Quantum discord for two-qubit systems

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Quantum discord, as introduced by Olliver and Zurek [Phys. Rev. Lett. **88**, 017901 (2001)], is a measure of the discrepancy between two natural yet different quantum analogs of the classical mutual information. This notion characterizes and quantifies quantumness of correlations in bipartite states from a measurement perspective, and is fundamentally different from the various entanglement measures in the entanglement vs separability paradigm. The phenomenon of nonzero quantum discord is a manifestation of quantum correlations due to noncommutativity rather than due to entanglement, and has interesting and significant applications in revealing the advantage of certain quantum tasks. We will evaluate analytically the quantum discord for a large family of two-qubit states, and make a comparative study of the relationships between classical and quantum correlations in terms of the quantum discord. We furthermore compare the quantum discord with the entanglement of formation, and illustrate that the latter may be larger than the former, although for separable states, the entanglement of formation always vanishes and thus is less than the quantum discord.

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I. INTRODUCTION

A generic bipartite quantum state ρ , mathematically represented by a density operator, is a hybrid object with both classical and quantum characteristics. It can encode classical as well as quantum correlations by means of superposition, entanglement, and mixing. How to distinguish these two kinds of correlations is of basic importance and interest in quantum information theory.

To address the above issue, one usually works in the widely used entanglement vs separability dichotomy scenario first formalized by Werner [1]. Numerous investigations exist concerning the detection, quantification, and applications of entanglement along this line [2-4]. However, entanglement is not the only aspect of quantum correlations, and it is found that there are tasks in which some quantum correlations other than entanglement are responsible for the quantum advantage. For instance, there are "quantum nonlocality without entanglement" [5–7] and quantum speedup with separable states [8–11]. Therefore, it is desirable to investigate quantum correlations from another perspective.

An appealing and significant approach different from the entanglement vs separability scenario is taken by Olliver and Zurek [12]. The idea is to take advantage of the observation that in pursuing quantum analogs of classical notions, equivalent classical expressions often lead to different quantum analogs due to noncommutativity of operators which represent quantum states and observables, and this difference can be exploited to characterize and quantify the "quantumness" of an object. In particular, Olliver and Zurek defined a quantity, called the quantum discord, as the difference of two natural quantum extensions of the classical mutual information, and exhibited its applications in revealing quantum aspect of correlations in bipartite states including separable ones. The quantum discord is further used by Zurek in analyzing Maxwell's demons [13]. A closely related and important quantity has also been introduced by Henderson and Vedral from a different perspective [14]. Other similar quantities with the same spirit have been extensively studied by Horodecki *et al.* [15].

We will consider the following setup that allows for introducing the relevant notions. Consider a classical bipartite state for a system with parties *a* and *b*, which is mathematically represented by a joint probability distribution p_{jk} with *j* and *k* indexing the measurement outcomes of parties *a* and *b*, respectively. Thus the marginal probabilities for parties *a* and *b* are $p_j^a \coloneqq \sum_k p_{jk}$ and $p_k^b \coloneqq \sum_j p_{jk}$, respectively. Let $H(\dots)$ be the Shannon entropy functional, e.g., $H(p) \coloneqq -\sum_{jk} p_{jk} \log_2 p_{jk}$. The classical mutual information is defined as [16,17]

$$I(p) := H(p^{a}) + H(p^{b}) - H(p),$$
(1)

which may be rewritten as

$$I(p) = H(p^{a}) - H(p|p^{b}),$$
(2)

where

$$H(p|p^{b}) := H(p) - H(p^{b}) = -\sum_{jk} p_{jk} \log_2 p_{j|k}$$
(3)

is the conditional entropy, while

$$p_{j|k} \coloneqq \frac{p_{jk}}{p_k^b} \tag{4}$$

is the conditional probability distribution given the marginal p^b .

Now consider quantum extensions of the above scenario. The classical probability distributions are replaced by density operators acting on a composite Hilbert space and the summation is replaced by the trace. Thus a bipartite density operator ρ shared by parties *a* and *b* plays the role of a joint probability *p*, while the marginal states (reduced density operators) $\rho^a = \text{tr}_b \rho$ and $\rho^b = \text{tr}_a \rho$ (partial trace) play the role of the marginal probabilities p^a and p^b , respectively. The Shannon entropy functional is replaced by the quantum entropy (von Neumann entropy) [18,19]

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$$S(\rho) \coloneqq -\operatorname{tr} \rho \log_2 \rho. \tag{5}$$

With these substitutions, the aim is to generalize the classical mutual information into the quantum scenario and investigate its consequences and implications.

The first natural quantum extension is of course the quantum mutual information

$$\mathcal{I}(\rho) \coloneqq S(\rho^a) + S(\rho^b) - S(\rho) \tag{6}$$

$$=S(\rho^a) - S(\rho|\rho^b), \tag{7}$$

which can be considered as a direct formal generalization of either Eq. (1) or Eq. (2), with the quantum conditional entropy being defined as

$$S(\rho|\rho^b) \coloneqq S(\rho) - S(\rho^b), \tag{8}$$

which in turn is a formal generalization of the classical conditional entropy defined by Eq. (3). The quantum mutual information has fundamental physical significance, and is usually used as a measure of total correlations [19–26]. See Refs. [24,25] for two recent operational justifications and Ref. [26] for a historical review.

In order to reveal the quantum nature of correlations, Olliver and Zurek considered another route of generalizing the classical mutual information by use of a measurement-based conditional density operator [12]. Here a measurement is always understood to be of von Neumann type which consists of a set of one-dimensional projectors that sum up to the identity. Let $\{B_k\}$ be such a measurement performed locally only on party *b*, then the quantum state, conditioned on the measurement outcome labeled by *k*, changes to

$$\rho_k = \frac{1}{p_k} (I \otimes B_k) \rho(I \otimes B_k) \tag{9}$$

with probability $p_k = \operatorname{tr}(I \otimes B_k) \rho(I \otimes B_k)$. Here *I* is the identity operator for party *a*. Clearly, ρ_k may be considered as a conditional density operator (conditioned on the measurement outcome labeled by *k*), which is a formal quantum generalization of the classical conditional probability distribution $p_{\cdot|k}$ defined by Eq. (4). With this conditional density operator, an alternative variant of quantum conditional entropy (with respect to the measurement $\{B_k\}$) is defined as

$$S(\rho|\{B_k\}) \coloneqq \sum_k p_k S(\rho_k), \tag{10}$$

and furthermore, a variant of quantum mutual information (based on the measurement $\{B_k\}$) may be defined as

$$\mathcal{I}(\rho|\{B_k\}) \coloneqq S(\rho^a) - S(\rho|\{B_k\}),\tag{11}$$

which is intuitively motivated by the classical Eq. (2). The quantity

$$\mathcal{C}(\rho) \coloneqq \sup_{\{B_k\}} \mathcal{I}(\rho | \{B_k\})$$
(12)

is interpreted, implicitly by Olliver and Zurek [12] and explicitly by Henderson and Vedral [14], as a measure of classical correlations. See Refs. [12,14,27] for further explanations.

Now, we have two quantum analogs of the classical mutual information: The original quantum mutual information $\mathcal{I}(\rho)$, and the measurement-induced quantum mutual information $\mathcal{C}(\rho)$. The difference

$$Q(\rho) \coloneqq \mathcal{I}(\rho) - \mathcal{C}(\rho) \tag{13}$$

is the so-called quantum discord, and is interpreted as a measure of quantum correlations by Olliver and Zurek [12]. It can be shown that the quantum discord is always nonnegative by expressing mutual information in terms of quantum relative entropy and invoking the monotonicity property of the latter [18,19].

Due to the complicated optimization involved, it is usually intractable to evaluate the quantum discord for generic cases. The purpose of this article is to evaluate the quantum discord analytically for a certain family of two-qubit states, and investigate the comparative relations between the total, quantum, and classical correlations, as measured by the quantum mutual information, the quantum discord, and the quantity defined in Eq. (12), respectively, for some specific two-qubit states. It is explicitly shown that it is not the case that for all states the classical correlations [defined by Eq. (12)] are greater than or equal to the quantum correlations [defined by Eq. (13)]. Thus states exist that have greater quantum correlations than classical correlations. Last, the quantum discord is compared to the entanglement of formation (which is a specific measure of entanglement) for some specific two-qubit states. This comparison shows that the quantum discord can be larger than the entanglement of formation for some states, whereas it can be smaller for other states. Thus, these measures of correlations are not only quantitatively but also qualitatively different.

The remainder of the article is arranged as follows. In Sec. II, we derive the analytical expressions of the quantum discord for a large family of two-qubit states, and in Sec. III, we compare various correlation measures based on the quantum mutual information and the quantum discord. We also compare the quantum discord and the entanglement of formation. Finally, Sec. IV is devoted to the summary.

II. TWO-QUBIT SYSTEMS

Pairs of two-level systems, e.g., two-qubit systems, are primary building blocks for encoding correlations via quantum systems [28]. Consider a two-qubit system with Hilbert space $C^2 \otimes C^2$ and computational base { $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$ }. Any state for such a system may be parametrized as [28]

$$\tau = \frac{1}{4} \left(I + \vec{u}\vec{\sigma} \otimes I + I \otimes \vec{v}\vec{\sigma} + \sum_{j,k=1}^{3} w_{jk}\sigma_j \otimes \sigma_k \right).$$
(14)

Here *I* is the identity operator on the composite system or on the marginal systems, depending on the context, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ with $\sigma_1, \sigma_2, \sigma_3$ being the Pauli spin observables in the *x*, *y*, *z* directions. $\vec{u} = (u_1, u_2, u_3)$, $\vec{v} = (v_1, v_2, v_3) \in \mathbb{R}^3$, $\vec{u}\vec{\sigma} = u_1\sigma_1 + u_2\sigma_2 + u_3\sigma_3$, etc., and w_{jk} are real numbers. According to the singular value decomposition theorem in linear algebras, the matrix $W = \{w_{jk}\}$ can always be written as $W = O^a \operatorname{diag}\{c_1, c_2, c_3\}O^b$ or, equivalently, as

$$\sum_{j,k=1}^{3} O_{jm}^{a} w_{jk} O_{nk}^{b} = \delta_{mn} c_{m}.$$
 (15)

Here $O^a = \{O^a_{jm}\}$ and $O^b = \{O^b_{nk}\}$ are orthogonal matrices in O(3). Moreover, there always exist unitary matrices U and V in U(2) such that $U\sigma_j U^{\dagger} = \sum_{m=1}^3 O^a_{jm}\sigma_m$ and $V\sigma_k V^{\dagger} = \sum_{n=1}^3 O^b_{nk}\sigma_n$ [28]. Letting $\vec{\alpha} = \vec{u}O^a$, $\vec{\beta} = \vec{v}(O^b)^T$ (T denotes transposition) and noting that

$$U \otimes V\left(\sum_{j,k=1}^{3} w_{jk}\sigma_{j} \otimes \sigma_{k}\right)U^{\dagger} \otimes V^{\dagger}$$

$$= \sum_{j,k=1}^{3} w_{jk}(U\sigma_{j}U^{\dagger}) \otimes (V\sigma_{k}V^{\dagger})$$

$$= \sum_{m,n=1}^{3} \left(\sum_{j,k=1}^{3} w_{jk}O_{jm}^{a}O_{nk}^{b}\right)\sigma_{m} \otimes \sigma_{n} = \sum_{m=1}^{3} c_{m}\sigma_{m} \otimes \sigma_{m},$$
(16)

one sees that the state τ is locally unitary equivalent to

$$\gamma = \frac{1}{4} \left(I + \vec{a}\vec{\sigma} \otimes I + I \otimes \vec{b}\vec{\sigma} + \sum_{j=1}^{3} c_j\sigma_j \otimes \sigma_j \right).$$
(17)

That is, a general two-qubit state can always be reduced, up to local unitary equivalence, to a state in the above form. For analytical simplicity and since we are only interested in the correlations in the bipartite states, we will only consider those states with the maximally mixed marginals, that is, we will only consider the following further simplified family of states:

$$\rho = \frac{1}{4} \left(I + \sum_{j=1}^{3} c_j \sigma_j \otimes \sigma_j \right), \tag{18}$$

where c_j are real constants satisfying certain constraints such that ρ is a well defined density operator (see below). Our primary aim is to evaluate the quantum discord $Q(\rho)$ defined by Eq. (13), which in turn requires us to evaluate $\mathcal{I}(\rho)$ defined by Eq. (6) and $C(\rho)$ defined by Eq. (12).

First, we evaluate the total correlations $\mathcal{I}(\rho)$. It can be directly checked that ρ have eigenvalues

$$\lambda_0 = \frac{1}{4} (1 - c_1 - c_2 - c_3), \tag{19}$$

$$\lambda_1 = \frac{1}{4} (1 - c_1 + c_2 + c_3), \qquad (20)$$

$$\lambda_2 = \frac{1}{4} (1 + c_1 - c_2 + c_3), \qquad (21)$$

$$\lambda_3 = \frac{1}{4} (1 + c_1 + c_2 - c_3), \tag{22}$$

from which we readily see the constraints of the coefficients c_i are such that $\lambda_l \in [0,1]$ for l=0,1,2,3. The marginal

states of ρ are $\rho^a = I/2$ and $\rho^b = I/2$. Consequently, the quantum mutual information in ρ is

$$\mathcal{I}(\rho) = 2 + \sum_{l=0}^{3} \lambda_l \log_2 \lambda_l.$$
⁽²³⁾

Next, we evaluate the classical correlations $C(\rho)$. Let

$$\{\Pi_k = |k\rangle\langle k|: k = 0, 1\}$$
(24)

be the local measurement for party *b* along the computational base $\{|k\rangle\}$; then any von Neumann measurement for party *b* can be written as

$$\{B_k = V\Pi_k V^{\dagger} : k = 0, 1\}$$
(25)

for some unitary $V \in U(2)$. But any unitary V can be written, up to a constant phase, as

$$V = tI + i\vec{y}\vec{\sigma} \tag{26}$$

with $t \in \mathbb{R}$, $\vec{y} = (y_1, y_2, y_3) \in \mathbb{R}^3$, and

$$t^{2} + y_{1}^{2} + y_{2}^{2} + y_{3}^{2} = 1.$$
 (27)

After the measurement $\{B_k\}$, the state ρ will change to the ensemble $\{\rho_k, p_k\}$ with

$$\rho_k \coloneqq \frac{1}{p_k} (I \otimes B_k) \rho(I \otimes B_k) \tag{28}$$

and $p_k = tr(I \otimes B_k)\rho(I \otimes B_k)$. We need to evaluate ρ_k and p_k . For this purpose, we write

$$p_{k}\rho_{k} = (I \otimes B_{k})\rho(I \otimes B_{k}) = [I \otimes (V\Pi_{k}V^{\dagger})]\rho[I \otimes (V\Pi_{k}V^{\dagger})]$$
$$= (I \otimes V)(I \otimes \Pi_{k})(I \otimes V^{\dagger})\rho(I \otimes V)(I \otimes \Pi_{k})(I \otimes V^{\dagger})$$
$$= \frac{1}{4}(I \otimes V)(I \otimes \Pi_{k})\left(I + \sum_{j=1}^{3} c_{j}\sigma_{j} \otimes (V^{\dagger}\sigma_{j}V)\right)$$
$$\times (I \otimes \Pi_{k})(I \otimes V^{\dagger}).$$
(29)

By use of the relations

$$V^{\dagger}\sigma_{1}V = (t^{2} + y_{1}^{2} - y_{2}^{2} - y_{3}^{2})\sigma_{1}$$

+ 2(ty_{3} + y_{1}y_{2})\sigma_{2} + 2(-ty_{2} + y_{1}y_{3})\sigma_{3}, \quad (30)

$$V^{\dagger}\sigma_{2}V = 2(-ty_{3} + y_{1}y_{2})\sigma_{1} + (t^{2} + y_{2}^{2} - y_{1}^{2} - y_{3}^{2})\sigma_{2}$$
$$+ 2(ty_{1} + y_{2}y_{3})\sigma_{3}, \qquad (31)$$

$$V^{\dagger}\sigma_{3}V = 2(ty_{2} + y_{1}y_{3})\sigma_{1} + 2(-ty_{1} + y_{2}y_{3})\sigma_{2} + (t^{2} + y_{3}^{2} - y_{1}^{2} - y_{2}^{2})\sigma_{3},$$
(32)

and $\Pi_0 \sigma_3 \Pi_0 = \Pi_0$, $\Pi_1 \sigma_3 \Pi_1 = -\Pi_1$, $\Pi_j \sigma_k \Pi_j = 0$ for j = 0, 1, k = 1, 2, we obtain $p_0 = p_1 = \frac{1}{2}$ and

$$\rho_0 = \frac{1}{2} (I + c_1 z_1 \sigma_1 + c_2 z_2 \sigma_2 + c_3 z_3 \sigma_3) \otimes (V \Pi_0 V^{\dagger}), \quad (33)$$

$$\rho_1 = \frac{1}{2} (I - c_1 z_1 \sigma_1 - c_2 z_2 \sigma_2 - c_3 z_3 \sigma_3) \otimes (V \Pi_1 V^{\dagger}), \quad (34)$$

where

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$$z_1 \coloneqq 2(-ty_2 + y_1y_3), \tag{35}$$

$$z_2 \coloneqq 2(ty_1 + y_2 y_3), \tag{36}$$

$$z_3 := t^2 + y_3^2 - y_1^2 - y_2^2.$$
(37)

Let

$$\theta \coloneqq \sqrt{|c_1 z_1|^2 + |c_2 z_2|^2 + |c_3 z_3|^2},\tag{38}$$

which depends on the measurement $\{B_k\}$ or, equivalently, on V. Then

$$S(\rho_0) = S(\rho_1) = -\frac{1-\theta}{2}\log_2 \frac{1-\theta}{2} - \frac{1+\theta}{2}\log_2 \frac{1+\theta}{2}.$$
(39)

Therefore, by defining Eq. (10),

$$S(\rho|\{B_k\}) = p_0 S(\rho_0) + p_1 S(\rho_1)$$

= $-\frac{1-\theta}{2} \log_2 \frac{1-\theta}{2} - \frac{1+\theta}{2} \log_2 \frac{1+\theta}{2}$, (40)

and by defining Eq. (11),

$$\mathcal{I}(\rho|\{B_k\}) = S(\rho^a) - S(\rho|\{B_k\})$$

= $1 + \frac{1-\theta}{2}\log_2\frac{1-\theta}{2} + \frac{1+\theta}{2}\log_2\frac{1+\theta}{2}$
= $\frac{1-\theta}{2}\log_2(1-\theta) + \frac{1+\theta}{2}\log_2(1+\theta).$ (41)

It can be directly verified that $z_1^2 + z_2^2 + z_3^2 = 1$. Let us put

$$c \coloneqq \max\{|c_1|, |c_2|, |c_3|\},\tag{42}$$

then

$$\theta \le \sqrt{|c|^2 (|z_1|^2 + |z_2|^2 + |z_3|^2)} = c, \tag{43}$$

and the equality can be readily attained by appropriate choice of t, y_j . More specifically, (1) if $c = |c_1|$, then the equality is achieved by taking $|z_1|=1$, $z_2=z_3=0$, e.g., $|t|=|y_2|=\frac{1}{\sqrt{2}}$, $y_1=y_3=0$; (2) if $c=|c_2|$, then the equality is achieved by taking $|z_2|=1$, $z_1=z_3=0$, e.g., $|t|=|y_1|=\frac{1}{\sqrt{2}}$, $y_2=y_3=0$; (3) if $c=|c_3|$, then the equality is achieved by taking $|z_3|=1$, $z_1=z_2=0$, e.g., $y_1=y_2=0$.

Therefore, we see that

$$\sup_{\{B_k\}} \theta = \sup_V \theta = c.$$
(44)

Now by defining Eq. (12), we obtain

$$\mathcal{C}(\rho) = \sup_{\{B_k\}} \mathcal{I}(\rho | \{B_k\}) = \frac{1-c}{2} \log_2(1-c) + \frac{1+c}{2} \log_2(1+c).$$
(45)

Finally, from Eqs. (23) and (45), we obtain the quantum discord

$$\begin{aligned} \mathcal{Q}(\rho) &= \mathcal{I}(\rho) - \mathcal{C}(\rho) \\ &= \frac{1}{4} [(1 - c_1 - c_2 - c_3) \log_2(1 - c_1 - c_2 - c_3) \\ &+ (1 - c_1 + c_2 + c_3) \log_2(1 - c_1 + c_2 + c_3) \\ &+ (1 + c_1 - c_2 + c_3) \log_2(1 + c_1 - c_2 + c_3) \\ &+ (1 + c_1 + c_2 - c_3) \log_2(1 + c_1 + c_2 - c_3)] \\ &- \frac{1 - c}{2} \log_2(1 - c) - \frac{1 + c}{2} \log_2(1 + c). \end{aligned}$$
(46)

It will be interesting to consider the particular case $c_1 = c_2 = c_3 = -c$. In this instance, the state ρ turns out to be the Werner state

$$\rho = (1 - c)\frac{I}{4} + c|\Psi^{-}\rangle\langle\Psi^{-}|, \quad c \in [0, 1]$$
(47)

with $|\Psi^{-}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. According to the preceding calculations, we have

$$\mathcal{I}(\rho) = \frac{3(1-c)}{4} \log_2(1-c) + \frac{1+3c}{4} \log_2(1+3c), \quad (48)$$

$$C(\rho) = \frac{1-c}{2}\log_2(1-c) + \frac{1+c}{2}\log_2(1+c), \quad (49)$$

and the quantum discord

$$Q(\rho) = \frac{1-c}{4} \log_2(1-c) - \frac{1+c}{2} \log_2(1+c) + \frac{1+3c}{4} \log_2(1+3c).$$
(50)

The graph of $\mathcal{Q}(\rho)$ versus c will be plotted in Fig. 2.

III. COMPARISONS

Recall that the quantum mutual information $\mathcal{I}(\rho)$ is a measure of total correlations, while $\mathcal{C}(\rho)$ and the quantum discord $\mathcal{Q}(\rho)$ are interpreted as measures of classical and quantum correlations, respectively [12,14]. The natural question arises as to the relationships among these three correlation measures.

Let us first consider some particular cases. In the extreme case of the maximally entangled Bell state $\rho = |\Psi^-\rangle\langle\Psi^-|$, we have

$$\mathcal{I}(\rho) = 2, \quad \mathcal{C}(\rho) = 1, \quad \mathcal{Q}(\rho) = 1.$$
(51)

Thus in this case, the total correlations are equally divided into the classical and quantum correlations. This equal distribution still holds for any pure state, which can be directly proved by means of the Schmidt decomposition. More precisely, for any bipartite pure state $\rho = |\Phi\rangle\langle\Phi|$ in any composite system (not necessarily a two-qubit system), if its Schmidt decomposition is written as $|\Phi\rangle = \sum_j \alpha_j |j\rangle \otimes |j\rangle$, and $S = -\sum_j |\alpha_j|^2 \log_2 |\alpha_j|^2$ is the reduced von Neumann entropy, then



FIG. 1. (Color online) Graph of $D(\rho)=Q(\rho)-C(\rho)$ versus $c_1, c_2 \in [-0.1, 0.1]$ for ρ defined by Eq. (18), with $c=-c_3=0.1$. Here we see clearly that $Q(\rho)$ can be larger, as well as smaller, than $C(\rho)$. The unit of $Q(\rho)$ is bit.

$$\mathcal{I}(\rho) = 2S, \quad \mathcal{C}(\rho) = S, \quad \mathcal{Q}(\rho) = S.$$
 (52)

On the other extreme, consider the case when ρ can be written as

$$\rho = \sum_{jk} p_{jk} \Pi_j^a \otimes \Pi_k^b, \tag{53}$$

where $p := \{p_{jk}\}$ is a bivariate probability distribution, and $\{\Pi_{j}^{a}\}$ and $\{\Pi_{k}^{b}\}$ are sets of orthogonal projections for parties *a* and *b*, respectively. Clearly, this state is essentially an operator formalism of the classical probability distribution *p* without any quantum nature [that is, *p* and ρ defined by Eq. (53) are in one to one correspondence], and one expects

$$\mathcal{I}(\rho) = I(p), \quad \mathcal{C}(\rho) = I(p), \quad \mathcal{Q}(\rho) = 0.$$
 (54)

This is indeed the case as can be directly checked. Thus, in this instance, all correlations are classical, and there are no quantum correlations.

Based on the above intuitive observations (that is, correlations in any maximally entangled Bell states are equally divided into classical and quantum parts, while all correlations in any classical bivariate probability distribution are of a classical nature, and in both cases, classical correlations are not less than quantum correlations), one may ask whether $C(\rho) \ge Q(\rho)$ holds true for all ρ . In fact, this is in general false, as demonstrated by the numerical results in Fig. 1. To gain an intuitive feeling of the relationships between $C(\rho)$ and $Q(\rho)$, we depict the graph of

$$D(\rho) = \mathcal{C}(\rho) - \mathcal{Q}(\rho) \tag{55}$$

for the states defined by Eq. (18) for some specified values of c_1, c_2, c_3 in Fig. 1. Without loss of generality, we may assume that $c=-c_3$, and consider $D(\rho)$ as a function of c_1, c_2 . Note that c_1, c_2, c_3 are constrained such that the eigenvalues $\lambda_i \in [0, 1]$.

We now further compare the quantum discord with the entanglement of formation which is customarily used as a



FIG. 2. (Color online) Graphs of $Q(\rho)$ and $\mathcal{E}(\rho)$ versus *c* for the Werner state $\rho = (1-c)\frac{l}{4} + c|\Psi^-\rangle\langle\Psi^-|$. Here we see that $Q(\rho)$ is smaller than $\mathcal{E}(\rho)$ when $c \in (0.879, 1)$. The unit of $Q(\rho)$ and $\mathcal{E}(\rho)$ is bit.

measure of entanglement [2–4]. Recall that the entanglement of formation of ρ is defined as

$$\mathcal{E}(\rho) \coloneqq \inf \sum_{l} p_{l} S(\operatorname{tr}_{a} |\Phi_{l}\rangle \langle \Phi_{l}|), \qquad (56)$$

where the infimum is taken over all pure state ensemble realizations of $\rho: \rho = \sum_l p_l |\Phi_l\rangle \langle \Phi_l|$. An elegant analytic formula for $\mathcal{E}(\rho)$ when ρ is a two-qubit state is ingeniously derived by Wootters [4,29]:

$$\mathcal{E}(\rho) = H\left(\frac{1+\sqrt{1-\theta^2}}{2}\right),\tag{57}$$

where

$$\theta \coloneqq \max\{0, \theta_1 - \theta_2 - \theta_3 - \theta_4\}$$
(58)

and $\theta_1 \ge \theta_2 \ge \theta_3 \ge \theta_4$ are the square root of eigenvalues of $\rho \tilde{\rho}$ with $\tilde{\rho} = \sigma_2 \otimes \sigma_2 \rho^* \sigma_2 \otimes \sigma_2$, while ρ^* is the complex conjugate of ρ in the computational base $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

Now for ρ defined by Eq. (18), it is readily checked that $\tilde{\rho} = \rho$. Consider the particular case $c_3 \le c_2 \le c_1 \le 0$; then

$$\theta = \max\left\{0, -\frac{1+c_1+c_2+c_3}{2}\right\};$$
 (59)

and $\mathcal{E}(\rho)$ is given by Eq. (57). One wants to inquire the relationship between $\mathcal{Q}(\rho)$ and $\mathcal{E}(\rho)$, in particular, one wants to know whether they give the same qualitative characterizations of quantum correlations.

To address this issue, let us consider ρ defined by Eq. (18) with $c_1=c_2=c_3=-c$, i.e., the Werner states. We depict the graphs of $Q(\rho)$ and $\mathcal{E}(\rho)$ versus $c \in [0,1]$ in Fig. 2. We see that the quantum discord is always positive except for the trivial cases (pure or maximally mixed), and in particular it is positive for any nondegenerate separable Werner states.

More interestingly, we observe that while the quantum discord dominates the entanglement of formation when $c \in (0, 0.879)$, the dominance is reversed when $c \in (0.879, 1)$. Consequently, there are no simple dominance relation between the quantum discord and the entanglement of formation, and they are incomparable in the sense that there exist states ρ_1 and ρ_2 such that $Q(\rho_1) > \mathcal{E}(\rho_1)$, while $Q(\rho_2)$ $< \mathcal{E}(\rho_2)$. They are different not only quantitatively, but also qualitatively.

IV. SUMMARY

We have evaluated the quantum discord for a family of two-qubit states, and obtained analytical formulas. The results are used to illustrate various comparative relations PHYSICAL REVIEW A 77, 042303 (2008)

among the total, quantum, and classical correlations. In particular, we have demonstrated that there are no simple dominance relations between the quantum and classical correlations in terms of the quantum discord, although both are entropic measures with intuitive operational meaning. Our results corroborate the general viewpoint that the quantum nature of correlations is very intricate and subtle, and many different quantities are needed in order to capture its various aspects.

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