Maximally discordant separable two-qubit $X$ states

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Abstract In a recent article, Gharibian (Phys Rev A 86:042106 2012) has conjectured that no two-qubit separable state of rank greater than two could be maximally non-classical (defined to be those which have normalized geometric discord $1/4$) and asked for an analytic proof. In this work, we prove analytically that among the subclass of $X$ states, there is a unique (up to local unitary equivalence) maximal separable state of rank two. For the general case, we derive some necessary conditions.

Keywords Geometric discord · $X$ states · Separability · Two qubit

1 Introduction

As it is well known, the basic tasks in quantum information theory are mainly characterization, quantification and possible applications of quantum correlations. Of these, the characterization part is naturally the elementary step where different notions of \textit{quantumness} emerge from different perspectives. It is always interesting to characterize the states having maximum quantumness (which obviously depends on both the notion as well as the measure), because in general, different notions induce different ordering on the state space. For example, given two entanglement measures $E_1$, $E_2$, in general there are states $\rho_1$, $\rho_2$ such that $E_1(\rho_1) > E_1(\rho_2)$, but $E_2(\rho_1) < E_2(\rho_2)$ [1]. Thus, maximally entangled states with respect to (w.r.t.) $E_1$ need not be maximally
entangled w.r.t. $E_2$. As a result, historically whenever a new measure was proposed, this question was raised subsequently. For some classic examples, see [1–4].

Naturally, the recently introduced quantum discord [5], or its well studied variant, the geometric discord [6–9] should not be any exception. It is known that the usual geometric discord reaches its maximum only on maximally entangled states [10]. However, a much advertised distinctive feature of quantum discord is that it can be nonzero even for separable states. Therefore, an obvious question would be: what is the maximum discord for separable states? To our knowledge, the first general bound on entropic discord [5] for separable states was $\delta_A \leq \min\{S_A, S_B, I(A : B)\}$, given by A. Datta (see p. 40 of [11]). Since then, a vast literature has appeared for characterization of maximally discordant states—applying both analytical [12–14] and numerical techniques [15–21], or even experimentally [22,23], mainly for two qubits. Very recently, Gharibian [24] has proved analytically that among rank-two separable states of two qubits, the maximum value of normalized geometric discord is $1/4$ and conjectured that no separable two-qubit state of higher rank could achieve this value. The aim of the present work is to explore this conjecture.

Before proceeding further, let us define the relevant quantities. The main object, the geometric discord (GD), for an $m \otimes n$ state is defined by (normalized to have maximum value 1)

$$D(\rho) = \frac{m}{m-1} \min_{\chi \in \Omega_0} \|\rho - \chi\|^2,$$

where $\Omega_0$ is the set of zero-discord or classical-quantum (CQ) states (given by $\sum p_k |\psi_k\rangle_A \langle \psi_k| \otimes \rho^B_k$) and $\|X\|^2 = \text{Tr}(X^\dagger X)$ is the Frobenius or Hilbert–Schmidt norm. Consider an arbitrary two-qubit state in the Bloch form

$$\rho = \frac{1}{4} \left[ I \otimes I + x^t \sigma \otimes I + I \otimes y^t \sigma + \sum T_{ij} \sigma_i \otimes \sigma_j \right]$$

(2a)

$$:= (x, y, T),$$

(2b)

where $x, y \in \mathbb{R}^3$, $T = (T_{ij}) \in \mathbb{R}^{3 \times 3}$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)^t$ is the usual vector of three Pauli matrices. Then, its GD can be calculated analytically [6],

$$D(\rho) = \frac{1}{2} \left[ \|x\|^2 + \|T\|^2 - \lambda_{\text{max}}(xx^t + TT^t) \right],$$

(3)

with the optimal CQ state given by $\chi = (e^t x e, y, ee^t T)$ [6,25] and $e$ being the eigenvector of

$$G := xx^t + TT^t$$

(4)

corresponding to its maximum eigenvalue $\lambda_{\text{max}}$. Denoting by $\lambda_{\text{↓}}^i(X)$ and $\lambda_{\text{↑}}^i(X)$ the eigenvalues (counting multiplicities) of $X$ in non-increasing and non-decreasing order, respectively, the conjecture thus becomes

$$\max_{\{\text{Separable } \rho\}} \sum_{i=2}^3 \frac{\lambda_{\text{↓}}^i(G)}{2} = \frac{1}{2}$$

(5)
Although geometric discord is a probable quantum resource, at least in some restricted scenario [26,27], we must emphasize that, irrespective of this, the present problem is interesting in its own right. As is evident from (5), this can be cast as an optimization problem among separable states, without any relation to discord. Also, we note the close resemblance with important inequalities:

\[ \|T\|_1 := \sum_{i=1}^{3} \sqrt{\lambda_i \left(T T^T \right)} \leq 1 \]  

(6a)

\[ M(\rho) := \sum_{i=1}^{2} \lambda_i \left(T T^T \right) \leq 1. \]  

(6b)

The first inequality is a necessary condition for separability for two-qubit states [28]. The last one is a sufficient condition for satisfaction of CHSH inequality for two-qubit states [29].

2 Maximally non-classical separable two-qubit X states

As it appears, solving the conjecture for general two-qubit case is difficult (some instances will be mentioned later); therefore, we explore the next general case, i.e., the class of X states. This family includes Bell-diagonal states, Werner states and due to its simple structure (in the sense that it has fewer parameters than a generic state) is often used to study evolution of correlation measures. A detailed study of discord of X states has been carried out recently in [30]. However, the analysis there is unnecessarily complicated due to consideration of completely irrelevant phases. Also, the present question was out of their purview.

**Proposition 1** The maximum of \( D \) among two-qubit separable X-states is 1/4. Moreover, all such maximal states have rank 2.

In computational basis, two-qubit X states are given by

\[ \rho = \begin{pmatrix} a & 0 & 0 & p \\ 0 & b & q & 0 \\ 0 & q & c & 0 \\ p & 0 & 0 & d \end{pmatrix}, \]  

(7)

where without loss of generality, we have taken all entries nonnegative because the local unitary (LU) transformation (i.e., renaming the basis)

\[ |0\rangle_k \rightarrow \exp \left( i \theta_p + (-1)^k \theta_q \right) |0\rangle_k \quad k = 1, 2 \]

will drive out the phases of \( p \) and \( q \) and neither \( D \) nor rank changes under LU.

The requirement \( \rho \geq 0 \) gives the constraints \( p^2 \leq ad \) and \( q^2 \leq bc \). We also need the separability constraints, i.e., positivity of partial transposition (PPT). Noting
that the partial transposition just interchanges \( p \) and \( q \), it follows that \( \rho \) represents a separable state iff
\[
\max\{p, q\} \leq \min\{\sqrt{bc}, \sqrt{ad}\}. 
\]

With explicit calculation, we have \( x = (0, 0, a + b - c - d) \) and \( G = \text{diag}\{4(p + q)^2, 4(p - q)^2, 2(a - c)^2 + 2(b - d)^2\} \). Therefore,
\[
\sum_{i=1}^{2} \lambda_i^2(G) \leq 8(p^2 + q^2) \leq 16 \min\{ad, bc\},
\]
where equality occurs in Eq. (9a) iff
\[
4(p + q)^2 \leq 2(a - c)^2 + 2(b - d)^2
\]
and equality occurs in Eq. (9b) iff
\[
p = q = \min\{\sqrt{ad}, \sqrt{bc}\}
\]
As we are seeking for maximum, it follows from Eq. (9b) that the maximum occurs iff
\[
ad = bc \quad \text{(12)}
\]
and the maximum value in Eq. (9) becomes \( \max\{16ad\} \) subject to
\[
ad = bc = \frac{1}{8} \left[(a - c)^2 + (b - d)^2\right]
\]
\[
a + b + c + d = 1,
\]
where the last equality (instead of being an ‘\( \leq \)’ inequality) in (13a) is due to the fact that it is an upper bound to the optimization function itself. (Note that if the two maximum exist, the maximum with a strict inequality is always strictly less than that of an equality). We show in Appendix that this maximum occurs at \( a = b = (2 \pm \sqrt{2})/8, c = d = 1/(32a) \), and hence, maximum possible value of \( D \) is 1/4.

We also note that the conditions (11) and (12) were necessary to achieve this maximum. Thus, it is necessary that the state has rank two, and up to LU, the unique separable \( X \) state having the maximum \( D \) is given by
\[
\rho = \frac{1}{4\sqrt{2}} \begin{pmatrix}
\sqrt{2} + 1 & 0 & 0 & 1 \\
0 & \sqrt{2} + 1 & 1 & 0 \\
0 & 1 & \sqrt{2} - 1 & 0 \\
1 & 0 & 0 & \sqrt{2} - 1
\end{pmatrix} 
\]
Quite surprisingly, the authors of Ref. [17] have obtained this state numerically as the optimal one, starting from a rank-two \( X \) state. On the other hand, it was shown in
Ref. [24] that the unique (up to LU) optimal state among rank-two separable state is given by
\[
\sigma = \frac{1}{2} (|00\rangle \langle 00| + |+1\rangle \langle +1|) = \frac{1}{4} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}.
\]
(15)

Although, \( \sigma \) apparently does not looks like an \( X \) state, we note that \( \rho \) and \( \sigma \) are LU equivalent, namely \( \sigma = (U \otimes V) \rho (U \otimes V)^\dagger \) with
\[
U = \begin{pmatrix} 1 + \sqrt{2} & 1 - \sqrt{2} \\ \sqrt{4 + 2\sqrt{2}} & \sqrt{4 - 2\sqrt{2}} \\ \sqrt{4 + 2\sqrt{2}} & \sqrt{4 - 2\sqrt{2}} \end{pmatrix}, \quad V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

Now let us give some necessary conditions for a two-qubit state to be a maximally geometric-discordant yet separable state (MGDSS).

3 Some necessary conditions for MGDSS

Proposition 2 No two-qubit separable state with \( x = 0 \), or \( TT^t = \lambda^2 I \) could be an MGDSS.

Proof. By Proposition 1, an MGDSS must have \( D(\rho) \geq 1/4 \).

Now, from (6a), a necessary condition for separability is \( \sum \sigma_i(T) \leq 1 \) [28]. So, assuming the singular values of \( T \) as \( a, b, c \geq 0 \), we must have for \( x = 0 \),
\[
a + b + c \leq 1
\]
(16a)
\[
a^2 + b^2 + c^2 - \max\{a^2, b^2, c^2\} \geq \frac{1}{2}
\]
(16b)

which is clearly impossible, as the maximum of \( a^2 + b^2 + c^2 - \max\{a^2, b^2, c^2\} \) subject to the constraints \( a + b + c \leq 1 \) and nonnegative \( a, b, c \) is \( 2/9 < 1/2 \).

The second assertion follows by noticing that the eigenvalues of \( G \) then become \( \{\|x\|^2 + \lambda^2, \lambda^2, \lambda^2\} \).

Remark. The separability condition can not be ignored in proposition 2, as for the Werner state
\[
\rho_w = p |\Psi^-\rangle \langle \Psi^-| + \frac{(1 - p)}{4} I
\]
where \( |\Psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2} \), we have \( x = 0 \) and \( D = p^2 \) thereby \( D > 1/4 \) whenever \( p > 1/2 \). The conjecture in (5) predicts the stronger result that \( D(\rho) > 1/4 \) implies the state is surely entangled, irrespective of \( x \). Note that this result also prohibits the separable Bell-diagonal states to be maximally discordant [17].

The separability condition in the conjecture is really important, even for existence of extrema.
Proposition 3 The function $D$ has no maximum among all (including the entangled) rank-2 two-qubit states.

Proof It is well known that the maximum of $D(\rho)$ is 1 and attained only at pure maximally entangled states (i.e., rank-one states)\[10\]. So, it suffices to show that for any given small $\epsilon > 0$, there is always a rank-two state $\rho_\epsilon$ having $D(\rho_\epsilon) = 1 - \epsilon$. Out of many possibilities, one such rank-two state is given by

$$\rho_\epsilon = \left(\frac{1}{2} + \sqrt{\frac{1}{4} - \frac{\epsilon}{3}}\right)|\Psi^\rangle\langle\Psi^-| + \left(\frac{1}{2} - \sqrt{\frac{1}{4} - \frac{\epsilon}{3}}\right)|00\rangle\langle00|$$

(17)

It is easy to verify that the optimal measurement operators $\Pi_{1,2} = (I \pm \sigma_x)/2$ give the required value of $D$.

We note that the state in (17) remains entangled for the entire range of $\epsilon \in [0, 3/4]$. Also, changing $\epsilon \to 3/4 - \epsilon$, it follows that there is always a rank-two (entangled) state having $D = 1/4 + \epsilon$.

4 Discussion

Before concluding, let us mention some of our attempts toward this conjecture. We have been able to prove the conjecture (including the uniqueness), under any one of the following assumptions:

i. An MGDSS $\rho$ must have at least one closest CQ state as $\rho^A \otimes \rho^B$

ii. An MGDSS should have $y = 0$

iii. $G$ has degenerate spectrum for any MGDSS

iv. $G$ is singular for any MGDSS

Although all these assumptions are heuristically reasonable, we do not know why (or how to establish) any one of these is necessary for MGDSS. A quite unpleasant situation occurs while trying to directly solve the optimization problem:

$$\max f(x, T) := \|x\|^2 + \|T\|^2 - e^t(xx^t + TT^t)e$$

Vanishing of the gradient gives

$$\frac{\partial f}{\partial x} = 0 \Rightarrow x = e^txe$$

$$\frac{\partial f}{\partial T} = 0 \Rightarrow T = ee^T$$

(18a) (18b)

These two equations are enough to determine a unique MDSS. But unfortunately, the Hessian matrix is block diagonal with block $2(I - ee^t) \geq 0$. Thereby, we can not guarantee that this is indeed the maxima, and hence, the conjecture for the general case remains open.
Appendix: Proof of the optimization in Proposition 1

We first note that the constraint (13a) implies \(abcd \neq 0\), \(a \neq c\), \(b \neq d\). Now, let us try to parameterize \((a, b, c, d)\) using the constraints. To absorb the first constraint, without loss of generality, we can take \(a = bk\), \(c = dk\), \(k > 0\). Then, the constraint (13b) becomes

\[
b + d = \frac{1}{k + 1},
\]

and we are left with only the following constraint

\[
(a - c)^2 + (b - d)^2 = 8bd
\]

\[
\Rightarrow (b - d)^2(k^2 + 1) = 8bdk,
\]

where we have just substituted \(a\) and \(c\) in terms of \(bk\) and \(dk\), respectively, in the first equation. Squaring (19) and subtracting (20) from it yields

\[
4bd = \frac{k^2 + 1}{(k + 1)^4}
\]

Noting that \(ad = bdk\), we have to find the maximum of the function

\[
f(k) = \frac{k(k^2 + 1)}{(k + 1)^4}
\]

subject to \(k > 0\). The derivatives are very easy to calculate. Indeed, \(f'(k) = 0\) only at \(k = 1\) and \(f''(1) = f'''(1) = f''''(1) = 0\), but \(f''''(1) = -3/16 < 0\). Hence, the unique maximum occurs at \(k = 1\). From (19) and (21), this corresponds to the solution \(a = b = (2 \pm \sqrt{2})/8, c = d = 1/(32a)\).

References

1. Eisert, J., Plenio, M.: A comparison of entanglement measures. J. Mod. Opt. 46, 145–154 (1999). doi:10.1080/09500349908231260
2. Verstraete, F., Audenaert, K., Moor, B.D.: Maximally entangled mixed states of two qubits. Phys. Rev. A 64, 012316 (2001). doi:10.1103/PhysRevA.64.012316
3. Munro, W.J., James, D.F.V., White, A.G., Kwiat, P.G.: Maximizing the entanglement of two mixed qubits. Phys. Rev. A 64, 030302(R) (2001). doi:10.1103/PhysRevA.64.030302
4. Miranowicz, A., Grudka, A.: Ordering two-qubit states with concurrence and negativity. Phys. Rev. A 70, 032326 (2004). doi:10.1103/PhysRevA.70.032326
5. Ollivier, H., Zurek, W.H.: Quantum discord: a measure of the quantumness of correlations. Phys. Rev. Lett. 88, 017901 (2001). doi:10.1103/PhysRevLett.88.017901
6. Dakić, B., Vedral, V., Brukner, C.: Necessary and sufficient condition for nonzero quantum discord. Phys. Rev. Lett. 105, 190502 (2010). doi:10.1103/PhysRevLett.105.190502
7. Luo, S., Fu, S.: Geometric measure of quantum discord. Phys. Rev. A 82, 034302 (2010). doi:10.1103/PhysRevA.82.034302
8. Rana, S., Parashar, P.: Tight lower bound on geometric discord of bipartite states. Phys. Rev. A 85, 024102 (2012). doi:10.1103/PhysRevA.85.024102
9. Hassan, A.S.M., Lari, B., Joag, P.S.: Tight lower bound to the geometric measure of quantum discord. Phys. Rev. A 85, 034302 (2012). doi:10.1103/PhysRevA.85.024302
10. Luo, S., Fu, S.: Measurement-induced nonlocality. Phys. Rev. Lett. 106, 120401 (2011). doi:10.1103/PhysRevLett.106.120401
11. Datta, A.: Studies on the role of entanglement in mixed-state quantum computation. Ph.D. Thesis. arXiv:0807.4490v1
12. Gharibian, S., Piani, M., Adesso, G., Calsamiglia, J., Horodecki, P.: Characterizing quantumness via entanglement creation. Int. J. Quantum Inf. 9, 1701 (2011). doi:10.1142/S0219749911008258
13. Okrasa, M., Walczak, Z.: On two-qubit states ordering with quantum discordos. EuroPhys. Lett. 98, 40003 (2012). doi:10.1209/0295-5075/98/40003
14. Adhikari, S., Banerjee, S.: Operational meaning of discord in terms of teleportation fidelity. Phys. Rev. A 86, 062313 (2012). doi:10.1103/PhysRevA.86.062313
15. Lang, M.D., Caves, C.M.: Quantum discord and the geometry of bell-diagonal states. Phys. Rev. Lett. 105, 150501 (2010). doi:10.1103/PhysRevLett.105.150501
16. Galve, F., Giorgi, G.L., Zambrini, R.: Maximally discordant mixed states of two qubits. Phys. Rev. A 83, 012102 (2011). doi:10.1103/PhysRevA.83.012102
17. Girolami, D., Adesso, G.: Interplay between computable measures of entanglement and other quantum correlations. Phys. Rev. A 84, 052110 (2011). doi:10.1103/PhysRevA.84.052110
18. Girolami, D., Paternostro, M., Adesso, G.: Faithful nonclassicality indicators and extremal quantum correlations in two-qubit states. J. Phys. A Math. Theor. 44, 352002 (2011). doi:10.1088/1751-8113/44/35/352002
19. Batle, J., Platino, A., Platino, A.R., Casas, M.: Peculiarities of quantum discord’s geometric measure. J. Phys. A Math. Theor. 44, 505304 (2011). doi:10.1088/1751-8113/44/50/505304
20. Al-Qasimi, A., James, D.F.V.: Comparison of the attempts of quantum discord and quantum entanglement to capture quantum correlations. Phys. Rev. A 86, 032101 (2011). doi:10.1103/PhysRevA.86.032101
21. Batle, J., Casas, M., Platino, A.: Correlated multipartite quantum states. Phys. Rev. A 87, 032318 (2013). doi:10.1103/PhysRevA.87.032318
22. Chiuri, A., Vallone, G., Paternostro, M., Mataloni, P.: Extremal quantum correlations: experimental study with two-qubit states. Phys. Rev. A 84, 020304(R) (2011). doi:10.1103/PhysRevA.84.020304
23. Fedrizzi, A., Skerlak, B., Paterek, T., de Almeida, M.P., White, A.G.: Experimental information complementarity of two-qubit states. New J. Phys. 13, 053038 (2011). doi:10.1088/1367-2630/13/5/053038
24. Gharibian, S.: Quantifying nonclassicality with local unitary operations. Phys. Rev. A 86, 042106 (2012). doi:10.1103/PhysRevA.86.042106
25. Miranowicz, A., Horodecki, P., Chhajlany, R.W., Tuziemski, J., Sperling, J.: Analytical progress on symmetric geometric discord: measurement-based upper bounds. Phys. Rev. A 86, 042123 (2012). doi:10.1103/PhysRevA.86.042123
26. Dakić, B., et al.: Quantum discord as resource for remote state preparation. Nat. Phys. 8, 666–670 (2012). doi:10.1038/nphys2377
27. Horodecki, P., Tuziemski, J., Mazurek P., Horodecki, R.: Can communication power of separable correlations exceed that of entanglement resource? arXiv:1306.4938v2
28. De Vicent, J.I.: Separability criteria based on the Bloch representation of density matrices. Quantum Inf. Comput. 7, 624–638 (2007)
29. Horodecki, R., Horodecki, M., Horodecki, P.: Violating Bell inequality by mixed spin-1/2 states: necessary and sufficient condition. Phys. Lett. A 200, 340 (1995). doi:10.1016/0375-9601(95)00214-N
30. Bellomo, B., et al.: Unified view of correlations using the square-norm distance. Phys. Rev. A 85, 032104 (2012). doi:10.1103/PhysRevA.85.032104