Witnessed entanglement and the geometric measure of quantum discord

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We establish relations between geometric quantum discord and entanglement quantifiers obtained by means of optimal witness operators. In particular, we prove a relation between negativity and geometric discord in the Hilbert-Schmidt norm, which is slightly different from a previous conjectured one [1]. We also show that, redefining the geometric discord with the trace norm, better bounds can be obtained. We illustrate our results numerically.

I. INTRODUCTION

Entanglement has been widely investigated in the last years [2], and is a resource that allows for tasks that cannot be performed classically, as teleportation [3], quantum key distribution [4], superdense coding [5], and speed-up of some algorithms [6], just to cite a few examples. Therefore entanglement is an indisputable signature of the non-classicality of a state. Nevertheless, some authors have argued that there is more to the quantumness of a state than just its entanglement [7–9]. This notion of quantumness beyond entanglement is captured by the quantum discord, which is defined as all the correlations contained in a state but the classical ones [7], or as a measure of disturbance of a state after local measurements [8], both definitions being compatible with a class of separable states with non-null quantum discord.

Recent investigations suggest that quantum discord can be considered a resource that gives a quantum advantage [10]. In order to deepen our understanding of both the usefulness of such a resource and how quantum it really is, it is important to devise operational means to quantify it, and also to relate it to quantum entanglement. In this respect, the geometric discord [11] defined as the distance between the state of interest and a properly defined classical state is an invaluable tool. Unhappily the classical states do not form a convex set [12], and therefore one cannot use the well known separating hyperplane theorem to characterize discord as is done with the witness operators in the case of the entanglement problem [2].

Interesting investigations relating entanglement and discord have been done recently [1, 13]. In [13], entanglement of formation is related to discord in a conservation equation, and in [1] geometric discord is conjectured to be bounded by the negativity. While entanglement of formation is not computable in general, many other interesting entanglement quantifiers can be expressed in terms of optimal entanglement witnesses [14] which, by its turn, can be calculated numerically by means of efficient semidefinite programs [15, 16]. In this work we will explore bounds for geometric discord by means of optimal entanglement witnesses. In particular, we will prove that negativity bounds the geometric discord.

This paper is organized as follows. In Sec.II we briefly revise quantum discord, and propose a redefinition of geometric discord using the Schatten $p$-norm. In Sec.III, we recall the witnessed entanglement, with special attention to both negativity and robustness. In Sec.IV, we derive bounds for geometric discord using witnessed entanglement. In Sec.V, we illustrate our results for Werner states and some families of bound entangled states. We conclude in Sec.VI.

II. QUANTUM DISCORD

The total amount of correlations of a bipartite system $AB$ is quantified by the well known mutual information, which in the classical case can be written in two equivalent forms linked by Bayes’ rule, namely: $I(A : B) = H(A) + H(B) - H(AB) = H(A) - H(A|B)$, being $H(X)$ the Shanon entropy of $X$ and $H(X|Y)$ the conditional entropy of $X$ given $Y$. For a quantum system $\rho_{AB}$, the mutual information is defined in terms of the von Neuman

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entropy $S(\rho) = -Tr(\rho \log \rho)$, and reads:

$$I(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}),$$  

(1)

with $\rho_A$ and $\rho_B$ being the marginals of $\rho_{AB}$. However, the definition of a quantum conditional entropy is dependent on the choice of a given POVM $\{\Pi_k\}$ to be measured on party B, and the two expressions for the mutual information are no longer equivalent. While Eq.5 still quantifies the total amount of correlations in the quantum state, the other expression involving the conditional entropy needs some attention. After the measurement of $\Pi_k$ on B, party A is left in the state $\rho_{A|k} = Tr_B(\mathbb{I} \otimes \Pi_k \rho_{AB})/p_k$, with probability $p_k = Tr(\mathbb{I} \otimes \Pi_k \rho_{AB})$. Now we can write the conditional entropy associated to the POVM $\{\Pi_k\}$ as:

$$S(\rho_{A|B}) = \sum_k p_k S(\rho_{A|k}).$$  

(2)

$J(\rho_{AB}, \{\Pi_k\}) = S(\rho_A) - S(\rho_{A|B})$ quantifies the classical correlations contained in $\rho_{AB}$ under measurements in the given POVM. Therefore, maximizing $J(\rho_{AB}, \{\Pi_k\})$ over all POVMs quantifies the classical correlations in the quantum state, namely [8, 9] :

$$J_{AB}(\rho) = S(\rho_A) - \min_{\Pi_k} \sum_k p_k S(\rho_{A|k}),$$  

(3)

where the POVMs can be chosen to be rank-one [17]. Finally, the quantum discord is the disagreement between the nonequivalent expressions of mutual information in the quantum case, namely [8, 9]:

$$D(\rho_{AB}) = I(\rho_{AB}) - J(\rho_{AB}).$$  

(4)

Note that $D(\rho_{AB})$ is non-negative and asymmetric with respect to $A \leftrightarrow B$.

As discord is supposed to measure the quantumness of a state, it is not wonder that the maximally entangled states Eq.8 are the most discordant, while states which are a mere encoding of classical probability distributions Eq.7 are concordant (i.e. $I(\rho_{AB}) = J(\rho_{AB})$) [18]. Bipartite maximally entangled states in $B(\mathbb{C}^{d=\text{size} \times \text{size}})$, with $d_A = d_B$, have the form:

$$\phi = \frac{1}{d_A} \sum_{i,j=1}^{d_A} |ii\rangle\langle jj|,$$  

(5)

while classical states can be written as:

$$\xi = \sum_{i,j=1}^{d_A} p_{ij} |e_i\rangle\langle e_i| \otimes |f_j\rangle\langle f_j|,$$  

(6)

where $|e_i\rangle$ and $|f_j\rangle$ are two orthonormal bases. Note however, that as discord is asymmetric, if the measurements are to be done in subsystem $B$, the following class of states are also concordant or classical:

$$\xi = \sum_{j=1}^{d_A} p_{j} \rho_j \otimes |f_j\rangle\langle f_j|.$$  

(7)

To distinguish these two classes of classical states, sometimes the former is referred to as classical-classical, while the latter is quantum-classical.

An alternative definition for quantum discord is based on the distance between the given quantum state and the closest classical state [11, 19, 22]. Adopting the Hilbert-Schmidt norm $\|\rho - \xi\|_2(2)$, we can write [11]:

$$D(2)(\rho_{AB}) = \min_{\xi \in \Omega} \|\rho - \xi\|_2(2),$$  

(8)

where $\Omega$ is the set of zero-discord states. This measure can be interpreted as the minimal disturbance after local measurements on subsystem $B$. In this case $\Omega$ contains the states in Eq.7 and $D(2)$ can be calculated analytically for some states [21].

Consider the Schatten $p$-norm for some matrix $A$ and positive integer $p$:

$$\|A\|_p = \{Tr[(A^*A)^{p/2}]\}^{1/p},$$  

(9)
which, for $p = 2$ is the Hilbert-Schmidt norm. In finite Hilbert spaces, these norms induce the same ordering \[23\]. Therefore we propose to extend the geometric discord for any $p$-norm, namely:

$$D_{(p)}(\rho_{AB}) = \min_{\xi \in \Omega} \|\rho_{AB} - \xi\|_p^p.$$  

(10)

Note that for $p \geq q$, we have $\|A\|_p \leq \|A\|_q$. It follows that the 1-norm is the most distinguishable distance in Hilbert space. Therefore, we shall investigate the geometric discord in the 1-norm ($D_{(1)}$), besides the usual $D_{(2)}$. As we shall see, it is easy to bound these geometric discords by entanglement witnesses.

### III. WITNESSED ENTANGLEMENT

Entanglement witnesses are Hermitian operators (observables - $W$) whose expectation values contain information about the entanglement of quantum states. The operator $W$ is an entanglement witness for a given entangled quantum state $\rho$ if the following conditions are satisfied \[24\]: its expectation value is negative for the particular entangled quantum state ($\text{Tr}(W\rho) < 0$), while it is non-negative on the set of separable states ($S$) ($\forall \sigma \in S$, $\text{Tr}(W\sigma) \geq 0$). We are particularly interested in optimal entanglement witnesses. $W_{\text{opt}}$ is the OEW for the state $\rho$ if

$$\text{Tr}(W_{\text{opt}}\rho) = \min_{W \in \mathcal{M}} \text{Tr}(W\rho),$$

(11)

where $\mathcal{M}$ represents a compact subset of the set of entanglement witnesses $\mathcal{W}$ \[14\].

OEWs can be used to quantify entanglement. Such quantification is related to the choice of the set $\mathcal{M}$, where different sets will determine different quantifiers \[14\]. We can define these quantifiers by:

$$E_w(\rho) = \max\{0, -\min_{W \in \mathcal{M}} \text{Tr}(W\rho)\}.$$  

(12)

An example of a quantifier that can be calculated using OEWs is the Generalized Robustness of entanglement \[25\] ($R_g(\rho)$), which is defined as the minimum required mixture such that a separable state is obtained. Precisely, it is the minimum value of $s$ such that

$$\sigma = \frac{\rho + s\varphi}{1 + s}$$

be a separable state, where $\varphi$ can be any state. We know that the Generalized Robustness can be calculated from Eq\[12\] using $\mathcal{M} = \{W \in \mathcal{W} \mid W \leq I\}$ \[14\], where $I$ is the identity operator; in other words,

$$R_g(\rho) = \max\{0, -\min_{\{W \in \mathcal{W} \mid W \leq I\}} \text{Tr}(W\rho)\}.$$  

(14)

A particular case of the Generalized Robustness is the Random Robustness, where $\varphi$ in Eq\[13\] is taken to be the maximally mixed state ($I/d$). In this case, the compact set of entanglement witnesses is $\mathcal{M} = \{W \in \mathcal{W} \mid \text{Tr}(W) = 1\}$. The Random Robustness $R_r(\rho)$ quantifies the resilience of the entanglement to white noise, and is given by \[16\]:

$$d \times R_r(\rho) = \max\{0, -\min_{\{W \in \mathcal{W} \mid \text{Tr}(W) = 1\}} \text{Tr}(W\rho)\}.$$  

(15)

The well known Negativity for bipartite states, which is the sum of the negative eigenvalues of the partial transpose of the given state, $N(\rho) \equiv (\|\rho^{T_A}\|_1 - 1)/2$, can also be expressed in terms of OEWs as \[14\]:

$$N(\rho) = \max\{0, -\min_{0 \leq \text{Tr}(W) \leq 1} \text{Tr}(W\rho)\}.$$  

(16)

The construction of entanglement witnesses is a hard problem. In an interesting method proposed by Brandão and Vianna \[15\], the optimization of entanglement witnesses is cast as a robust semidefinite program (RSDP). Despite RSDP is computationally intractable, it is possible to perform a probabilistic relaxation turning it into a semidefinite program(SDP), which can be solved efficiently \[26\].
IV. BOUNDING GEOMETRIC DISCORD WITH WITNESSED ENTANGLEMENT

In this section we show that geometric discord, in any norm, is lower bounded by entanglement. In particular, we show that norm-2 geometric discord is bounded by negativity, but the relation is slightly different from that conjectured by Girolami and Adesso [12].

For any two operators $A, B \in B(\mathbb{C}^d)$ and the Schatten $p$-norm $\|A\|_p = \text{Tr}[(AA^\dagger)^{p/2}]^{1/p}$, the following inequality holds:

$$\|A\|_p\|B\|_q \geq |\text{Tr}[AB^\dagger]|,$$  \hspace{1cm} (17)

where $1/q + 1/p = 1$.

The geometrical discord for a state $\rho \in B(\mathbb{C}^{d_A \times d_B})$ is:

$$D_p(\rho) = \|\rho - \bar{\xi}\|_p^p,$$ \hspace{1cm} (18)

where $\bar{\xi}$ is the closest non-discordant state. The witnessed entanglement of $\rho$ can be written as:

$$E_w(\rho) = \min\{0, -\text{Tr}[W\rho]\},$$ \hspace{1cm} (19)

where $W$ is the optimal entanglement witness of $\rho$. Plugging $A = \|\rho - \bar{\xi}\|_p$ and $B = W$ in Eq.17, we get:

$$\|\rho - \bar{\xi}\|_p\|W\|_q \geq |\text{Tr}[\rho - \bar{\xi}]W\rho]|.$$

(20)

If $\rho$ is entangled and $\bar{\xi}$ is separable we have $|\text{Tr}[\rho - \bar{\xi}]W\rho]| \geq |\text{Tr}[\rho W\rho]|$, thus:

$$\|\rho - \bar{\xi}\|_p \geq \frac{|\text{Tr}[\rho W\rho]|}{\|W\|_q},$$ \hspace{1cm} (21)

which in terms of geometric discord (Eq.2) reads:

$$D_p(\rho) \geq \left(\frac{E_w(\rho)}{\|W\|_q}\right)^p.$$ \hspace{1cm} (22)

Therefore, given any entanglement witness (it does not need to be optimal), we have a bound for geometric discord in any norm. Note that Eq.6 is also valid for multipartite states. For norm-1 and norm-2, Eq.6 reduces to:

$$D_1(\rho) \geq \frac{E_w(\rho)}{\|W\|_\infty},$$ \hspace{1cm} (23)

$$D_2(\rho) \geq \frac{E_w^2(\rho)}{\text{Tr}[W^2\rho]}.$$ \hspace{1cm} (24)

If $W$ is the entanglement witness for the negativity, $N(\rho) = E_w(\rho)$ (see Eq.19), then $\text{Tr}[W^2\rho] = n_-$, where $n_-$ is the number of negative eigenvalues of the partial transpose of $\rho$ ($\rho^{T_A}$). Thus, in norm-2, discord is lower bounded by negativity as:

$$D_2(\rho) \geq \frac{N^2(\rho)}{n_-},$$ \hspace{1cm} (25)

where $0 < n_- \leq d - 1$ (remember $d = d_A \times d_B$). For norm-1 discord, one has to calculate $\|W\|_\infty$, which is simply the largest eigenvalue of $W$ in absolute value, and use Eq.23. Note that it is easy. One has just to form a rank-$n_-$ projector with the eigenstates of $\rho^{T_A}$ associated to the $n_-$ negative eigenvalues, then $W$ is the partial transpose of this projector.

V. NUMERICAL APPLICATIONS

In this section we illustrate our results with numerical calculations on maximally entangled pure states, Werner states and bound entangled states. We consider the negativity and random robustness.
A. Werner states

Werner states \((d_A \otimes d_A)\) [27], which are of the Bell diagonal type, can be written as:

\[
\rho_w = \frac{d_A + k}{d_A^2 - d} \mathbb{I}_d - \frac{d_A k - 1}{d_A^2 - d} |\psi^+\rangle\langle\psi^+|,
\]

where \(|\psi^+\rangle = \sum_{i,j=0}^{d_A-1} (|ij\rangle + |ji\rangle). The parameter \(k\) is in the interval \([-1, 1]\), and the state is entangled for \(k > 0\).

In (Fig.1) we compare negativity, random robustness and 1-norm geometric discord. Note that negativity and random robustness coincide in the entangled region and are always less than the discord. Note also that the random robustness in the non-entangled region \((Tr(\rho_w W_{\rho_w}) \geq 0)\) has a functional behavior similar to the discord.

B. Bound-entangled states

Bound entangled states have positive partial transpose (ppt) and are known to be undistillable [28]. The negativity is useless in this case, but the random robustness can give an interesting bound for the discord.

1. Horodecki’s ppt-entangled states

Consider a Hilbert space \(\mathbb{C}^3 \otimes \mathbb{C}^3\), and a canonical orthonormal basis \(|i\rangle\)\(_{0,1,2}\). Take the following three states [28, 29]:

\[
Q = I \otimes I - \left[ \sum_{i=0}^2 |i\rangle\langle i| \otimes |i\rangle\langle i| + |2\rangle\langle 2| \otimes |0\rangle\langle 0| \right],
\]

\[
|\psi\rangle = \frac{1}{3} \left[ |0\rangle|0\rangle + |1\rangle|1\rangle + |2\rangle|2\rangle \right]
\]

and

\[
|\phi_k\rangle = |2\rangle \otimes \left[ \sqrt{\frac{1 + k}{2}} |0\rangle + \sqrt{\frac{1 - k}{2}} |2\rangle \right],
\]

where \(0 \leq k \leq 1\). The following convex combination is a ppt-entangled state for \(0 \leq k < 1\), and is separable for \(k = 1\):

\[
\varrho_k = \frac{k}{8k + 1} \left[ 3|\psi\rangle\langle\psi| + Q \right] + \frac{1}{8k + 1} |\phi_k\rangle\langle\phi_k|.
\]

Note, in Fig.2a, that the most discordant state of this family is the less entangled one, and vice-versa. However, it is not a general characteristic of bound entangled states, as can be seen in the next example (Fig.2b).
FIG. 2: (Color online) 1-norm geometric discord and random robustness for $3 \otimes 3$ (a) and $4 \otimes 4$ (b) ppt-entangled states.

![Diagram](image)

TABLE I: Entanglement and some properties of the corresponding entanglement witness. $W_n$ and $W_r$ are the entanglement witnesses for negativity and random robustness, respectively.

| $(d = 2 \otimes 2)$ $\rho = |\Phi^+\rangle\langle \Phi^+|$ | $\text{Tr}(\rho W_n)$ | $\text{Tr}(\rho W_r)$ | $\text{Tr}(W_n^2)$ | $\text{Tr}(W_r^2)$ | $\| W_n \|_\infty$ | $\| W_r \|_\infty$ |
|---|---|---|---|---|---|---|
| $(d = 4 \otimes 4)$ $\rho = |\Phi^+\rangle\langle \Phi^+|$ | -1.5000 | -0.2500 | 6 | 0.1677 | 1.5000 | 0.2503 |
| $(d = 8 \otimes 8)$ $\rho = \rho_w(8, -1)$ | -0.1250 | -0.1250 | 1 | 1.0000 | 0.1250 | 0.1250 |
| $(d = 2 \otimes 32)$ $\rho = \rho_w(8, -1)$ | -0.1786 | -0.0179 | 10 | 0.1013 | 0.5000 | 0.0600 |

2. UPB entangled states

In a bipartite Hilbert space $\mathcal{H} = \mathbb{C}^d_A \otimes \mathbb{C}^d_B$, an orthogonal product basis (PB) is an $l$-dimensional set of separable states spanning a subspace $\mathcal{H}_l$ of $\mathcal{H}$. When the complement of this PB in $\mathcal{H}$ has only entangled states, we say that the complete basis containing PB is a unextendible product basis (UPB) [30].

Consider the following three classes of vectors in $\mathcal{H} = \mathbb{C}^4 \otimes \mathbb{C}^4$:

$$|v_j\rangle = |j\rangle \otimes \frac{|(j + 1) \mod 4\rangle - |(j + 2) \mod 4\rangle}{\sqrt{2}},$$

$$|u_j\rangle = \frac{|(j + 1) \mod 4\rangle - |(j + 2) \mod 4\rangle}{\sqrt{2}} \otimes |j\rangle,$$

$$|w\rangle = \frac{1}{4} \sum_{i,j=0}^{3} |i\rangle \otimes |j\rangle.$$ 

Now define the following vectors: $|\psi_k\rangle = |v_k\rangle$ for $k = 0, 1, 2, 3$, $|\psi_k\rangle = |u_{k \mod 4}\rangle$ for $k = 4, 5, 6, 7$, and $|\psi_k\rangle = |w\rangle$ for $k = 8$. Finally, a ppt-entangled state is given by:

$$\rho = \frac{1}{7} \left( I - \sum_{k=0}^{8} |\psi_k\rangle\langle \psi_k| \right).$$ (31)

In (Fig.2b), we plotted random robustness and 1-norm geometric discord for the convex mixture:

$$\sigma = \frac{s}{16} I + (1 - s) \rho,$$ (32)

which is separable for $s > 0.169$. We see that the discord is always greater than the entanglement, and the most discordant states are also the most entangled.

C. Pure states versus Werner states

In Tabs. I and II, we compare the bounds for norm-1 and norm-2 in two maximally entangled states, an $8 \otimes 8$ Werner state, and a $2 \otimes 8$ mixed state whose density matrix coincides with the $8 \otimes 8$ Werner state. The norm-1 bounds are much better than the norm-2 ones. Tab.III is an Erratum for the published version of this paper.
We obtained bounds for geometric discord, in any norm, in terms of entanglement witnesses (EW). Many known measures of entanglement can be expressed by Optimal EWs, which implies that our bounds are quite general. We note that, in a previous work [31], we showed how to calculate entanglement and geometric discord in systems of indistinguishable fermions, and we checked that the geometric discord was also bounded by the witnessed entanglement in that case.

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VI. CONCLUSION

| $D_2$ | $T_{\infty}^{(\rho W_2)}$ | $T_{01}^{(\rho W_2)}$ | $D_1$ | $T_{\infty}^{(\rho W_1)}$ | $T_{01}^{(\rho W_1)}$ |
|-------|-----------------|-----------------|-------|-----------------|-----------------|
| $d = 2 \otimes 2$ $\rho = |\Phi^+\rangle \langle \Phi^+|$ | 0.5000 | 0.2500 | 1.0000 | 1.0000 | 1.0000 |
| $d = 4 \otimes 4$ $\rho = |\Phi^+\rangle \langle \Phi^+|$ | 0.7500 | 0.3750 | 1.5000 | 1.0000 | 0.9988 |
| $d = 8 \otimes 8$ $\rho = \rho_w(8,-1)$ | 0.0179 | 0.0156 | 0.0156 | 1.0000 | 1.0000 |
| $d = 2 \otimes 32$ $\rho = \rho_w(8,-1)$ | 0.0102 | 0.0032 | 0.0032 | 0.5714 | 0.3580 |

TABLE II: Bounding geometric discord with witnessed entanglement.

| $d = 2 \otimes 2$ $\rho = |\Phi^+\rangle \langle \Phi^+|$ | $T_{\infty}^{(\rho W_2)}$ | $T_{01}^{(\rho W_2)}$ | $D_1$ | $T_{\infty}^{(\rho W_1)}$ | $T_{01}^{(\rho W_1)}$ |
|-------|-----------------|-----------------|-------|-----------------|-----------------|
| $d = 4 \otimes 4$ $\rho = |\Phi^+\rangle \langle \Phi^+|$ | 0.7500 | 0.1500 | 1.5000 | 0.0938 | 0.2500 |
| $d = 8 \otimes 8$ $\rho = \rho_w(8,-1)$ | 0.0179 | 0.0002 | 1.0000 | 0.0020 | 0.0020 |
| $d = 2 \otimes 32$ $\rho = \rho_w(8,-1)$ | 0.0102 | 0.0005 | 0.5714 | 0.0028 | 0.0179 |

TABLE III: Errata for Eqs. 21, 27 and 28 in [Phys. Rev. A 86, 024302 (2012)].
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