well can both be interrelated to such properties of open systems. Encouraged by the hierarchy pointed out in this paper, we believe it becomes even more meaningful to keep searching for simple but universal, physically motivated and mathematically accessible, unifying measures of "quantumness" of the correlations, along the spirit of Refs. [13,15,16,22].

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possess an unnormalized geometric discord of $1/6$, which would correspond, in our notation, to $D_G = 1/3$ (thus apparently higher than the tight bound $D_G = 1/4$ that we find here). However, such a reported value is unfortunately wrong, as following the very same analysis of [14], one finds instead for those edge separable Bell diagonal states an unnormalized value of the discord equal to $1/18$, corresponding to $D_G = 1/9$ in our notation. Our analysis and extensive numerical investigation confirm that no separable two-qubit state can achieve a higher (normalized) geometric discord than $1/4$, and in particular, no Bell diagonal separable state can even come close to saturating such a bound.

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