Properties of a geometric measure for quantum discord

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We discuss some properties of the quantum discord based on the geometric measure advanced by Dakic, Vedral, and Brukner [Phys. Rev. Lett. 105, 190502 (2010)], with emphasis on Werner- and MEM-states. By recourse to a systematic survey of the two-qubits state-space we ascertain just how good the measure is in representing quantum discord. We explore the dependence of quantum discord on the degree of mixedness of the bipartite states, and also its connection with non-locality as measured by the maximum violation of a Bell inequality within the CHSH scenario.

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I. INTRODUCTION

One of the most fundamental concepts in the quantum description of Nature is that of entanglement, that in recent years has been the subject of intense research efforts [1–4]. All entangled pure states of bipartite systems exhibit non-local features that manifest themselves through the violation of Bell inequalities [1–4]. On the other hand, there exist entangled mixed states that comply with all Bell inequalities. Therefore, entanglement encompasses a concept of quantum correlations broader than the one associated with non-locality. Entanglement, however, does not describe all aspects of the quantum correlations exhibited by multipartite physical systems. In this regard, an important concept that has been receiving much attention lately is that of quantum discord, that refers to quantum correlations different from those involved in entanglement [5–11]. Besides its intrinsic conceptual interest, the study of quantum discord may also have technological implications: examples of improved quantum computing tasks that take advantage of quantum correlations but do not rely on entanglement have been reported [see for instance, among a quite extensive references-list, 6–11]. The aim of the present contribution is to investigate various features of a recently advanced geometric measure of quantum discord and its relationships with the degree of mixture of the quantum state describing a multi-partite system. The connection between discord and non-locality will also be addressed.

Quantum discord [7] constitutes a quantitative measure of the “non-classicality” of bipartite correlations as given by the discrepancy between the quantum counterparts of two classically equivalent expressions for the mutual information. More precisely, quantum discord is defined as the difference between two ways of expressing (quantum mechanically) such an important entropic quantifier. If $S$ stands for the von Neumann entropy, for a bipartite state $A-B$ of density matrix $\rho$ and reduced (“marginals”) ones $\rho_A, \rho_B$, the quantum mutual information (QMI) $M_q$ reads [7]

$$M_q(\rho) = S(\rho_A) + S(\rho_B) - S(\rho),$$

which is to be compared to its associated classical notion $M_{\text{class}}(\rho)$, that is expressed using conditional entropies. If a complete projective measurement $\Pi_B^i$ is performed on $B$ and (i) $p_i$ stands for $Tr_{AB} \Pi_B^i \rho$ and (ii) $\rho_{A|\Pi_B^i}$ for $[\Pi_B^i \rho \Pi_B^i / p_i]$, then our conditional entropy becomes

$$S(A|\{\Pi_j^B\}) = \sum_i p_i S(\rho_{A|\Pi_B^i}),$$

so that $M_{\text{class}}(\rho)$ adopts the appearance

$$M_{\text{class}}(\rho|\{\Pi_j^B\}) = S(\rho_A) - S(A|\{\Pi_j^B\}).$$

Now, if we minimize over all possible $\Pi_B^i$ the difference $M_q(\rho) - M_{\text{class}}(\rho|\{\Pi_j^B\})$ we obtain the quantum discord $\Delta$, that quantifies non-classical correlations in a quantum system, including those not captured by entanglement. One notes then that only states with zero $\Delta$ may exhibit strictly classical correlations. An interesting explorative work is that of Zambrini et al. [8] that illustrate on several interesting aspects of quantum discord for a large family of states. A. Ferraro et al. [9] have shown that such kind of these states has negligible Hilbert space (HS) volume. In other words, a state picked out at random from HS must exhibit positive discord. In this reference, a simple necessary criterion for zero quantum discord is also given. Intuitively, quantum discord may be viewed as the minimal correlations’ loss (as measured by the quantum mutual information) due to measurement, an interpretation entirely analogous to the original one of Ollivier and Zurek [9–11].

Despite increasing evidences for relevance of the quantum discord (Qd) in describing non-classical resources in information processing tasks, there was until quite recently no straightforward criterion to verify the presence
of discord in a given quantum state. Since its evaluation involves an optimization procedure and analytical results are known only in a few cases, such criteria become clearly desirable. Last year Datta advanced a condition for nullity of quantum discord \cite{Datta2009}, and progress was also achieved in \cite{Luo2011} by introducing an interesting geometric measure of quantum discord (GQD). Let \( \chi \) be a generic \( \Delta = 0 \)-state. The GQD measure is then given by

\[
D(\rho) = \text{Min}_\chi \{ ||\rho - \chi||^2 \},
\]

where the minimum is over the set of zero-discord states \( \chi \). We deal then with the square of Hilbert-Schmidt norm of Hermitian operators, \( ||\rho - \chi||^2 = Tr[(\rho - \chi)^2] \). Dakic et al. show how to evaluate this quantity for an arbitrary two-qubit state \cite{Dakic2010}. Moreover, they demonstrate their geometric distance contains all relevant information associated to the notion of quantum discord. This was a remarkable feat given that, despite robust evidence for the pertinence of the Qd-notion, its evaluation involves optimization procedures, with analytical results being known only in a few cases.

Now, given the general form of an arbitrary two-qubits’ state in the Bloch representation

\[
4\rho = I \otimes I + \sum_{i=1}^{3} x_i \sigma_i \otimes I + \sum_{i=1}^{3} y_i I \otimes \sigma_i + \sum_{u,v=1}^{3} T_{uv} \sigma_u \otimes \sigma_v,
\]

with \( x_u = Tr(\rho(\sigma_u \otimes I)) \), \( y_u = Tr(\rho(I \otimes \sigma_u)) \), and \( T_{uv} = Tr(\rho(\sigma_u \otimes \sigma_v)) \), it is found in Ref. \cite{Dakic2010} that a necessary and sufficient criterion for witnessing non-zero quantum discord is given by the rank of the correlation matrix

\[
1/4 \begin{pmatrix} 1 & y_1 & y_2 & y_3 \\ x_1 & T_{11} & T_{12} & T_{13} \\ x_2 & T_{21} & T_{22} & T_{23} \\ x_3 & T_{31} & T_{32} & T_{33} \end{pmatrix},
\]

that is, a state \( \rho \) of the form \cite{Dakic2010} exhibits finite quantum discord iff the matrix \cite{Datta2009} has a rank greater than two. It is seen that the geometric measure \cite{Luo2011} is of the final form \cite{Datta2009} to elucidate further, hopefully interesting, Qd-facets, beginning by ascertaining just how well the measure represents the quantum discord notion.

\section{II. Typical Features of the Geometrical Measure of Quantum Discord (GQD)}

\subsection{A. Preliminaries}

We shall perform a systematic numerical survey of the properties of arbitrary (pure and mixed) states of a given quantum system by recourse to an exhaustive exploration of the concomitant state-space \( \mathcal{S} \). To such an end it is necessary to introduce an appropriate measure \( \mu \) on this space. Such a measure is needed to compute volumes within \( \mathcal{S} \), as well as to determine what is to be understood by a uniform distribution of states on \( \mathcal{S} \). The natural measure that we are going to adopt here is taken from the work of Zyczkowski et al. \cite{Zyczkowski2001}. An arbitrary (pure or mixed) state \( \rho \) of a quantum system described by an \( N \)-dimensional Hilbert space can always be expressed as the product of three matrices,

\[
\rho = UD[\{\lambda_i\}]U^\dagger.
\]

Here \( U \) is an \( N \times N \) unitary matrix and \( D[\{\lambda_i\}] \) is an \( N \times N \) diagonal matrix whose diagonal elements are \( \{\lambda_1, \ldots, \lambda_N\} \), with \( 0 \leq \lambda_i \leq 1 \), and \( \sum \lambda_i = 1 \). The group of unitary matrices \( U(N) \) is endowed with a unique, uniform measure: the Haar measure \( \nu \) \cite{Zyczkowski2001}. On the other hand, the \( N \)-simplex \( \Delta \), consisting of all the real \( N \)-uples \( \{\lambda_1, \ldots, \lambda_N\} \) appearing in \( \rho \), is a subset of a \( (N - 1) \)-dimensional hyperplane of \( R^N \). Consequently, the standard normalized Lebesgue measure \( \mathcal{L}_{N-1} \) on \( R^{N-1} \) provides a natural measure for \( \Delta \). The aforementioned measures on \( U(N) \) and \( \Delta \) lead then to a natural measure \( \mu \) on the set \( \mathcal{S} \) of all the states of our quantum system \cite{Zyczkowski2001}, namely,

\[
\mu = \nu \times \mathcal{L}_{N-1}.
\]

All our present considerations are based on the assumption that the uniform distribution of states of a quantum system is the one determined by the measure \cite{Zyczkowski2001}. Thus, in our numerical computations we are going to randomly generate states according to the measure \cite{Zyczkowski2001}.

\subsection{B. Probability density distributions associated with \( D(\rho) \)}

Let us emphasize that quantum discord quantifies non-classical correlations in a quantum system and one is most interested in those not captured by entanglement.
Only states with zero discord exhibit strictly classical correlations. As stated above, Ferraro et al. [9] proved that these number of such states is “negligible” for the whole of Hilbert’s space (HS), so that a quantum state picked up at random has positive discord, a result that holds for any HS-dimension and has straightforward implications for quantum computation.

Maximally-entangled mixed states (MEMS) were first studied by Munro et al. [17] and are of special interest for quantum communication purposes. For them, the quantum discord can be easily obtained. Their connection with quantum discord has been recently studied by Zambrini et al. [8]. We will find these states below.

We ask ourselves first of all for the question of how well does the values of the distance $D$ represent the presence of quantum discord. For the answer we refer the reader to Fig. 1, which plots the Qd-amount versus the geometric Qd values $D$ of states picked at random from the 2-qubits space. Absolute correspondence would be represented by the diagonal at 45 degrees. Crosses represent Qd and GQd for an arbitrary state. We see that there is a good correlation between both quantities, the plane being mostly populated for low values of the either quantum discord measures. The upper dashed line represents the MEMS states. The diagonal (solid line) is closely followed by the curve (dotted line) representing Werner states.

How are finite $D$—states distributed in Hilbert space? We refer the reader to Fig. 2, that depicts the probability density distribution of finding a given value of the discord $\text{GQd}$. The lower curve corresponds to all states, while the upper curve depicts the same distribution for separable states only (PPT states). Notice the strong bias of both curves towards low values of $\text{GQd}$. The inset depicts similar probability (density) distributions for states with a particular value of the participation ratio only. As we increase the value of $R$ (values for $R=1$, 1.3, 1.6, 2, 2.3, 2.6, 3, 3.3 and 3.8, from right to left), the range of available $\text{GQd}$s diminishes. The distribution for pure states ($R=1$) generated according to the Haar measure is analytic. See text details.

![FIG. 1: (Color online) Sample plot of discord measures Qd vs GQd (crosses) for two qubit mixed states. There exists a strong correlation between both quantities, the plane being mostly populated for low values of the either quantum discord measures. The upper dashed line represents the MEMS states. The diagonal (solid line) is closely followed by the curve (dotted line) representing Werner states.](image)

![FIG. 2: (Color online) Plot of the probability (density) distribution of finding a state $\rho$, pure or mixed, of two qubits with a given value of the discord $\text{GQd}$. The lower curve corresponds to all states, while the upper curve depicts the same distribution for separable states only (PPT states). Notice the strong bias of both curves towards low values of $\text{GQd}$. The inset depicts similar probability (density) distributions for states with a particular value of the participation ratio only. As we increase the value of $R$ (values for $R=1$, 1.3, 1.6, 2, 2.3, 2.6, 3, 3.3 and 3.8, from right to left), the range of available $\text{GQd}$s diminishes, as expected. The distribution for pure states ($R=1$) generated according to the Haar measure is analytic. See text details.](image)
this maximum is attained by Werner states. That is, these states maximize the geometric measure of Ref. [6]. This graph constitutes a nice illustration of the fact that zero-discord is a rather rare event.

Let us delve into the case of Werner states. Since we seek maximum correlations (quantal + classical), we shall consider states which are diagonal in the Bell basis, since nonlocal correlations tend to concentrate after some depolarizing process [13]. If we do so, states [5] should possess null values for \( x \) and \( y \). In other words, we have Bell diagonal states. We consider the paradigmatic case of Werner states of the type \( \text{diag}(1 - 3x, x, x, x) \) \( (x \in [0, \frac{1}{3}] ) \) in the Bell basis \( \{ |\Phi^+ \rangle, |\Phi^- \rangle, |\Psi^+ \rangle, |\Psi^- \rangle \} \). These are a special case of the ones considered in Ref. [6] (states of maximally mixed marginals with \( T_{11} = 0, T_{33} = 1 - 4x, T_{22} = -T_{33} \)). Thus, we have \( D = \frac{1}{2}(1 - 4x)^2 = \frac{1}{6}(\frac{3}{4} - 1) \), which is optimal.

We pass now to the mean value of the geometric measure \( \text{GQd} \) as a function of the participation ratio \( R \) for all the space of two qubits (Fig. 4). The monotonic behavior of the \( \text{GQd} \) is apparent. The value for pure states is analytic \( \langle \frac{\sqrt{D}}{\sqrt{1 + D}} \rangle \). The inset depicts the same quantity \( \text{GQd} \), but only for separable states. Notice the expected behavior for the quantum discord (null for separable and maximally mixed states). Both curves coincide in the range \( R \in [3, 4] \).

Since we encounter the Werner states to be most “discordant” ones for a given value of the participation ratio \( R \), we may wonder why this is not the case for the original quantum discord measure \( \text{Qd} \) of [7]. In point of fact, states \( \text{diag}(1 - 3x, x, x, x) \), with \( x \in [\frac{1}{3}, \frac{1}{4}] \) happen to be of maximal \( \text{Qd} \) in the region \( R \in [3, 4] \), where all states are separable! This implies that a depolarizing process would concentrate quantum correlations for \( \text{Qd} \) only where just classical correlations exist, which seems to be a contradiction. Therefore, we are forced to abandon the initial assumption that a state \( \rho \), who has been through some depolarizing channel, concentrates quantum discord. This fact is sustained by the evidence that Bell diagonal states do not optimize \( \text{Qd} \) for a given \( R \). In point of fact, states that concentrate entanglement for a given \( R \), that is, MEMS states, possess the form

\[
\begin{pmatrix}
g(x) + \frac{x}{2} & 0 & 0 & 0 \\
0 & g(x) - \frac{x}{2} & 0 & 0 \\
0 & 0 & 1 - 2g(x) & 1 - 2g(x) \\
0 & 0 & \frac{1 - 2g(x)}{2} & \frac{1 - 2g(x)}{2}
\end{pmatrix}, \quad (12)
\]

in the Bell basis, with \( g(x) = 1/3 \) for \( 0 \leq x \leq 2/3 \), and \( g(x) = x/2 \) for \( 2/3 \leq x \leq 1 \) (the quantity \( x \) being equal to the concurrence \( C \)). Notice the aforementioned tendency of states to concentrate correlations (here entirely from an entanglement origin) in view of the quasi diagonal form of [12]. In addition, MEMS maximize \( \text{Qd} \) in the R-range \( [1, 1.8] \). Thus, maximum discord and maximum entanglement coincide for low-purity values.

Fig. 2 should be now compared to Fig. 5, that gives, in the fashion of Zambrini et al. [8], the probability (density) distribution for the true discord \( \text{Qd} \) for all two-qubits’ states (lower curve). The more peaked curve corresponds to separable states only. The inset refers to a more original scenario and depicts the density distribution of the classical correlations (CC). Classical and quantum correlations are distributed in rather similar fashion because most states exhibit very small

![FIG. 3: (Color online) Plot of the GQd vs the participation ratio R for a sample of \( 10^6 \) mixed states of two qubits. The lower curve corresponds to MEMS states, while the solid line corresponds to the maximum GQd value compatible with a given R. This maximum is attained by Werner states for the measure GQd of quantum discord. See text for details.](image)

![FIG. 4: (Color online) Plot of the mean value of the quantum discord measure GQd vs the participation ratio R for all the space of two qubits. The monotonic behavior of GQd is apparent. The value for pure states is analytic \( \langle \frac{\sqrt{D}}{\sqrt{1 + D}} \rangle \). The inset depicts the same quantity GQd only for separable states. Notice the expected behavior for the quantum discord (null for separable and maximally mixed states). Both curves coincide in the range R \( \in [3, 4] \). Since we encounter the Werner states to be most “discordant” ones for a given value of the participation ratio R, we may wonder why this is not the case for the original quantum discord measure Qd of [7]. In point of fact, states \( \text{diag}(1 - 3x, x, x, x) \), with \( x \in [\frac{1}{3}, \frac{1}{4}] \) happen to be of maximal Qd in the region R \( \in [3, 4] \), where all states are separable! This implies that a depolarizing process would concentrate quantum correlations for Qd only where just classical correlations exist, which seems to be a contradiction. Therefore, we are forced to abandon the initial assumption that a state \( \rho \), who has been through some depolarizing channel, concentrates quantum discord. This fact is sustained by the evidence that Bell diagonal states do not optimize Qd for a given R. In point of fact, states that concentrate entanglement for a given R, that is, MEMS states, possess the form](image)
We pass now to Fig. 6. It is a sample plot for Qd vs. R for $10^6$ mixed states of two qubits. The upper dashed curve corresponds to MEMS states, while the solid one is that for Werner states. The inset depicts the mean value of Qd vs R. Notice the change in the curve for all states being separable ($R \geq 3$). The horizontal line represents the analytic value for pure states generated according to the Haar measure ($\frac{1}{3\log2}$).

**FIG. 6:** (Color online) Sample plot for Qd vs R for $10^6$ mixed states of two qubits. The upper dashed curve corresponds to MEMS states, while the solid one is that for Werner states. The inset depicts the mean value of Qd vs R. Notice the change in the curve for all states being separable ($R \geq 3$). The horizontal line represents the analytic value for pure states generated according to the Haar measure ($\frac{1}{3\log2}$). See text for details.

**III. BELL INEQUALITIES AND GEOMETRIC MEASURE FOR QUANTUM DISCORD**

Most of our knowledge on Bell inequalities and their quantum mechanical violation is based on the CHSH inequality \[19\]. With two dichotomic observables per party, it is the simplest nontrivial Bell inequality for the bipartite case with binary inputs and outcomes. Quantum mechanically, these observables reduce to $A_j(B_j) = a_j(b_j) \cdot \sigma$, where $a_j(b_j)$ are unit vectors in $\mathbb{R}^3$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ the Pauli matrices. Violation of CHSH inequality requires the expectation value of the operator $B_{CHSH} = A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2$ to be greater than two. In this vein one should make reference to the Tsirelson-bound, also known as Tsirelson’s inequality. It is indeed an inequality that imposes an upper limit to quantum mechanical correlations between distant events. It relates to the discussion and experimental determination of whether local hidden variables are required for, or even compatible with, the representation of experimental results. This is of particular relevance to EPR’s thought experiment and to the CHSH inequality. It is named for B. S. Tsirelson, who derived it \[20\].

Let us now consider the case of the maximum violation of a Bell inequality, in the form of the CHSH Bell inequality for two qubits, Fig. 7 depicts the nonlocality measure $B_{CHSH}^{max}$ vs $GQd$ for a random sample of uniformly generated two qubit-mixed states. The horizontal curve at the height of two” represents the limit for local variable model theories (LVM) to hold, whereas the upper one at $2\sqrt{2}$ represents the Tsirelson-bound for quantum mechanics. As we can appreciate, each quantum state lies between the two curves, and the general trend is a certain correlation between both quantities. This remarkable behavior can be explained as follows. Since we seek maximum violation of the CHSH inequality, those states necessarily must concentrate their nonlocal correlations. Therefore, a considerable subset of states that fills the entire region between these curves is that of Bell diagonal states. In point of fact, those Bell diagonal states that are less nonlocal are precisely the previously discussed Werner states, that is, diag$(1 - 3x, x, x, x) \ (x \in [0, \frac{1}{2}])$, which exhibit a maximum amount of GQd. Therefore, when calculating their nonlocality measure, we find it to be \[21\] (J. Batle and M. Casas, e-print arXiv:quant-ph/1102.4653.) $B_W = 2\sqrt{2} (1 - 4x)$, which implies that the lower curve in Fig. 7 is of the form $B_{CHSH}^{max} = 4\sqrt{GQd}$.

Now, what is the nature of the upper curve in Fig. 7? As explained in Ref. \[21\] there is a limit to those states that maximize the CHSH inequality. These states are given in the form in Eq. (17) of \[21\], namely, diag$(1 - x, x, 0, 0) \ (x \in [0, \frac{1}{2}])$ also in the Bell basis. These maximally nonlocal mixed states (MNMS) maximally violate the CHSH inequality for a given value of
the participation ratio $R$. Their nonlocality is given by $B = 2\sqrt{2(1-x)^2 + x^2}$. Obtaining their concomitant $GQd$ measure in the usual manner, we obtain $GQd = \frac{1}{2}(1-2x)^2$. Combining both relations, we naturally obtain $B_{\text{CHSH}}^{\text{max}} = 2\sqrt{1-2GQd}$.

**IV. CONCLUSIONS**

We have performed a systematic survey of the two qubits Hilbert’s space so as to assess the main features of the geometric measure of quantum discord $D$ advanced in [6]. We have shown that, when considering the typical behavior of general (pure or mixed) states of two qubits, the geometric measure of quantum discord is strongly correlated with the measure of quantum discord originally advanced by Zurek and Ollivier. We investigated the connection between quantum discord and degree of mixedness as measured by the participation ratio $R$. As a general trend we observed that as $R$ increases the range of possible values of the discord decreases, only small vales of $D$ becoming available. We showed that the maximum values of $D$ compatible with given values of $R$ are attained by the Werner states. The behaviour of MEMS in connection with quantum discord and degree of mixedness was also addressed. Finally, we examined the connection between the geometric measure of quantum discord and non-locality (as measured by the maximum violation of a bell inequality within the CHSH scenario). Our results indicate that there exists a clear tendency of non-locality to increase as one considers two-qubits states exhibiting increasing values of quantum discord.

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