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Entanglement and discord for qubits and higher spin systems

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Abstract. We discuss aspects of entanglement and quantum discord, two of the quantum correlations that are of much interest in the field of quantum information. Their definitions and handling will be discussed, with simple illustrative examples. A specific example is of entanglement decay resulting from a simple dissipative process and how to alter that decay. An analytical prescription for computing quantum discord when a qubit (spin-1/2 or two-level quantum system) is involved is presented along with applications, and its generalization to higher spins (many levels) indicated.

Keywords. Quantum information; quantum computing; qubit; entanglement; quantum discord; mixed states; density matrix; X-states; entropy; quantum mutual information; geometric discord.

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1. Introduction

Quantum information, an umbrella term to embrace quantum computing, quantum teleportation, and quantum key distribution, exploits fundamental principles of quantum physics:superposition, entanglement, and identity of particles [1]. Each of these non-classical features makes possible certain calculations, or of speed up in them, that is not achievable with classical objects or phenomena. Thus, the principle of superposition, which speaks to the linearity of quantum physics at its fundamental level, allows a qubit (a quantum two-level system) to be in a superposition with complex coefficients of the two base states $|0\rangle$ and $|1\rangle$. This amounts to a three-parameter (normalization fixes one of the four real parameters in the two complex coefficients) infinity of states, a vastly larger state space than the two states of a classical bit. There lies the potential both for a vastly larger memory and for the speed-up of calculations that lend excitement to the field of quantum computing.

Next, a quantum system built-up of at least two parts, such as a pair of qubits, exhibits unique correlations between them, entanglement being the best known [2]. Such pairs lead to logic gates for quantum computation [1], and a shared entangled state is the way to teleport a quantum state [1,3] or securely exchange a cryptographic key between two parties [4]. Other types of quantum correlations may also be useful for some applications. In this paper, after §2 that sets out definitions and notation, §3 will consider an entangled pair of qubits and a phenomenon called finite end of that entanglement under dissipative processes [5] and how to alter that end through unitary operations individually on the two qubits [6]. Section 4 presents a correlation called discord between two subsystems [7], along with an analytical procedure for calculating it when one of the subsystems is a qubit [8,9]. A generalization for higher-dimensional 'qudits' will be briefly discussed.

This paper will not consider the hardware for implementing qubits. Many candidate systems are being explored: Nuclear magnetic resonance, Josephson junctions, trapped atoms and ions, electron spins, quantum dots, photon polarization, nitrogen vacancies in diamond, impurities embedded in silicon, etc. This paper was presented in a laser workshop, laser technology being involved in some of these alternatives being explored. But it focusses on 'software' questions, namely the quantum principles behind the applications of quantum information that are common to whatever specific hardware may be used.

2. Pure and mixed states and their density matrices

Pure states of a qubit, such as $|0\rangle$, $|1\rangle$, or their superposition such as $(|0\rangle + |1\rangle)/\sqrt{2}$ can be represented by column vectors with two entries as $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, and $\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$, respectively. Corresponding to these kets, their density matrices ρ that are in the form of a ket-bra are $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, and $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$, respectively. Density matrices are normalized so as to have unit trace and for all such pure states, the trace remains invariant upon squaring ρ.

Generally, one has access not to pure states but mixed states. They cannot be represented by ket vectors but only through density matrices and for them, $\mathrm{Tr}(\rho^2) < \mathrm{Tr}(\rho) = 1$. An example is $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$. No column vector representation is available for such a mixed state. Rather, one may regard states such as this as resulting from a random averaging of the phases in superposing the two base states with complex coefficients, thus rendering the off-diagonal entries to be zero. One can also define a von Neumann entropy analogous to thermodynamic entropy or Shannon's information entropy through [1,10]

$$S = -\mathrm{Tr}(\rho \log \rho), \tag{1}$$

the logarithm taken to base 2. The trace involves a sum over the eigenvalues of ρ; for all pure states, with these eigenvalues always 0 or 1, S vanishes. On the other hand, mixed states have non-zero entropy, the example above having $S = 1$.

This terminology and notation extends to all quantum states. Moving to a bipartite system such as two qubits, we have four base states. Taking product states of the two qubits, a 'separable' basis may be represented as $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$, with entries for the first and second qubit shown inside the ket. Their wave functions are direct products of those of the individual qubits and may be represented by column vectors with four entries, successive unit entries in the four positions starting from the top with all other entries being zero. Their density matrices will be 4×4 with a unity in one of the diagonal positions and all other entries zero. On the other hand, taking the simple superposition state $(|0\rangle + |1\rangle)/\sqrt{2}$ mentioned above for each qubit, a product of them gives a column vector with 1/2 in each of the four entries or a density matrix with 1/4 in all the 16 entries. Again, the eigenvalues are all 0 or 1 and the entropy zero.

There are also other pure states such as the 'singlet' state $(|01\rangle - |10\rangle)/\sqrt{2}$. Its ket column vector has entries, in order, $(0, 1/\sqrt{2}, -1/\sqrt{2}, 0)$, with the corresponding density matrix that has four non-zero entries in the middle, and again has $S = 0$. It differs, however, from the states previously mentioned by not being separable, the state vectors not factorizing as a product of those for each qubit. The state is 'entangled'. The spin state of the helium atom in its ground state is such a singlet, a state with definite quantum number, namely zero, for the total spin operator $\vec{S}^2$ and its projection S_z, which commute with the total Hamiltonian and with each other. On the other hand, this set of mutually commuting operators cannot accommodate the individual spin operators s_z of the electrons so that no definite value attaches to them, both $\pm 1/2$ occurring with equal probability, only with the proviso that when one is 1/2, the other is necessarily $-1/2$. The spins are entangled. Its 'triplet' counterpart, with a plus sign in place of the minus, is also similarly entangled, with definite total values (spin = 1, projection $S_z = 0$) but the individual spin projections undetermined. Along with the two other linear superpositions, $((|00\rangle \pm |11\rangle)/\sqrt{2}$, of the base states (these are also triplets but without definite S_z), these four states also provide a basis for the two qubits but now each of the four is non-separable. Indeed, they are maximally entangled and are the so-called 'Bell states' (§1.3.6 of [1]). Note again that all are pure states and thus have both a ket vector and density matrix representation, the latter having all eigenvalues zero or unity and thus with zero entropy. In §4, we consider how another type of quantum correlation called quantum discord distinguishes between entangled and unentangled states through a further consideration of entropy.

With entanglement for pure states defined in terms of whether the wave function factorizes or not, we consider next mixed states of a bipartite system AB. A natural generalization is whether the density matrix for the total ρ^{AB} decomposes into the direct product of individual density matrices ρ^{A} and ρ^{B} or, in a further extension, to a sum of such direct products with positive definite coefficients,

$$\rho^{\mathrm{AB}} = \sum_{i=1}^{d_{\mathrm{A}}} p_i \rho_i^{\mathrm{A}} \otimes \rho_i^{\mathrm{B}}, \tag{2}$$

with $p_i \geq 0$. p_i may be interpreted as the probability of each separable component i. Such a density matrix is said to describe a separable, unentangled mixed state. As such a constructive decomposition of a separable mixed state may not always be easy to obtain, other methods are necessary to determine whether a density matrix is separable. For a pair of qubits, two convenient methods are to compute the 'concurrence' [11] through the eigenvalues of $\rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$ or by examining the eigenvalues of the 'partially transposed' density matrix in which just one of the spins is transposed [12]. For higher-dimensional spins, no such measures on mixed state density matrices are available for determining whether a bipartite system is entangled or not [13]. This remains a major open question in the topic of entanglement.

3. Entanglement dissipation and its avoidance

As a simple pedagogical example to illustrate the aspects of entanglement and its time evolution, consider two qubits where the excited state $|0\rangle$ decays spontaneously to the ground state $|1\rangle$ with a rate Γ for each qubit [5]. This is the only dynamics postulated and there is no coupling between the qubits. We shall follow the time evolution of various initial density matrices $\rho(0)$. It is clear at the outset that, whatever the initial state, entangled or not, at asymptotically large time, both qubits will be in the ground state and, therefore, the system will be in $|11\rangle$ with no entanglement. What makes this system interesting, however, is that for certain initial configurations, the entanglement can vanish at a finite time even though there is still some population in the excited states [5]. Thus, entanglement can decay away even when excitation has not completely dissipated.

Consider, for instance, a density matrix

$$\begin{pmatrix} a(t) & 0 & 0 & 0 \\ 0 & b(t) & z(t) & 0 \\ 0 & z^*(t) & c(t) & 0 \\ 0 & 0 & 0 & d(t) \end{pmatrix}, \tag{3}$$

with unit trace, $a(t)+b(t)+c(t)+d(t)=1$. With many zero entries, this is a subset of the general two-qubit density matrix, indeed a further subset of what are called X-states [5,14,15] which have non-zero entries only along the diagonal and antidiagonal. The time evolution under the postulated decay is easily followed. Each $|0\rangle$ amplitude decays exponentially to $|1\rangle$ so that the only off-diagonal element's evolution is immediate: $z(t)=z(0)\exp(-\Gamma t)$. The four diagonal elements are coupled, a decreasing at a rate 2Γ while 'feeding' with rate Γ into b and c, while b and c decrease with rate Γ as they feed into d.

Such a set of coupled equations is readily solved. An initial Bell state, with $a(0)=d(0)=0, b(0)=c(0)=1/2, z(0)=\pm 1/2$, retains its entanglement at all t, reducing to the final unentangled state with $d=1$ and all other coefficients zero only in the limit of infinite time. On the other hand, an initial state such as $d(0)=0$ and all other coefficients initially equal to $1/3$, loses its entanglement at a finite time t_0, given by $\Gamma t_0=\ln(1+1/\sqrt{2})\approx 0.535$ [5]. Using photon polarization as the two states of a qubit, such a finite time end of entanglement of certain density matrices has been experimentally demonstrated [16].

A next interesting question is whether external intervention can alter the decay of entanglement. It is in the nature of entanglement that individual unitary operations on the qubits cannot change the amount of entanglement correlation between them. But there is an asymmetry with respect to the time evolution of the system in that only the upper state decays while the lower one does not. Therefore, a unitary transformation of one or both qubits that switches the base states $|0\rangle$ and $|1\rangle$ into each other, while leaving the entanglement unaffected at that instant, nevertheless, can alter the subsequent evolution. Indeed, as illustrated in figure 1, depending on when the switch is made, further evolution can be altered in many ways [6]. Once launched from $t=0$ with coefficients such as to have entanglement die at t_0, if a switch is made between t_A and t_0, entanglement will end even sooner, while for switches between t_B and t_A, the entanglement persists past t_0 although still terminating at a later finite time. Should the switch be made early enough,

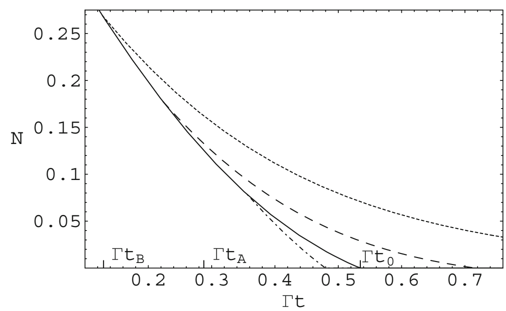

Figure 1. Evolution of negativity N, an index of entanglement, of a mixed state density matrix of two qubits [6]. The solid line shows evolution to zero entanglement at time t_0. The dash–dot line shows an even faster end of entanglement if base states of both qubits are switched at a time $t_A < t < t_0$. The large-dash line shows a delay in the end for switches made at $t_B < t < t_A$. The short-dash line shows a complete avoidance of a finite end, N decaying only asymptotically, for switch times $t < t_B$.

before t_B, then the finite time end can be completely averted, entanglement vanishing only asymptotically. The values t_A and t_B of critical times depend, of course, on the initial values of the parameters in eq. (3) [6]. There have been many studies of different dissipative mechanisms and couplings between the two qubits and of switchings done at one or both ends to study such entanglement decay and revival [17].

4. Quantum discord

As in classical physics with many types of correlations between subsystems, many quantum correlations besides entanglement have been discussed [18]. A prominent one is called quantum discord [7], the name itself not illuminating and perhaps unfortunate. It is a very different type of correlation from entanglement with no simple relationship between them as we shall see now. It rests on the definition of entropy introduced earlier in §2 both for the full system and for the subsystems and on extracting out all the classical correlations so that what is left is ascribed to 'quantum discord'. Compared to entanglement based on separability of the density matrix with measures available only for spin-1/2 but not higher-dimensional subsystems, entropies and quantum discord can be calculated, at least in principle, for any dimensional density matrices and systems. On the other hand, the subtraction of all classical correlations poses a major challenge in calculating quantum discord, especially for larger dimensions. More recently, a variant called geometrical discord [19] that is more accessible has been advanced and we shall consider both in this section.

4.1 *Entropic measure*

With entropy as defined in eq. (1), correlations in a bipartite quantum state are quantified by their 'quantum mutual information' defined as [20]

$$\mathcal{I}(\rho^{AB}) = S(\rho^{A}) + S(\rho^{A}) - S(\rho^{AB}), \tag{4}$$

in terms of the entropies of the composite system AB and of the individual subsystems A and B upon tracing over one of them. Thus, for a separable, pure state $|00\rangle$, whose ρ^{AB} is a 4×4 matrix with 1 in the first element and all others zero, ρ^{A} and ρ^{B} are both 2×2 matrices with entry 1 in the first element and three zeroes, and all S and thereby $\mathcal{I}$ in eq. (4) vanish. On the other hand, a pure entangled Bell state $|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ has ρ^{AB} as in eq. (3) with $a = d = 0, b = z = c = 1/2$, with vanishing S while ρ^{A} and ρ^{B} are $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$ which are mixed states with $S = 1$. Therefore, the quantum mutual information is 2. This same value applies to all the maximally entangled Bell states and the quantity $\mathcal{I}$ proves convenient for distinguishing separable from entangled pure states. It also represents the maximum amount of information that A can send to B using the correlated quantum state between them as the key for one-time pad cryptography [21].

Clearly, there is also classical correlation in such a coupled state AB, namely one classical bit of information that can be exchanged between A and B. This leads to the concept of quantum discord as the correlation that exists beyond the classical,

$$\mathcal{Q}(\rho^{\mathrm{AB}}) = \mathcal{I}(\rho^{\mathrm{AB}}) - \mathcal{C}(\rho^{\mathrm{AB}}), \tag{5}$$

its maximum amount, achieved in Bell states, being unity.

In extending to mixed states, eq. (4) continues unchanged. There remains the definition of the classical correlation to obtain quantum discord. The logic followed is that any measurement carried out on A alone with no involvement of B cannot affect a quantum correlation between them. Therefore, the classical correlation is defined as

$$\mathcal{C}(\rho^{\mathrm{AB}}) = \sup_{A_i} \left(S(\rho^{\mathrm{B}}) - S(\rho^{\mathrm{AB}}|\{A_i\}) \right), \tag{6}$$

where the supremum is to account for the maximum possible classical correlation by considering all possible measurements A_i on A, and $S(\rho^{\mathrm{AB}}|\{A_i\}) = \Sigma_i p_i S(\rho_i)$ with the conditional density operator defined as

$$\rho_i = \frac{(A_i \otimes \mathcal{I})\rho^{\mathrm{AB}}(A_i \otimes \mathcal{I})}{p_i}. \tag{7}$$

Here, $\mathcal{I}$ stands for the identity operator for the second subsystem, and the measurement operators $A_i = U|i\rangle\langle i|U^\dagger$ are chosen by transforming the orthogonal projectors $\Pi_i = |i\rangle\langle i|$, $i = 0, 1$ for subsystem A along the computational basis kets $|i\rangle$ by a general unitary transformation U, and $p_i = \mathrm{Tr}((A_i \otimes \mathcal{I})\rho^{\mathrm{AB}}(A_i \otimes \mathcal{I}))$ [22]. More generally, to embrace all possible measurements on A, one would use positive operator valued measures (POVM) E_i (§2.2.6 of [1]) rather than orthogonal projectors Π_i but for qubits, this is not necessary, the latter being sufficient.

For a qubit A, the unitary operator U can be parametrized in terms of the Pauli matrices as $U = tI + i\vec{y}\cdot\vec{\sigma}$, where the four parameters t, $\vec{y}$ are constrained by unitarity: $t^2 + y_1^2 + y_2^2 + y_3^2 = 1$ [22]. The three independent parameters can be redefined into the unit vector $\vec{z}$ defined as [22]

$$\vec{z} = \{2(-ty_2 + y_1 y_3), 2(ty_1 + y_2 y_3), t^2 + y_3^2 - y_1^2 - y_2^2\}. \tag{8}$$

This unit vector is relevant for the choice of measurement directions $i = \pm\hat{z}$. For any vector $\vec{V}$ and direction $\pm\hat{z}$, the vector identity, $A_i(\vec{\sigma}\cdot\vec{V})A_i = \pm(\vec{z}\cdot\vec{V})A_i$, together with $A_i = U|i\rangle\langle i|U^\dagger = (1\pm\vec{z}\cdot\vec{\sigma})/2$, leads to the standard polar decomposition

$$A_+ = \begin{pmatrix} \cos^2(\theta/2) & \frac{1}{2}\sin\theta \mathrm{e}^{-i\phi} \\ \frac{1}{2}\sin\theta \mathrm{e}^{i\phi} & \sin^2(\theta/2) \end{pmatrix}, \tag{9}$$

and A_-, its parity conjugate, obtained by the substitution $(\theta,\phi)\to(\pi-\theta,\pi+\phi)$.

The algebra involved [8,22] in calculating the post-measurement state in eq. (7) finally boils down to the following very simple prescription [9]. So long as A is a qubit, whatever the dimension d_{B} of B, view the density matrix ρ^{AB} as a block 2×2 matrix of four equal blocks each of dimension $d_{\mathrm{B}}\times d_{\mathrm{B}}$. $(A_+\otimes\mathcal{I})\rho^{\mathrm{AB}}(A_+\otimes\mathcal{I})$ is calculated by multiplying the four blocks, considered in a clockwise manner from the top left, by the elements in eq. (9), that is, $\cos^2(\theta/2)$, $(1/2)\sin\theta\mathrm{e}^{-i\phi}$, $\sin^2(\theta/2)$ and $(1/2)\sin\theta\mathrm{e}^{i\phi}$, respectively. To trace out subsystem A, add the four blocks together. Compute the entropy of the resulting matrix to enter into the second term on the right-hand side of eq. (6). As the eigenvectors depend only on the unit vector $\vec{z}$, they are only functions of two parameters, the polar angles (θ,ϕ) of $\vec{z}$. Therefore, the classical correlation calculation in eq. (6) involves a maximization over just these two parameters, a feasible proposition [8,9].

Experience with thousands of randomly chosen density matrices has shown that in many cases such as for the density matrices in eq. (3), the supremization involves only θ and not ϕ and in others that the supremum is achieved for the special values of $\theta = 0, \pi/2$ [9,23]. Indeed, this is so for over 99% of randomly chosen density matrices of qubit–qubit and three qubits as illustrated in figure 2. This makes for easy calculation of quantum discord.

As an illustration of differences between entanglement, classical correlation and quantum discord, figures 3 and 4 show these quantities for mixed states obtained by 'diluting' Bell states with a simple separable state or with the completely mixed unit density matrix [8]. Figure 3 shows the former for

$$\rho = a|\psi^+\rangle\langle\psi^+| + (1-a)|11\rangle\langle 11|, \tag{10}$$

where $|\psi^+\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$ is the triplet Bell state. Entanglement, as measured by concurrence $C'(\rho)$, diminishes linearly from its maximum of 1 to zero in terms of the dilution parameter $1-a$. The values of classical correlation and quantum discord are shown. For other Bell states, the relative order of the three quantities can be different and that there is no simple ordering is illustrated in figure 4 which is for the 'Werner state' [24]

$$\rho = a|\psi^-\rangle\langle\psi^-| + (1-a)\mathcal{I}/4. \tag{11}$$

In particular, for the region $0 < a < 1/3$, where the Werner state is well known to have zero entanglement and the density matrix is separable, classical correlation and quantum discord still remain non-vanishing.

We make brief remarks on extension of quantum discord calculations to systems AB when neither subsystem is a qubit but is of higher dimension. The definitions given earlier remain valid but the construction of the operators A_i is of course more complicated. For a qutrit of dimension 3, there are three orthogonal projectors Π_i instead of two. Even more, whereas for qubits the two orthogonal projectors suffice, this is no longer true in

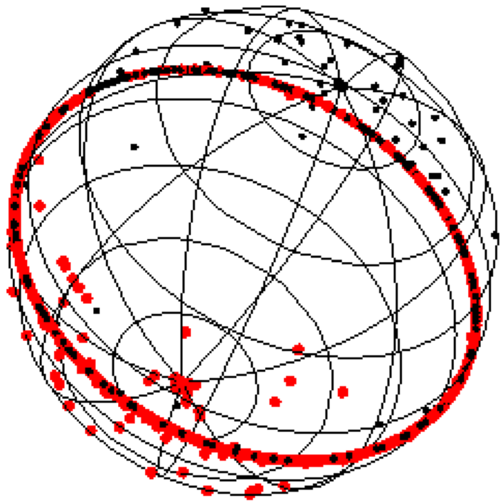

Figure 2. Points (θ, ϕ) on the Bloch sphere for 10,000 randomly chosen qubit–qubit (fuzzy, light) and qubit–qutrit (sharp, dark), obtained by optimization, for quantum discord. Because of antipodal symmetry, only half of the sphere suffices for each case. 99.8% and 99.5%, respectively, of the points lie at the poles or Equator (from [9]).

higher dimension d and one has to consider POVMs of which there are $d(d+1)/2$ and thus 6 for A, a qutrit [25]. These can be chosen to be the symmetric Gell–Mann or other matrices for $d = 3$ and higher [26], just as the two symmetric Pauli σ_x and σ_z can be used, along with the unit matrix, to define POVM for qubits [8]. The final supremum to get the classical correlation with more parameters is also numerically more cumbersome. For these reasons, an alternative correlation is increasingly being discussed.

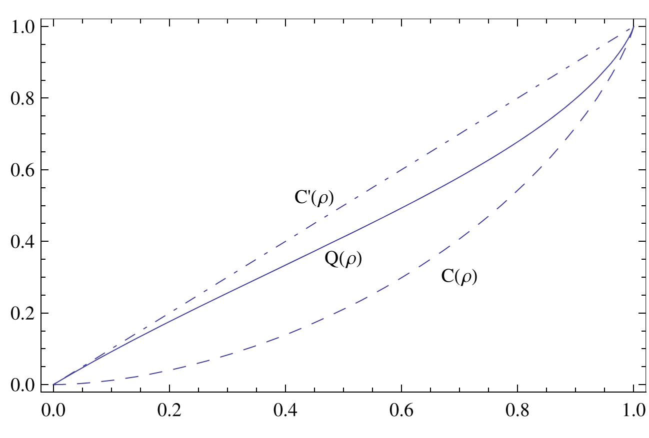

Figure 3. Concurrence $C'(\rho)$, quantum discord $\mathcal{Q}(\rho)$ and classical correlation $\mathcal{C}(\rho)$ for the mixed state in eq. (10) (from [8]).

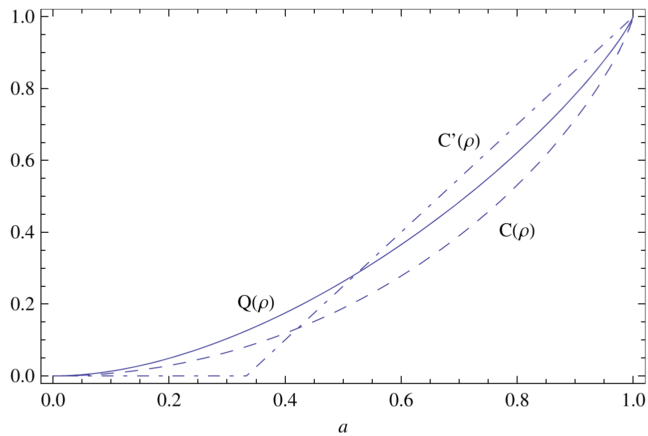

Figure 4. Concurrence $C'(\rho)$, quantum discord $\mathcal{Q}(\rho)$ and classical correlation $\mathcal{C}(\rho)$ for the mixed state in eq. (11). Contrast with figure 3. Note that concurrence or entanglement vanishes for $0 < a < 1/3$ while the other correlations remain non-zero (from [8]).

4.2 *Geometric discord*

An alternative formula for quantum discord for $2 \otimes d$ systems, a geometric measure, is defined as [19]

$$D_{\mathrm{A}}^{(2)}(\rho) = \min_{\chi \in \mathcal{C}} \|\rho - \chi\|^2, \tag{12}$$

where χ is a classical state. Such a classical state, in general, can be written as

$$\chi = \sum_{i=1}^{d_{\mathrm{A}}} p_i \Pi_i^{\mathrm{A}} \otimes \rho_i^{\mathrm{B}}, \tag{13}$$

where d_{A} is the dimensionality of subsystem A and Π_i^{A} are its projectors. ρ_i^{B} are density matrices describing states of subsystem B. Contrast with eq. (2). The logic of the definition is to take the distance to the nearest classical state as a measure of the discord [19].

For two-qubit systems, classical states are defined in terms of one p_i, two angles defining the projectors Π_i^A and two sets of three parameters defining each ρ_i, a total of nine parameters. The minimization in eq. (12) can be carried out analytically to give an accessible closed form expression [19]. Remarkably, the same can be extended to qubit–qudit states in spite of the larger number of parameters involved [9]. This is what makes calculations of the geometric discord more tractable than of its entropic counterpart.

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