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Comparison of the attempts of quantum discord and quantum entanglement to capture quantum correlations

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Measurements of quantum systems disturb their states. To quantify this nonclassical characteristic, Zurek and Ollivier [Phys. Rev. Lett. **88**, 017901 (2001)] introduced the *quantum discord*, a quantum correlation that can be nonzero even when entanglement in the system is zero. Discord has aroused great interest as a resource that is more robust against the effects of decoherence and offers the exponential speed-up of certain computational algorithms. Here, we study general two-level bipartite systems and give general results on the relationship between discord, entanglement, and linear entropy. We also identify the states for which discord takes a maximal value for a given entropy or entanglement, thus placing strong bounds on entanglement-discord and entropy-discord relations. We find out that although discord and entanglement are identical for pure states, they differ when generalized to mixed states as a result of the difference in the method of generalization.

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I. INTRODUCTION

Since the emergence of quantum mechanics at the beginning of the 20th century, physicists have been intrigued and puzzled by its interpretation and consequences. The characteristics that distinguish quantum from classical systems have been investigated extensively. To be able to study quantum correlations in a system, it is important to quantify them. Although this is a challenging task for multicomponent quantum systems, progress has been made in the case of two-level bipartite quantum systems. One method suitable for pure states [1,2] involves calculating the entropy of the reduced density matrix of the system, also known as the entanglement of formation (EOF). To extend this concept to mixed states, the entanglement is defined to be equal to the weighted sum of the entanglement of the pure states involved in the decomposition of the mixed states, minimized over all decompositions [3–5]. The restriction enforced by this minimization places a bound on the entanglement for mixed states; indeed, when a certain level of disorder of the state is attained, it is known that entanglement must disappear [6,7]. It is, therefore, not surprising that for some systems as they reach a certain level of mixture, the entanglement is completely lost, a phenomena which in the study of state dynamics is commonly known as entanglement sudden death (ESD) [8].

Another approach to capture quantum correlations was taken by Zurek and Ollivier [9], where they used the fact that the measurement of quantum systems, unlike classical systems, disturbs their state. To quantify the correlations based on this idea, one looks at the mutual information function $I(\hat{\rho})$, where $\hat{\rho}$ is the density matrix describing the state of the whole system. Given a system C composed of two subsystems A and B, $I(\hat{\rho})$ is a measure of how much information is shared between the two subsystems. In other words, it is can viewed as an indication of the degree of correlation between them. The correlations between the two subsystems can be classical and/or quantum. However, if the correlations are quantum in nature, then calculating $I(\hat{\rho})$ *after* a measurement is performed on one of the subsystems (for instance, B) yields a *different* result than that calculated *before* the measurement is performed. This disagreement is the basis for defining discord; the definition is finalized after optimizing over all possible measurement bases. One of the major reasons in the aroused interest [10–23] in this novel correlation is that, as was shown in [9], even when entanglement is zero in a system, discord can still be finite. This led to the hope that using discord instead of entanglement as a resource, in fields like quantum computation, can lead to more efficient computations. In [23], discord was characterized in the deterministic quantum computation with 1 bit (DQC1) model [25], calling for experimental verifications of its powers, which was demonstrated in [22].

In this paper, we look at the relationship between discord, entanglement, and linear entropy to investigate the connection between these quantities. We perform the study on the most general density matrices representing two-level bipartite systems. Since we lack an analytic expression for discord for these general states, the heart of the work is numeric in nature, involving optimization over all possible measurements that can be performed on one of the subsystems under study. Our numerical work facilitates the principal results presented here: the analytic form of the states for which the discord takes extreme values. As will be shown, one can place definite boundaries on the relationships between entanglement and discord, and mixture [quantified by the linear entropy using Eq. (8)] and discord.

II. DISCORD, ENTANGLEMENT, AND LINEAR ENTROPY FOR TWO-LEVEL BIPARTITE SYSTEMS

To consider discord, let us look at system C, which is composed of two subsystems A and B, both of which are two-level quantum systems. The effects of measurements on one of the subsystems (B in the following analysis) is captured by looking at the mutual-information function defined as follows:

$$I(\hat{\rho}) = S(\hat{\rho}^A) + S(\hat{\rho}^B) - S(\hat{\rho}), \tag{1}$$

where $\hat{\rho}^i$ is the reduced-density matrix of subsystem i and $S(\hat{\rho}) = -\mathrm{Tr}\{\hat{\rho}\log_2\hat{\rho}\}$ [26]. Then, defining all set of projectors on B by $\{\hat{B}_k\}$, the measurement-induced mutual-information function for each of these sets takes the following form:

$$I(\hat{\rho} \mid \{B_k\}) = S(\hat{\rho}^A) - \sum_k p_k S(\hat{\rho}_k), \tag{2}$$

where $\hat{\rho}_k$ is the density matrix of the system after B_k is applied on B, $k \in \{1,2\}$, and $p_k = \mathrm{Tr}\{(\hat{I}\otimes\hat{B}_k)\hat{\rho}(\hat{I}\otimes\hat{B}_k)\}$. To obtain the final form for the measurement-induced density matrix, Eq. (2) is maximized over all possible $\{\hat{B}_k\}$ to obtain the following expression for discord:

$$Q(\hat{\rho}) = I(\hat{\rho}) - \max_{\{B_k\}}\left\{S(\hat{\rho}^A) - \sum_k p_k S(\hat{\rho}_k)\right\}. \tag{3}$$

To start the comparison between discord and entanglement, we compute the EOF and the discord for pure states in two-level bipartite systems $|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$, where $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$. It is convenient to use the Schmidt decomposition [27] to write the state as $|\psi\rangle = \sqrt{\lambda}\,|1_A\rangle\,|1_B\rangle + \sqrt{(1-\lambda)}\,|2_A\rangle\,|2_B\rangle$, where λ and $(1-\lambda)$ are the eigenvalues of the reduced density matrices, and $|1_i\rangle$ and $|2_i\rangle$ are the corresponding eigenvectors of the reduced density matrix of subsystem i. Using local unitary operations, which do not affect the quantum correlations present in the system, one can show that this state is equivalent to $|\psi\rangle = \sqrt{\lambda}\,|00\rangle + \sqrt{(1-\lambda)}\,|11\rangle$. In this case, the EOF as well as the discord, which can be computed analytically, are found to be identical and are given by $E(\hat{\rho}) = Q(\hat{\rho}) = h(\lambda)$, where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$. Therefore, discord and EOF amount to the same set of correlations in the case of pure states [16]. In the mixed state case, there is no explicit analytic expression for discord. The most general analytic expression so far was presented in a very interesting paper by Luo [28] for the mixed states with maximally mixed marginals (MMMs) (i.e, the reduced density matrices $\hat{\rho}^A$ and $\hat{\rho}^B$ are both maximally mixed).

Going back to system C described above, with A and B each being two-level quantum systems, we parametrize all the possible measurements that can be performed on B by two variables θ and ϕ. Each complete set of possible measurements, which is composed of two elements, is defined as follows:

$$\begin{aligned}\hat{B}_1 &= |\psi\rangle\langle\psi|,\\ \hat{B}_2 &= |\psi_\perp\rangle\langle\psi_\perp|,\end{aligned} \tag{4}$$

where

$$\begin{aligned}|\psi\rangle &= \cos\theta|0\rangle + e^{i\phi}\sin\theta|1\rangle,\\ |\psi_\perp\rangle &= -\sin\theta|0\rangle + e^{i\phi}\cos\theta|1\rangle.\end{aligned} \tag{5}$$

The resultant of the density operator when such measurements are performed on subsystem B is

$$\hat{\rho}_k = \frac{1}{p_k}(\hat{I}\otimes\hat{B}_k)\hat{\rho}(\hat{I}\otimes\hat{B}_k). \tag{6}$$

To obtain the final form of Eq. (3), we numerically search the θ and ϕ space for the set of values that maximizes Eq. (2).

For a given density matrix $\hat{\rho}$, the EOF is given in terms of concurrence $\mathcal{C}(\hat{\rho})$ by the formula [5]

$$E(\hat{\rho}) = h\left(\frac{1+\sqrt{1-\mathcal{C}^2(\hat{\rho})}}{2}\right), \tag{7}$$

where $\mathcal{C} = \max = \{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}$, where λ_i are the eigenvalues, in decreasing order, of the matrix $\hat{R} = \hat{\rho}(\hat{\sigma}_y\otimes\hat{\sigma}_y)\hat{\rho}^T(\sigma_y\otimes\sigma_y)$.

For a comparison of discord with entropy, we calculate the linear entropy, defined as follows:

$$S_L = \tfrac{4}{3}[1 - \mathrm{Tr}(\hat{\rho}^2)]. \tag{8}$$

III. RESULTS

Figures 1 and 2 provide the plots that give the relationship between discord and entanglement, and discord and linear entropy for the two-level bipartite systems, respectively. As noted above, in the case of pure states, discord and entanglement are *identical*. For mixed states, the two quantities are loosely related; generally speaking, the higher the entanglement, the higher the discord. The region with high-quantum correlations has a narrower relationship than the one in a lower-correlation regime. This results in a plot that resembles a horn (Fig. 1). The difference between discord and entanglement that arises in the mixed-state case is due to the optimization that was done to extend the pure-state case to the mixed-state case. In the low-quantum regime and for a large number of systems, the minimization that is done over the pure-state decomposition in defining entanglement has a trend of giving a more pessimistic measure for quantum correlations than the maximization

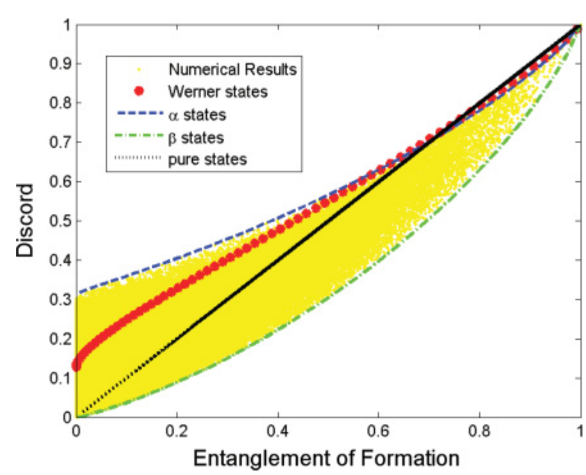

FIG. 1. (Color online) Discord-entanglement horn. Discord increases as entanglement increases. In the case of pure states, the two quantities are identical. While in the mixed-state case, the relationship broadens. However, notice that this relationship narrows in the high-quantum correlated regime and is the broadest in the low-correlation regime. This gives the plot its "horn" shape. The upper bound of this relationship is given by the α states [Eq.(10)] (for $0 \leqslant \mathrm{EOF} \leqslant 0.620$ and $0 \leqslant Q \leqslant 0.644$), the Werner states [Eq.(9)] [24] (for $0.620 \leqslant \mathrm{EOF} \leqslant 0.746$ and $0.644 \leqslant Q \leqslant 0.746$), and the pure states (for $0.740 \leqslant \mathrm{EOF}$ and $Q \leqslant 1$). The lower bound is given by the β states [Eq.(11)].

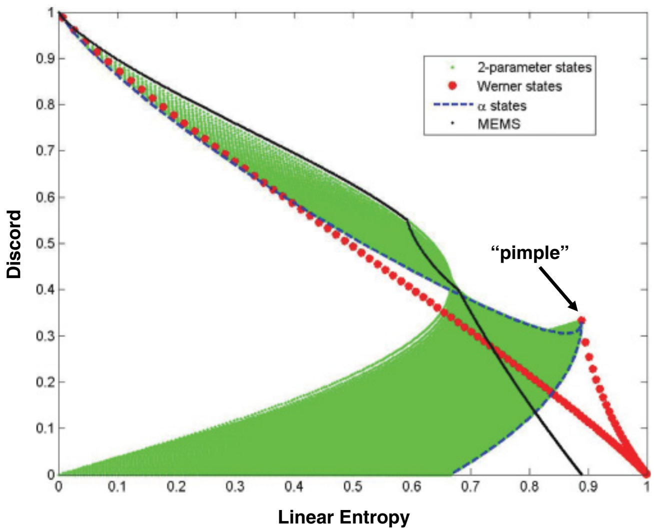

FIG. 2. (Color online) Boundaries on the relationship between discord and linear entropy. To easily illustrate the boundaries, this plot only includes the states that are involved in defining them. The two-parameter states [Eq. (14)] bound the curve from above up to $Q = 1/3$ and $S_L = 8/9$, after which the Werner states take over. Discord and linear entropy, as expected, display an inverse relationship: more randomness implies less quantum correlations. One of the interesting phenomena occurs at the pimple, where there exists states in which an increase in their entropy results in an increase in their discord. This is also the point that defines the value of linear entropy after which no entanglement can exist in the system [7]. Unlike entanglement, states exist that are very close to the maximally mixed states, but still have nonzero discord. In fact, the only value for entropy such that discord cannot be finite is for it being equal to one, in the case when the system is maximally mixed.

over all possible projectors on subsystem B that is done in defining discord. Discord and entanglement, therefore, are *not* different quantum correlations. They are two different ways to quantify these correlations. The disagreement between them, in the general mixed-state case, comes from limitations of optimization methods

The upper bound for the discord-entanglement plot is given for the most part by two classes of MMMs: the Werner states [Eq. (9)] and the α states [Eq. (10)]. In the highly correlated regime, it is bound by the pure states. The lower bound is given by another class of MMMs: the β states [Eq. (11)]. The Werner states, the α states, and the β states are given, respectively, as follows:

$$\hat{\rho}(\xi) = (1-\xi)\frac{I}{4} + \xi|\psi^-\rangle\langle\psi^-|, \tag{9}$$

where $-\frac{1}{3} \leqslant \xi \leqslant 1$ and $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$,

$$\hat{\rho}(\alpha) = \begin{pmatrix} \frac{\alpha}{2} & 0 & 0 & \frac{\alpha}{2} \\ 0 & \frac{(1-\alpha)}{2} & 0 & 0 \\ 0 & 0 & \frac{(1-\alpha)}{2} & 0 \\ \frac{\alpha}{2} & 0 & 0 & \frac{\alpha}{2} \end{pmatrix}, \tag{10}$$

where $0 \leqslant \alpha \leqslant 1$, and

$$\hat{\rho}(\beta) = \begin{pmatrix} \frac{\beta}{2} & 0 & 0 & \frac{\beta}{2} \\ 0 & \frac{(1-\beta)}{2} & \frac{(1-\beta)}{2} & 0 \\ 0 & \frac{(1-\beta)}{2} & \frac{(1-\beta)}{2} & 0 \\ \frac{\beta}{2} & 0 & 0 & \frac{\beta}{2} \end{pmatrix}, \tag{11}$$

where $0 \leqslant \beta \leqslant 1$. The analytic result for quantum discord in these cases can easily be obtained from the general expression for the MMMs in [28]. For the α and β states, it is given, respectively, as follows:

$$\begin{aligned} Q(\alpha,\zeta) = {} & (1-\alpha)\log_2(1-\alpha) + \alpha\log_2(\alpha) + (1+\alpha) \\ & - (1-\zeta)[\log_2(1-\zeta)]/2 \\ & - (1+\zeta)[\log_2(1+\zeta)]/2, \end{aligned} \tag{12}$$

where $\zeta = \max\{|\alpha|, |2\alpha - 1|\}$, and

$$Q(\beta) = \beta\log_2(\beta) + (1-\beta)\log_2(1-\beta) + 1. \tag{13}$$

Since these states also fall under the class of X states, expressions for their concurrence, from which the EOF is calculated, can be found, for example, in [29]. The concurrence of the α and β states, is given, respectively, by $C(\alpha) = \max\{0, 2\alpha - 1\}$ and $C(\beta) = |2\beta - 1|$. To prove that theses are indeed the boundaries, we performed two numeric calculations. First, we generated 10^6 random density matrices to find that the relationship between their discord and entropy all fall within these bounds. The algorithm involved creating a complex and random matrix $\hat{T}$, and from it, obtaining a well-behaved density matrix $\hat{\rho}$ by the relation $\hat{\rho} = \hat{T}\hat{T}^\dagger/\mathrm{Tr}\{\hat{T}\hat{T}^\dagger\}$. We also generated 10^5 points very close to the vicinity of each of the boundaries, with the result that none of the points fell outside the bounds imposed on them.

In Fig. 2, where the plot shows how much discord can be present in the system for a given amount of mixture, the boundaries are given by a different set of states. Beyond linear entropy being 8/9, it is bound from above by the Werner states. The rest of the plot is bound from above by a class of two-parameter density matrices described as follows:

$$\hat{\rho}(a,b) = \frac{1}{2}\begin{pmatrix} a & 0 & 0 & a \\ 0 & 1-a-b & 0 & 0 \\ 0 & 0 & 1-a+b & 0 \\ a & 0 & 0 & a \end{pmatrix}, \tag{14}$$

where $0 \leqslant a \leqslant 1$ and $a - 1 \leqslant b \leqslant 1 - a$. We find the analytic result for discord in this case to be

$$Q(a,b) = \min\{a,q\}, \tag{15}$$

where

$$\begin{aligned} q = {} & -\frac{b}{2}\log_2\left[\frac{(1+b)(1-a-b)}{(1-b)(1-a+b)}\right] + \frac{a}{2} \\ & \times \log_2\left[\frac{4a^2}{(1-a)^2 - b^2}\right] - \frac{\sqrt{a^2+b^2}}{2} \\ & \times \log_2\left[\frac{1+\sqrt{a^2+b^2}}{1-\sqrt{a^2+b^2}}\right] \end{aligned}$$

$$+ \frac{1}{2}\log_2\left[\frac{4[(1-a)^2-b^2]}{(1-b^2)(1-a^2-b^2)}\right], \tag{16}$$

and the expression for concurrence in this case is $\mathcal{C}(a,b) = \max\{0,|a| - \sqrt{(1-a)^2-b^2}\}$.

As can be seen in Fig. 2, the maximally entangled mixed states (MEMSs) [7] and the α states, both of which fall under this class of states, bound the plot at different regions. There is no lower bound to the relationship between discord and entropy, as the area below the two-parameter states as well as the Werner states becomes filled up when the whole range of density matrices is included. Also, note that the case when $a = q$ is what gives the bounding line that slopes down from the "pimple." Again, as is the case with discord and EOF, to verify these boundaries, points representing 10^6 random density matrices were generated, as well as 10^5 points in the near vicinity of these bounds. Other points to note about the figure is, first, that at the pimple, after which no entanglement can exist in the system [7], a rise in linear entropy results in a rise in discord. The states in this region are interesting to investigate, since experimentally speaking, more noise in the system at that stage enhances the quantum correlations. Also, unlike the case with entanglement, even for cases where linear entropy is arbitrarily close to the maximally mixed states at unit entropy, discord can still be finite. It is, therefore, not surprising that for states in which ESD occurs, similar behavior is not observed for discord [14,21].

IV. CONCLUSION

In conclusion, this work describes the relationship between discord and entanglement for the general two-level bipartite system. We have shown that in the general case of mixed states, the two quantum correlations vary, with the relationship broadening in the low-quantum regime. We conclude that they describe the same set of quantum correlations, as can be seen in the pure-state case, and although they vary in the case of mixed states, this is due to different methods of optimization used to extend the correlations from the pure-state case to the mixed-state case. Some questions arise. One is what is the optimal method to quantify quantum correlations? The answer to this question depends on the application of the quantum correlations. There is no universal definition for these correlations. An operational view is therefore recommended in order to define them. Another question is what is the meaning of the values for discord and EOF that are between the extreme cases of zero and one? We also reveal the general relationship between discord and linear entropy, highlighting interesting differences with a similar analysis done for entanglement [7]: At the point where entanglement disappears from the system, discord increases in value, and discord can be nonzero unless linear entropy is identically equal to one.

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