Geometric quantum discord for two-qubit X-states

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Geometric quantum discord with Bures distance, a kind of correlations in geometric point of view, is defined as the minimal Bures distance between the quantum state and the set of zero-discord states in bipartite quantum system. Comparing to other geometric distance, Bures distance is monotoonous and Riemannian and the minimal Bures distance to zero-discord states satisfies all criteria of an discord measure. Furthermore, Bures geometric quantum discord is closely linked to a minimal error quantum state discrimination. So far, geometric quantum discord with Bures distance has been calculated explicitly only for a rather limited set of two-qubit quantum states and expression for more general quantum states are unknown. In this paper, we derive explicit expression for Bures geometric quantum discord and classical correlation, together with all closest zero-discord states and closest product state for a five-parameter family of states. For general X-states, a seven-parameter family of that have been of interest in a variety of contexts in the field, we not only calculate the Bures geometric quantum discord for a wide class of this kind of states, but also provide a analytic upper bound for entirety.

I. INTRODUCTION

Correlations infiltrate our interpretation and understanding of the quantum world. Quantum correlations are also regarded as resources needed in quantum algorithms and quantum communication protocols which reveals the quantum advantages over their classical counterpart \cite{1–3}. To extract correlation information from quantum system, whether classical or quantum, one has to perform measurement. A key difference between the classical and quantum is the characteristics of measurements: while a classical measurement can extract information without disturbance in principle, a quantum measurement often unavoidably break the measured system. Actually, quantum measurement lie at very heart of quantum mechanics, and are the pivotal feature in both theoretical and experimental investigation of quantum information. The theory of non-locality, entanglement and quantum steering, all depend on quantum measurement \cite{4–7}.

To some extent, disturbance under quantum measurements signifies quantumness. From the information perspective, the existence of quantum correlation in quantum states will give rise to unavoidable loss of information after quantum measurements. Discord, which was explicitly introduced by Ollivier, Zurek \cite{8} and Henderson, Vedral \cite{9}, to quantify the quantumness of correlations, exactly arise from the loss of information caused by local measurements.

The total correlations (quantum and classical) in a bipartite quantum system are measured by the quantum mutual information defined as

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

where $\rho_{A(B)}$ and $\rho$ are the reduced density matrix of subsystem $A(B)$ and the density matrix of the total system, respectively, and $S(\rho) = -\text{Tr}(\rho \log \rho)$ is the von Neumann entropy.

Motivated by the idea that classical correlations (CC) are those that can be extracted via quantum measurement, i.e., the maximum amount of correlations extractable by local measurements, a measurement of classical correlations in a bipartite quantum system maybe defined as

\[
C^A(\rho_{AB}) := S(\rho_B) - \min_{\{\sigma_i^A\}} \sum_i p_i S(\rho_{B|i}),
\]

where the minimum is over all von Neumann measurements on subsystem $A$ and $p_i = \text{Tr}(\sigma_i^A \otimes I) \rho$ is the probability of the measurement outcomes $i$, $\rho_{B|i} = p_i^{-1} \text{Tr}_A(\sigma_i^A \otimes I) \rho$ is the corresponding conditional state of $B$. The second term in the right side of Eq.\eqref{2} represents the minimal remain information of system $B$ after a measurement is made on $A$. In other words $C^A(\rho_{AB})$ quantify the maximal amount of information can be extracted by local measurement on $A$ subsystem. For the direct definition of quantum conditional entropy, i.e., $S(\rho_{AB}) - S(\rho_B)$ which can be negative, the left term of Eq.\eqref{2} can be viewed as the corresponding quantum mutual information.

Based on the idea that the total correlations on quantum system including classical and quantum correlations, therefore, as a measure of quantum correlation, discord can be defined as

\[
\delta_A(\rho) := I(\rho_{AB}) - C^A(\rho_{AB}).
\]

The right part of Eq.\eqref{3} characterize the amount of mutual information which is not accessible by local measurements on the subsystem $A$. It can be shown that $\delta(\rho) \geq 0$ and $\delta_A(\sigma_{A-cl}) = 0$ iff

\[
\sigma_{A-cl} = \sum_{i=1}^{n_A} p_i |\alpha_i\rangle \langle \alpha_i| \otimes \sigma_{B|i},
\]

with $\{|\alpha_i\rangle_{i=1}^{n_A}\}$ is an orthonormal basis for subsystem $A$ and $\sigma_{B|i}$ are arbitrary states of $B$ depending on the index $i$, and $p_i \geq 0$ are some probabilities. We call A-classical states the zero-discord states of this form. In some sense, A-classical states can be viewed as a kind of classical states whose classical correlations can be extracted after a quantum measurements made by $A$ subsystem without any disturbance to the states themselves.

With the set of A-classical states, it is natural to characterize the quantum correlations from a geometric point of view like...
what happens in the theory of entanglement. The set of quantum states can be equipped with various distance [10]. In [11], the authors calculate the geometric quantum discord for two-qubit quantum states with Hilbert-Schmidt distance which is not a good distance in state spaces. From the information perspective, it is natural to study the geometry induced by the Bures distance [12–16]

\[ d_B(\rho, \sigma) = \sqrt{2(1 - \sqrt{F(\rho, \sigma)})}, \]

with fidelity [14]

\[ F(\rho, \sigma) = \|\sqrt{\rho} \sqrt{\sigma}\|_1^2 = |\text{tr} \sqrt{\rho \sigma} \sqrt{\rho}|^2. \]

The geometric quantum discord (GQD) is by definition the square distance of \( \rho \) to the set \( C_A \) of A-classical states,

\[ D_A(\rho) = d_B(\rho, C_A)^2 = \min_{\sigma_{A \rightarrow C} \in C_A} d_B(\rho, \sigma_{A \rightarrow C})^2. \]

More than the Bures distance is monotonous and Riemannian [17], the Bures-GQD is also jointly convex in state space [18]. The evaluation of the GQD for the mixed states \( \rho \) turns out to be related to an ambiguous quantum state discrimination (QSD) task [19, 20]. Indeed, the fidelity between \( \rho \) and the closest A-classical state (CCS) is given by the maximum success probability

\[ F_A(\rho) = \max_{\rho_{A \rightarrow C} \in C_A} F(\rho, \rho_{A \rightarrow C}) = \max_{\{\alpha_i\} \in \{\rho_{A \rightarrow C}\}} P^{\text{opt (N)}}(\{\rho_i, \lambda_i\}). \]

(5)

In the right-hand, the maximum is over all orthonormal basis \( \{\alpha_i\}_{i=1}^{n_A} \) of A and \( \{\rho_i, \lambda_i\}_{i=1}^{n_A} \) is the ensemble of states depending on \( \{\alpha_i\} \) and \( \rho \) defined by

\[ \lambda_i = \langle \alpha_i | \rho_A | \alpha_i \rangle, \rho_i = \lambda_i^{-1} \sqrt{\rho} \alpha_i \langle \alpha_i | \sqrt{\rho}. \]

Moreover, let us denote by \( \{\alpha_i^{\text{opt}}\} \) and \( \{\Pi_{i}^{\text{opt}}\} \) the basis and projective measurement(s) maximizing \( P^{\text{opt (N)}}(\{\rho_i, \lambda_i\}) \) in Eq.(5). Then the CCS(s) to \( \rho \) is (are)[20]

\[ \sigma_{\rho} = \frac{1}{F_A(\rho)} \sum_{i=1}^{n_A} |\alpha_i^{\text{opt}}\rangle \langle \alpha_i^{\text{opt}}| \otimes |\lambda_i^{\text{opt}} \sqrt{\rho} \Pi_{i}^{\text{opt}} \sqrt{\rho}. \]

(6)

As we known, the analytic solution of ambiguous QSD has been given for \( n_A = 2 \), then the geometric discord for a \( (2, n_B) \) system can be also calculated as follows. Firstly, if the subsystem A is a qubit, the expression of the success probability is

\[ P^{\text{opt (N)}}(\{\rho_i, \lambda_i\}) = \lambda_0 \text{tr}(\Pi_0 \rho_0) + \lambda_1 \text{tr}((1 - \Pi) \rho_1) \]

\[ = \frac{1}{2}(1 - \text{tr} \Lambda) + \text{tr}(\Pi \Lambda) \]

(7)

with \( \Lambda = \lambda_0 \rho_0 - \lambda_1 \rho_1 \). Furthermore, because of the min-mix principle, we can get

\[ F_A(\rho) = \frac{1}{2} \max_{|u| = 1} 1 - \text{tr} \Lambda(u) + 2 \sum_{i=1}^{n_B} \lambda_i(\mathbf{u}) \]

(8)

where \( \lambda_i(\mathbf{u}) \) are the eigenvalues in non-increasing order of the \( 2n_B \times 2n_B \) Hermitian matrix \( \Lambda(u) = \sqrt{\rho} \sigma_u \otimes I \sqrt{\rho} \) and \( \sigma_u \equiv \sum_{i=1}^{n_B} u_m \sigma_m \) for some unit vector \( \mathbf{u} \in \mathbb{R}^3 \). If \( \rho > 0 \) then Eq.(8) reduce to the well-known expression [21]

\[ F^{\text{opt (N)}}(\{\rho_i, \lambda_i\}) = F^{\text{opt (C)}}(\{\rho_i, \lambda_i\}) = \frac{1}{2}(1 + \text{tr} \Lambda(u)). \]

(9)

Two-qubit X-states, a class of states with natural symmetry structure [22], play an important role in studying dissipative dynamical evolution of quantum system, such as the sudden transitions discussed in [23, 24] and frozen phenomenon of quantum correlations [25]. This class of states includes Werner states [26] and Bell-diagonal states which also play a key role in entanglement theory. In [27], the author calculate the original quantum discord (3) for Bell-diagonal states. For a general two-qubit X-state, Mazhar Ali [28] provided an explicit expression for original quantum discord (3) and the quantification of Bures geometric quantum discord is still missing with only partial results available for subsets of three parameters [21, 29]. We derive a analytic expression of Bures quantum discord for a large subset of X-states and a tight upper bound is given for the whole class with Eq.(8).

The paper is organised as follows. In section II we compute the Bures quantum correlations for two-qubit X-state with \( a = d, b = c \) and determine the closest A-classical states of this kind of state. Moreover, we also calculate the Bures classical correlations and find the corresponding closest classical state. In section III we evaluate the Bures quantum correlations for general two-qubit X-state and study the corresponding CCS a large class of X-states. We conclude in Section IV with a summary and outlook.

II. GEOMETRIC QUANTUM DISCORD FOR A CLASS OF X-STATES

A. GQD of X-states with \( a=d, \ b=c \)

In this section, let us consider a class of five-parameter family states, two-qubit X-state with \( a = d, b = c \). The matrices \( \rho \) is given in the standard basis \{00, 01, 10, 11\} by

\[ \rho = \begin{pmatrix} a & 0 & 0 & y \\ 0 & b & x & 0 \\ 0 & \bar{y} & b & 0 \\ \bar{x} & 0 & 0 & a \end{pmatrix}. \]

(10)

The eigenvalues and corresponding eigenvectors of \( \rho \) are

\[ \rho_{1(2)}(\bar{a}) = b \mp |x|, \rho_{3(4)}(a) = a \mp |y|, \]

\[ |\phi_{1(2)}(\bar{a})\rangle = \frac{1}{\sqrt{2}}(0, 1, \mp/x|0\rangle, 0)^T, \]

\[ |\phi_{3(4)}(a)\rangle = \frac{1}{\sqrt{2}}(1, 0, 0, \mp/y|0\rangle)^T. \]

To calculate the geometric quantum discord of \( \rho \), one consider the eigenvalue of \( \Lambda(u) = \sqrt{\rho} \sigma_u \otimes I \sqrt{\rho} \) with the help of
Eq. (8). As $A(u)$ and $\sigma_u \otimes I \rho$ has the same eigenvalues, we can just pay attention to the latter which is easier to calculate. Let $u = (\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta)$, then in the standard basis, the matrix

$$\sigma_u \otimes I \rho = \begin{pmatrix} am & \frac{\pi}{\sqrt{\cm}} & \frac{\pi}{\sqrt{\cm}} & \frac{\pi}{\sqrt{\cm}} \\ \frac{\pi}{\sqrt{\cm}} & bm & mx & an \\ \frac{\pi}{\sqrt{\cm}} & bn & nx & am \end{pmatrix},$$

with eigenvalues come in opposite pairs $(\lambda_+(u), -\lambda_+(u))$,

$$\lambda_\pm(u) = \sqrt{\frac{1}{2} \mu \pm \frac{1}{2} \sqrt{\mu^2 - 4(a^2 - |y|^2)(b^2 - |x|^2)}},$$

where $\mu = \cos^2 \theta(a^2 + b^2 - |x|^2 - |y|^2) + 2ab \sin^2 \theta + 2|xy| \sin \theta \cos(2\psi + \eta + \xi)$. Moreover, the fidelity between $\rho$ and $\sigma_\rho$ is

$$F_A(\rho) = \frac{1}{2} + \max_{\theta, \psi}(\lambda_+(u) + \lambda_-(u)).$$

We notice that if $\mu$ reach the maximum then it is also true for $F_A(\rho)$. Actually, it is easy to see that

$$(\lambda_+(u) + \lambda_-(u))^2 = \mu = (a^2 - |y|^2)(b^2 - |x|^2).$$

Denoting $xy = |x|e^{i\phi}, y = |y|e^{i\xi}$, one can rewrite $\rho$ in the Bloch representation

$$\rho = \frac{1}{4}(I \otimes I + \sum_{i=1}^{3} c_i|\xi_i \otimes \sigma_i + c_{12}|\sigma_1 \otimes \rho + c_{21}|\sigma_2 \otimes \sigma_1),$$

(14) with $c_{12} = 2(|x| \cos \eta \pm |y| \cos \xi), c_{21} = 2(|x| \sin \eta - |y| \sin \xi)$ and $c_3 = 2(a - b)$. Any such state can be written up to a conjugation by a local unitary $U_A \otimes U_B$ as $[30, 31]$

$$\rho' = \frac{1}{4}(I \otimes I + \sum_{i=1}^{3} c'_i|\sigma_i \otimes \sigma_i)$$

(15) which means that $F_A(\rho') = \frac{1}{2} + \sqrt{|a + |y||b + |x|| + \sqrt{|a - |y||b - |x||}}$.

Theorem 1. If a quantum state $\rho'$ and $\rho$ in bipartite system are invariant up to a local unitary transformation, i.e., $\rho' = U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger$ for some $U_A \otimes U_B$, the same is true for their closest $A$-classical states.

Proof. On one hand, assuming $\{\sigma_{\rho'}\}$ are the CCS of $\rho'$ and $\sigma_{\rho}$ is a CCS of $\rho$, then

$$F(\rho, \sigma_{\rho}) = F(\rho, U_A \otimes U_B \sigma_{\rho} U_A^\dagger \otimes U_B^\dagger) \leq F(\rho', \sigma_{\rho'})$$

where in the first and last equality we use the invariance of the fidelity under unitary matrices and in the $\leq$ we use the definition of CCS. Because $U_A^\dagger \otimes U_B^\dagger \sigma_{\rho'} U_A \otimes U_B$ is a $A$-classical state, then the above $\leq$ become to $\leq$ and each $U_A^\dagger \otimes U_B^\dagger \sigma_{\rho'} U_A \otimes U_B$ is a CCS of $\rho$.

On the other hand, we want to show that each CCS of $\rho$ can be written as $U_A^\dagger \otimes U_B \sigma_{\rho'} U_A \otimes U_B$ for a $\sigma_{\rho'} \in \{\sigma_{\rho'}\}$. To prove this conclusion, supposing $\sigma_{\rho'}$ is a CCS of $\rho$ with
$U_A \otimes U_B \sigma_{\rho}' U_A^\dagger \otimes U_B^\dagger \notin \{\sigma_{\rho}\}$. Then,
\[
F(\rho, \sigma_{\rho}') = F(\rho', U_A \otimes U_B \sigma_{\rho}' U_A^\dagger \otimes U_B^\dagger) < F(\rho', \sigma_{\rho}) = F(\rho, U_A^\dagger \otimes U_B^\dagger \sigma_{\rho} U_A \otimes U_B) = F(\rho, \sigma_{\rho})
\]
where in the first two equality we use the unitary-invariance of fidelity and in the last equality we use the result of the first part of the proof. The ”<” is based on the assumption that $U_A \otimes U_B \sigma_{\rho}' U_A^\dagger \otimes U_B^\dagger \notin \{\sigma_{\rho}'\}$. The inequality $F(\rho, \sigma_{\rho}') < F(\rho, \sigma_{\rho})$ contradict with that assumption which indicates that each CCS of $\rho$ can be written as $U_A^\dagger \otimes U_B^\dagger \sigma_{\rho} U_A \otimes U_B$ for a $\sigma_{\rho}' \in \{\sigma_{\rho}\}$.

Based on the thm.(1) and the corresponding result about BD states in [21], we can deduce the formula of CCS for case(10):
\[
\sigma_{\rho}(r) = \frac{q_{\max}'(\alpha_0', \beta_0')}{2} [\langle \alpha_0', \beta_0' | \alpha_0', \beta_0' \rangle + |\alpha_0', \beta_0' \rangle \langle \alpha_0', \beta_0' |] + \frac{1 - q_{\max}'(\alpha_0', \beta_0')}{2} \times [(1+r) |\alpha_0', \beta_1' \rangle \langle \alpha_0', \beta_1' | + (1-r) |\alpha_0', \beta_0' \rangle \langle \alpha_0', \beta_0' |]
\]
if $p_0'p_{\max}' = 0$ and $p_m' > 0, \forall m \neq m_{\max}$, and
\[
\sigma_{\rho}(r) = \frac{q_{\max}'(\alpha_0, \beta_0')}{2} [\langle \alpha_0, \beta_0' | \alpha_0, \beta_0' \rangle + (1-r) |\alpha_0, \beta_0' \rangle \langle \alpha_0, \beta_0' |] + \frac{1 - q_{\max}'(\alpha_0, \beta_0')}{2} \times (\alpha_1', \beta_1' | \alpha_0', \beta_0' \rangle \langle \alpha_1', \beta_1' | + \alpha_0', \beta_0' \rangle \langle \alpha_0', \beta_0' |]
\]
if $p_0'p_{\max}' > 0$ and $p_1'p_{\max}' = 0$. In this equation $r \in [-1, 1], |\alpha_{0(1)}', U_A^\dagger | \alpha_{0(1)} U_A, |\beta_{0(1)}' \rangle = U_B^\dagger | \beta_{0(1)} U_B$ with $\{ |\alpha_{0(1)} \rangle, |\beta_{0(1)} \rangle \}$ defined in [21] and

\[
q_m' = \frac{1}{2} + \frac{2 \sqrt{p_n'p_k'} - 2 \sqrt{p_{\max}p_{\max}'}}{4 \sqrt{p_n'p_k'} + 4 \sqrt{p_{\max}p_{\max}'}} + 2,
\]
\[
p_0' = \frac{1}{4}(1-c_1' - c_2' - c_3'),
\]
\[
p_i' = \frac{1}{4}(1 + c_1' + c_2' + c_3' - 2c_i'), i = 1, 2, 3,
\]
where $\{m, n, k\}$ is a permutation of $\{1, 2, 3\}$.

C. classical correlation of X-states with a=d, b=c

It is different from quantum entropy case which can be defined with the maximally deviation of quantum entropy after a measurement, the classical correlation is not natural for geometric quantum discord with Bures distance. In [32], the classical correlation based on geometric point of view was defined as
\[
C_{d}(\rho) = \inf_{\chi_{\rho} \in \text{CCS}} \inf_{\pi_{\rho} \in \mathcal{P}} D_{d}(\chi_{\rho}, \pi) = \inf_{\chi_{\rho} \in \text{CCS}} D_{d}(\chi_{\rho}, \pi_{\chi_{\rho}}),
\]
with $\mathcal{P}$ is the set of product states, and $\pi_{\chi_{\rho}}$ is any of the closest product states to $\chi_{\rho}$. The subscribe $d$ can be any well-defined distance on state space, there we choose Bures distance.

As we can see, for two qubit X-state $\rho$ with $a = d, b = c$, we can consider the classical correlation(cc) and the corresponding classical correlated state(ccS). Due to $\rho' = U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger$ is a BD states, one have
\[
\max_{\pi \in \mathcal{P}} F(\rho, \pi) = \max_{\pi \in \mathcal{P}} F(\rho', \pi),
\]
where in equality we use the fact that $U_A \otimes U_B \pi U_A^\dagger \otimes U_B^\dagger$ is still a product state for any product state $\pi$. Obviously, the classical correlated state of this five-parameter family is the same as BD states up to a local unitary. Based on the corresponding result about BD states in [32], the closest product state $\pi_{\chi_{\rho}}$ for such state(10) is also $\frac{1}{2} \mathbb{I} \otimes \mathbb{I}$ and
\[
C_{Bu}(\rho) = 2 - \sum_{i} \sqrt{p_i} = 2 - \left( \sqrt{a + |y|} + \sqrt{a - |y|} + \sqrt{b + |x|} + \sqrt{b - |x|} \right)
\]
(19)

III. GEOMETRIC QUANTUM DISCORD OF X-STATES

A. A-classical state of two-qubit

In this section, we will talk about the general formula of A-classical states of two-qubit. Let
\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]
be the Pauli matrices acting on $\mathbb{C}^2$. Because $\{I, \sigma_1, \sigma_2, \sigma_3\}$ constitutes an operator base for the space of all operators on $\mathbb{C}^2$, any two-qubit state can be written as
\[
\rho = \frac{1}{4}(I \otimes I + \sum_i c_i \sigma_i \otimes I + I \otimes \sum_j c_j \sigma_j + \sum_{m,n} c_{mn} \sigma_m \otimes \sigma_n)
\]
(20)

Here $I$ is the identity operator on the composite system or on the component systems, depending on the context.

Therefore, each two qubit state has a one-to-one correspondence to a 15-dimensional vector
\[
(c_{10}, c_{20}, c_{30}, c_{01}, c_{02}, c_{03}, c_{11}, c_{12}, c_{13}, c_{21}, c_{22}, c_{23}, c_{31}, c_{32}, c_{33}),
\]
sometimes we identify the two-qubit state and corresponding vector. In particular, for a two-qubit X-state, the corresponding vector is
\[
(0, 0, c_{30}, 0, 0, c_{03}, c_{11}, c_{12}, 0, c_{21}, c_{22}, 0, 0, 0, c_{33}).
\]

In general, each two-qubit A-classical state can be written as
\[
\rho_{A-cl} = p |\alpha_0 \rangle \langle \alpha_0 | \otimes \rho_0 + (1 - p) |\alpha_1 \rangle \langle \alpha_1 | \otimes \rho_1,
\]
with $p \in [0, 1/2]$. Assuming $|\alpha_{0(1)}\rangle \langle \alpha_{0(1)}| = \frac{1}{2}(I \pm r \cdot \vec{a})$ with $r = (r_1, r_2, r_3)$ a unit 3-dimensional real vector and $\rho_0 = \frac{1}{2}(I \pm s \cdot \vec{a})$, $\rho_1 = \frac{1}{2}(I \mp t \cdot \vec{a})$, any two-qubit A-classical state $\sigma_{A-ct}$ has the following form

$$
\frac{1}{4}[p(I + r \cdot \vec{a}) \otimes (I + s \cdot \vec{a}) + (1-p)(I - r \cdot \vec{a}) \otimes (I + t \cdot \vec{a})]
$$

with $\vec{a} = (2p-1)r, \vec{b} = (ps + (-1)p)t, \vec{c} = (ps - (-1)p)t$. Based on above analysis, we have the following result.

**Proposition 2.** Each A-classical states of two qubit has following form

$$
\frac{1}{4}(I \otimes I + \sum_i c_{i0}\sigma_i \otimes I + I \otimes \sum_j c_{0j}I \otimes \sigma_j + \sum_{mn} c_{mn}\sigma_m \otimes \sigma_n),
$$

with

$$
c_{i0} = (2p - 1)r_i, i = 1, 2, 3
$$

$$
c_{0j} = ps_j + (1-p)t_j, j = 1, 2, 3
$$

$$
c_{mn} = r_m(ps_n - (1-p)t_n), m, n = 1, 2, 3
$$

where $p \in [0, 1/2], s_i, r_i, t_i \in R and |s| \leq 1, |t| \leq 1, |r| = 1$.

**B. the form of A-classical X-state**

In this section, we limit our discussion to initially prepared arbitrary two-qubit X-states. The density matrix of a two-qubit X-state in the standard basis $\{|00\}, |01\}, |10\}, |11\}$ is of the general form

$$
\rho_X = \begin{pmatrix}
a & 0 & 0 & y \\
0 & b & x & 0 \\
0 & x & c & 0 \\
y & 0 & 0 & d
\end{pmatrix},
$$

with eigenvalues

$$
p_{1(2)} = \frac{1}{2}(b + c \mp \sqrt{(b - c)^2 + 4|x|^2}),
$$

$$
p_{3(4)} = \frac{1}{2}(a + d \mp \sqrt{(a - d)^2 + 4|y|^2}),
$$

and the corresponding eigenvector is

$$
|\phi_{1(2)}\rangle = (0, (b - c) \mp \sqrt{(b - c)^2 + 4|x|^2}, 2x, 0)^T,
$$

$$
|\phi_{3(4)}\rangle = ((a - d) \pm \sqrt{(a - d)^2 + 4|y|^2}, 0, 0, 2y)^T.
$$

This class of states has underlying symmetry structure and its CCS is also like this for some special case.

**Theorem 3.** If a two-qubit X-state has only one closest A-classical state, the CCS is also a X-state.

**Proof.** Assuming $\sigma_{pX}$ is a closest A-classical state of a X-state $\rho_X$, which corresponding vector is

$$(c_{10}, c_{20}, c_{30}, c_{11}, c_{21}, c_{22}, c_{23}, c_{31}, c_{32}, c_{33}).$$

Owing to $\sigma_3 \otimes \sigma_3 \sigma_3 \otimes \sigma_3 = \rho$, one have

$$F(\rho_X, \sigma_{pX}) = F(\rho_X, \sigma_3 \otimes \sigma_3 \sigma_3 \otimes \sigma_3) = F(\rho_X, \sigma'_{pX})$$

with

$$\sigma'_{pX} = (-c_{01}, -c_{02}, -c_{03}, -c_{10}, -c_{20}, -c_{30},$$

$$c_{11}, c_{12}, c_{13}, c_{21}, c_{22}, c_{23}, -c_{31}, -c_{32}, c_{33}).$$

Obviously, $\sigma'_{pX}$ is also a CCS of $\rho_X$. For the assumption that $\rho_X$ has only one CCS, namely $\sigma_{pX} = \sigma'_{pX}$, therefore

$$c_{01} = c_{02} = c_{10} = c_{20} = c_{13} = c_{23} = c_{31} = c_{32} = 0,$

(23)

which means that $\sigma'_{pX}$ is also a X-state. \(\square\)

Replacing the result of Proposition (2) into Eq. (23), one finds that for these A-classical state as the unique CCS for some $\rho_X$,

$$(2p - 1)r_1 = (2p - 1)r_2 = 0,$$

$$ps_1 + (1-p)t_1 = ps_2 + (1-p)t_2 = 0,$$

$$r_3(ps_1 - (1-p)t_1) = r_3(ps_2 - (1-p)t_2) = 0,$$

$$r_1(ps_3 - (1-p)t_3) = r_2(ps_3 - (1-p)t_3) = 0.$$ To determine the parameters $c_{ij}$ of the unique $\sigma_{pX}$ for these $\rho_X$, we discuss for different $p$.

(i). for case $0 < p < 1/2$, one have that $r_1 = r_2 = 0$, $r_3 = 1$, and $s_i = \frac{1}{p}t_i, i = 1, 2$. Then

$$c_{11} = c_{12} = c_{21} = c_{22} = 0, c_{33} = ps_3 - (1-p)t_3,$$

$$c_{30} = 2p - 1, c_{03} = ps_3 + (1-p)t_3,$$

and the corresponding A-classical states can be written as

$$\frac{1}{4}
\begin{pmatrix}
\rho_{11} & 0 & 0 & 0 \\
0 & \rho_{22} & 0 & 0 \\
0 & 0 & \rho_{33} & 0 \\
0 & 0 & 0 & \rho_{44}
\end{pmatrix},$$

with $\rho_{11} = 1+c_{33}+c_{30}+c_{03}, \rho_{22} = 1-c_{33}+c_{30}-c_{03}, \rho_{33} = 1-c_{33}-c_{30}+c_{03}, \rho_{44} = 1+c_{33}+c_{30}-c_{03}.$

(ii). for case $p = 0$, it is easy to deduce that $r_1 = r_2 = t_1 = t_2 = 0, r_3 = 1$, and then

$$c_{11} = c_{12} = c_{21} = c_{22} = 0, c_{33} = -t_3,$$

$$c_{30} = -1, c_{03} = t_3,$$

and the corresponding A-classical states is also a diagonal state with $\rho_{11} = 1+c_{33}+c_{30}+c_{03}, \rho_{22} = 1-c_{33}+c_{30}-c_{03}, \rho_{33} = 1-c_{33}-c_{30}+c_{03}, \rho_{44} = 1+c_{33}+c_{30}-c_{03}.$

(iii). for case $p = 1/2$, there has three different case.

(1). if $s_3 \neq t_3$, one infer that $r_1 = r_2 = 0, r_3 = 1$ which is also corresponding to the diagonal states.
(2), if $s_3 = t_3$ and $r_3 \neq 0$, then $s_1 = s_2 = t_1 = t_2 = 0$ which means that
\[
\begin{align*}
\sigma_3 &= s_3, \sigma_{30} = 0, \\
\sigma_{11} &= c_{12} = c_{21} = c_{22} = 0, c_{33} = 0,
\end{align*}
\]
and the corresponding A-classical state is still a diagonal state.

(3). if $s_3 = t_3$ and $r_3 = 0$, then $s_1 = -t_1, s_2 = -t_2$ which means that
\[
\begin{align*}
\sigma_{03} &= s_3, \sigma_{30} = 0, \\
\sigma_{11} &= r_1 s_1, \sigma_{12} = r_1 s_2, \sigma_{21} = r_2 s_1, \sigma_{22} = r_2 s_2, c_{33} = 0,
\end{align*}
\]
and the corresponding A-classical states can be written as
\[
\frac{1}{4} \begin{pmatrix}
\rho_{11} & 0 & 0 & \rho_{14} \\
0 & \rho_{22} & \rho_{23} & 0 \\
0 & \rho_{32} & \rho_{33} & 0 \\
\rho_{41} & 0 & 0 & \rho_{44}
\end{pmatrix}
\]
with
\[
\begin{align*}
\rho_{11} &= \rho_{33} = 1 + c_{03}, \rho_{22} = \rho_{44} = 1 - c_{03}, \\
\rho_{14} &= c_{11} - c_{22} = i(c_{12} + c_{21}), \rho_{41} = c_{11} - c_{22} + i(c_{12} + c_{21}), \\
\rho_{23} &= c_{11} + c_{22} + i(c_{12} - c_{21}), \rho_{32} = c_{11} + c_{22} - i(c_{12} - c_{21}).
\end{align*}
\]

In conclusion, the closest A-classical state for these X-states with only one CCS is neither diagonal state or X-state. This result will help to derive the corresponding Bures GQD for these class of state with Eq.(6).

Now, we consider these X-states which have more than one closest A-classical state. In the Section II, the optimal local measurement in subsystem A of CCS has three kind of formula, i.e., $r = (\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta)$ for

(1). $\rho \in [0, 2\pi]$ with fixed $\theta.$

(2). $\theta \in [0, \pi],$ with fixed $\psi,$

(3). $\psi \in [0, 2\pi], [0, \pi].$

For X-states $\rho_X$ with $a = d, b = c$, the above (2) and (3) is the case. For case (1), if $\theta \neq \{0, \frac{\pi}{2}\}$, maybe no CCS is a X-state for these states and we will discuss this situation in next subsection.

As we can see in Eq.(6), the CCS of a quantum state $\rho$ depend on both the choice of optimal basis $\{|\alpha_i^{\text{opt}}\rangle\}$ and optimal projector $\Pi^{\text{opt}}$ of $\Lambda_u$. In fact, for these states which has unique optimal measurement and two different optimal projector, namely $\sum_i |\alpha_i \rangle \langle \alpha_i | \otimes \sigma_{Bi}$ and $\sum_i |\alpha_i \rangle \langle \alpha_i | \otimes \sigma'_{Bi}$ are the corresponding CCS, then $p \sum_i |\alpha_i \rangle \langle \alpha_i | \otimes \sigma_{Bi} + (1 - p) \sum_i |\alpha_i \rangle \langle \alpha_i | \otimes \sigma'_{Bi}$ is also a CCS for $\rho$ for any $p \in [0, 1]$[21]. Next, we will consider the Bures GQD for unique optimal measurement firstly and then pay attention to the different situation of optimal projector.

### C. Geometric quantum discord of X-states

Comparing to Eq.(6), the measurement vector $u$ of the optimal measurement is $(0, 0, 1)$ or $(\cos \psi, \sin \psi, 0)$ for a fixed $\psi$ when the CCS of $\rho$ is diagonal states or general X-state. Now, let us estimate the Bures geometric quantum discord and determine the corresponding closest A-classical state.

(i). If the optimal measurement $|\alpha_{0(1)} \rangle \langle \alpha_{0(1)} | = \frac{1}{2} (I \pm \sigma_3)$, i.e. $|\alpha_{0(1)} \rangle = |0(1) \rangle$. Then, for the eigenvalues and eigenvectors of
\[
\sigma_3 \otimes I \rho_X = \begin{pmatrix}
a & 0 & 0 & y \\
b & 0 & x & 0 \\
0 & -x & c & 0 \\
-\bar{y} & 0 & 0 & -d
\end{pmatrix}
\]
are $\lambda_{1(2)} = \frac{1}{2} (b - c \pm \sqrt{(b + c)^2 - 4|x|^2}, \lambda_{3(4)} = \frac{1}{2} (a - d \mp \sqrt{(a + d)^2 - 4|y|^2})$ and
\[
\begin{align*}
&|\psi_{1(2)} \rangle = (0, (b + c) \pm \sqrt{(b + c)^2 - 4|x|^2}, -2\pi, 0)^T, \\
&|\psi_{3(4)} \rangle = ((a + d) \mp \sqrt{(a + d)^2 - 4|y|^2}, 0, 0, -2\pi)^T.
\end{align*}
\]
the fidelity between $\rho_X$ and the CCS is
\[
F'(\rho_X) = \frac{1}{2} (1 + |\text{tr} |\Lambda_u \rangle \langle \Lambda_u|) = \frac{1}{2} (1 + \sqrt{(b + c)^2 - 4|x|^2} + \sqrt{(a + d)^2 - 4|y|^2}).
\]
We normalize the eigenvectors $|\psi_i \rangle$ and still denote it $|\psi_i \rangle$ for $i = 1, 2, 3, 4$. Due to the $\Lambda(u) = \sqrt{\rho_X} \sigma_3 \otimes I \rho_X$, since $\Lambda(u)$ has the same eigenvalues as $\sigma_3 \otimes I \rho_X$ and the corresponding eigenvectors are $\{\sqrt{\rho_X} |\psi_i \rangle, i = 1, 2, 3, 4 \}$, one gets the optimal projector, $\Pi^{\text{opt}} =$
\[
\begin{pmatrix}
\sqrt{\rho_X} |\psi_1 \rangle \langle \psi_2 | + |\psi_4 \rangle \langle \psi_4 | \sqrt{\rho_X} \\
\sqrt{\rho_X} |\psi_2 \rangle \langle \psi_2 | + |\psi_3 \rangle \langle \psi_3 | \sqrt{\rho_X} \\
\sqrt{\rho_X} |\psi_4 \rangle \langle \psi_4 | + |\psi_4 \rangle \langle \psi_4 | \sqrt{\rho_X} \\
\sqrt{\rho_X} |\Upsilon_1 \rangle \langle \Upsilon_1 | + |\Upsilon_2 \rangle \langle \Upsilon_2 | \sqrt{\rho_X}
\end{pmatrix}
\]
with $|\Phi \rangle \in \text{span} \{ |\psi_3 \rangle, |\psi_4 \rangle \}, |\Psi \rangle \in \text{span} \{ |\psi_1 \rangle, |\psi_2 \rangle \}$ and $|\Upsilon_1 \rangle, |\Upsilon_2 \rangle \in \text{span} \{ |\psi_i \rangle, i = 1, 2, 3, 4 \}$. Due to $|\Phi \rangle = |\Psi \rangle = |\Upsilon_1 \rangle = |\Upsilon_2 \rangle = 1$. If $\det(\rho_X) = (bc - |x|^2)(ad - |y|^2) \neq 0$, denoting $|\psi_i \rangle = (|\psi_{1(2)} \rangle, |\psi_{3(4)} \rangle)^T$, the corresponding closest A-classical state
\[
|\sigma_X \rangle = \frac{1}{\sqrt{2}} \left( |0 \rangle \otimes |\psi_1 \rangle + |1 \rangle \otimes |\psi_2 \rangle \right)|\psi_2 \rangle + |\psi_4 \rangle \langle \psi_4 | \rho_X |i\rangle
\]
is a diagonal state.

Moreover, even if $\det(\rho_X) = 0$, $\sqrt{\rho_X} |\psi_2 \rangle + |\psi_4 \rangle \langle \psi_4 | \sqrt{\rho_X}$ is also a optimal projector and the corresponding CCS is a diagonal state, of course X-state. In other words, supposing the optimal measurement of the CCS for a X-state
\[ \rho_X = \{ |0\rangle, |1\rangle \}, \text{we can always find a CCS to be a diagonal state and the corresponding Bures geometric quantum discord} \]
\[ D_A(\rho_X) = 1 - \sqrt{b + c - 4|y|^2 + (a + d - 4|y|^2)^2}, \quad (27) \]

(ii). If the optimal measurement \[ |o_{0(1)} \rangle \langle o_{0(1)} | = \frac{1}{2}(I \pm (r_1\sigma_1 + r_2\sigma_2)) \]. Then, on account of the eigenvalues of \[ (r_1\sigma_1 + r_2\sigma_2) \otimes I_{\rho_X} = \begin{pmatrix} 0 & mx & nc & 0 \\ ny & 0 & 0 & nd \\ na & 0 & 0 & ny \\ 0 & nb & nx & 0 \end{pmatrix} \]
are
\[ \lambda_{1(2)} = \pm \frac{1}{\sqrt{2}} \sqrt{h + \sqrt{h^2 - 4(ad - |y|^2)(bc - |x|^2)}} \]
\[ \lambda_{3(4)} = \pm \frac{1}{\sqrt{2}} \sqrt{h - \sqrt{h^2 - 4(ad - |y|^2)(bc - |x|^2)}} \]

where \( h = 2\text{Re}\{a^*xy\} + ac + bd \) and \( n = r_1 + ir_2, r_1^2 + r_2^2 = 1 \), the fidelity between \( \rho_X \) and its CCS can be calculated with Eq.(9): \[ F''_A(\rho_X) = \max_{r = (r_1, r_2, 0)} \frac{1}{2}(1 + 2\lambda_1 + 2\lambda_3). \]

We notice that if \( h \) reach the maximum then it is also true for \( F''_A(\rho_X) \). Actually, it is easy to see that \[ (\lambda_1 + \lambda_3)^2 = h + 2\sqrt{k}, \]
with \( k = (ad - |y|^2)(bc - |x|^2) \).

For general \( h \), let \( r_1 = \cos \psi, r_2 = \sin \psi, \psi \in [0, 2\pi] \) and \( xy = |xy|e^{i\phi}, \phi \in [0, 2\pi] \), then
\[ h(\psi) = 2|xy|(\cos 2\psi \cos \phi - \sin 2\psi \sin \phi) + ac + bd, \]
\[ = 2|xy| \cos(2\psi + \phi) + ac + bd, \]
and the derivation of \( h(\psi) \) is
\[ \frac{dh(\psi)}{d\psi} = -4|xy| \sin(2\psi + \phi). \]

If \( |xy| \neq 0 \), then \( h \) reaches the maximum when \( \psi = -\frac{\phi}{2} \), i.e., the vector corresponding to the optimal measurements is \( (\cos(\phi/2), -\sin(\phi/2), 0) \) with \( \phi \) is the phase of \( xy \). Therefore, \( h_{\text{max}} = 2|xy| + ac + bd \) and the fidelity is \[ F''_A(\rho_X) = \frac{1}{2} + \sqrt{2|xy| + ac + bd + 2 \sqrt{(ad - |y|^2)(bc - |x|^2)}}. \]

Assuming the eigenvector of \( \Lambda(u) \) is \( |\psi_i \rangle \) correspond to \( \lambda_i \), then the optimal projector can be also represented as (25). If \( bc \neq |x|^2, ad \neq |y|^2, \rho_X \) has only one CCS which is a X-state based on the theorem 3. In the other case, we can also choose \( \sqrt{\rho_X}(|\psi_2 \rangle \langle \psi_2 |) + \sqrt{\rho_X}(|\psi_4 \rangle \langle \psi_4 |) \) as the optimal projector like in case \((0, 0, 1)\) and the corresponding CCS is a X-state.

If \( |xy| = 0, h \) reaches the maximum for any \( \psi \in [0, 2\pi] \) which means that there are infinite optimal basis measurement \( \frac{1}{4}(I \pm (\cos \psi \sigma_1 + \sin \psi \sigma_2)) \) for \( \psi \in [0, 2\pi] \). However, it is not clear whether there are always exist a X-state CCS for \( \rho_X \) in this case.

Therefore, for these X-state \( \rho_X \) whose CCS \( \sigma_{\rho_X} \) is a X-state, the corresponding fidelity is the maximum of above \( F''_A(\rho_X) \) and \( F''_A(\rho_X) \). In other words, denoting \( \tau = (b + c)^2 - 4|x|^2, \kappa = (a + d)^2 - 4|y|^2, \)
(i), if \( \sqrt{\tau + \sqrt{\kappa}} \geq 2\sqrt{h + 2\sqrt{k}}, \) i.e., \( F''_A(\rho_X) > F''_A(\rho_X), \)
the Bures GQD is \[ D_A(\rho) = 2(1 - \sqrt{F''_A(\rho_X)}) \]
\[ = 2 - \sqrt{2(1 + \sqrt{(b + c)^2 - 4|x|^2} + \sqrt{(a + d)^2 - 4|y|^2}^2}, \]
and at least one of CCSs is Eq.(26).

(ii). If \( \sqrt{\tau + \sqrt{\kappa}} < 2\sqrt{h + 2\sqrt{k}}, \) i.e., \( F''_A(\rho_X) < F''_A(\rho_X), \)
the Bures GQD is \[ D_A(\rho) = 2(1 - \sqrt{F''_A(\rho_X)}) \]
\[ = 2 - 2 \sqrt{\frac{1}{2} + \sqrt{2|xy| + ac + bd + 2 \sqrt{(ad - |y|^2)(bc - |x|^2)}}. \]

Therefore, the corresponding fidelity and Bures geometric quantum discord of these kind of states \[ F_A(\rho_X) = \max\{F''_A(\rho_X), F''_A(\rho_X)\}, \]
\[ D_A(\rho_X) = \max\{2(1 - \sqrt{F''_A(\rho_X)}), 2(1 - \sqrt{F''_A(\rho_X)})\}. \]

In conclusion, if the CCS for a two-qubit X-state \( \rho_X \) is unique, then the corresponding optimal measurement is \((0, 0, 1)\) or \((\cos \psi, \sin \psi, 0)\) with \( \psi \) fixed. On the other hand, if the corresponding optimal measurement is \((0, 0, 1)\) or \((\cos \psi, \sin \psi, 0)\) with a unique \( \psi \), there are always exist a X-state CCS for \( \rho \) and the corresponding Bures GQD is given by Eq.(30).

In fact, for a general X-state \( \rho_X \), it is very difficult to judge whether a measurement is the optimal. Therefore, we will try to evaluate Bures GQD for X-state through exploring the relationship between the seven parameters in the next subsection.

## D. Bures GQD based on optimal projector

This part, we will study the optimal measurement and projector of two-qubit X-state \( \rho_X \) with the characteristic polynomial of \( \Lambda(u) \). As the \( \sigma_\rho \times \rho_X \) has the same eigenvalues as \( \Lambda(u) = \sqrt{\rho_X} \sigma_\rho \times \sqrt{\rho_X} \), then we focus on the former
\[ \sigma_\rho \times \rho_X = \begin{pmatrix} ma & mb & mc & my \\ na & mb & mc & ny \\ -mb & mx & nd & ny \\ -mc & nx & nd & my \end{pmatrix}. \]
The corresponding characteristic polynomial of $\Lambda(u)$ is
\[ P[\lambda] = \lambda^4 + t_3\lambda^3 + t_2\lambda^2 + t_1\lambda + t_0, \quad (31) \]
with
\[ t_3 = m(-a - b + c + d), \]
\[ t_2 = m^2(ab - bc - ad + cd + |x|^2 + |y|^2) - h, \]
\[ t_1 = m((a - d)(bc - |x|^2) + (b - c)(ad - |y|^2)), \]
\[ t_0 = (ad - |y|^2)(bc - |x|^2), \]
where $h = 2\text{Re}(a^2xy) - ac - bd$. The coefficient $t_2$ is the only one dependent on both $m$ and $n$, and the constant term of $P[\lambda]$ is the determinant of $\rho$, i.e. $t_0 = \det(\rho)$. Supposing $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the eigenvalues of $\Lambda(u)$, the $\Pi^{\text{opt}}$ is the spectral projector associated to the two highest eigenvalues, i.e., $\lambda_1, \lambda_2$, on the basis of the result of QSD[18].

If $\det(\rho_X) = 0$, namely (1) $\text{ad} = |y|^2$ or $bc = |x|^2$ or both, then at least one of the eigenvalue is 0 and the state $\rho_X$ has infinite optimal projectors. Moreover, if $t_1 = 0$ also holds, i.e. $\text{ad} = |y|^2$ and $bc = |x|^2$, $a = d = |y|$ or $b = c = |x|$, two non-zero real roots of $P[\lambda]$ are $\lambda_{1(4)} = \frac{-t_3 \pm \sqrt{t_3^2 - 4t_2}}{2}$. Therefore, the fidelity between $\rho$ and its CCS $F(\rho_X) = \frac{1}{2} + \max_{m} \{\lambda_1(m)\}$ with
\[ 2\lambda_1(m) = \sqrt{m^2 g(a, b, c, d) + 8|xy| + 4ac + 4bd - m|} \]
and the derivation of $2\lambda_1(m)$ is
\[ \frac{2d\lambda_1(m)}{dm} = \frac{mg(a, b, c, d)}{m^2 g(a, b, c, d) + 8|xy| + 4ac + 4bd} - \Delta \]
where $g(a, b, c, d) = 2(a^2 + b^2 + c^2 + d^2) - 1 - 4(|x|^2 + |y|^2 - ad - bc) - 8|xy|$ and $\Delta = c + d - a - b$. Denoting $g = g(a, b, c, d)$, to get the maximum eigenvalue $\lambda_1$, the corresponding optimal $m$ is
\[ m_{\text{opt}} = \begin{cases} 
1 & g \geq 0, \Delta < 0 \\
0 & g \leq 0, \Delta \geq 0 \\
-2\sqrt{2|xy| + ac + bd}\Delta & g \geq 0, \Delta \geq 0 \\
\sqrt{g^2 - (c + d - a - b)^2} & g < 0, \Delta < 0 
\end{cases} \]
Therefore, the corresponding fidelity $F(\rho_X)$ is
\[ \frac{1 + \sqrt{2(a + c)^2 + 2(b + d)^2 - 1}}{2} - \Delta \quad g \geq 0, \Delta < 0 \]
\[ \frac{1}{2} + \sqrt{ac + bd} \quad g \leq 0, \Delta \geq 0 \]
\[ \frac{1}{2} + \max\{\lambda_1(0), \lambda_1(1)\} \quad g \geq 0, \Delta \geq 0 \]
\[ \frac{1}{2} + \lambda_1\left(\frac{-2\sqrt{2|xy| + ac + bd}\Delta}{\sqrt{g^2 - (c + d - a - b)^2}}\right) \quad g < 0, \Delta < 0 \]

(i), in case the CCS is unique, so is the optimal measurement $[\alpha_{\text{opt}}^i]$. This situation has been dealt with in Section III.C.

(ii), in case the CCS is infinite, so is the optimal measurement $[\alpha_{\text{opt}}^i]$. and the corresponding measurement should be $(\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta, \psi) \in [0, 2\pi]$ for fixed $\theta$. For example, if $|xy| = 0$, then the coefficients of $P[\lambda]$ are all independent of the value of $\psi$ which means that the optimal measurement happen to be $(\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta, \psi) \in [0,2\pi]$ for some $\theta$.

Furthermore, if $a = d, b = c$, the X-state reduce to (10).
In this case, $t_3 = t_1 = 0$, and then $\lambda_1 = \sqrt{-t_2 + \sqrt{t_2^2 - 4t_0}}$ which consistence to the result in Section II.

In consequence, for two-qubit X-state, if the characteristic polynomial of $\Lambda(u)$ has at most two non-zero roots or has unique optimal measurement, the corresponding fidelity are (32) and (30), respectively.

E. a analytic bound for two-qubit X-states

For more general X-states, it is not the case that there exist a X-state CCS for each $\rho_X$. In fact, for the A-classical X-states is the subset of A-classical states, the minimal Bures distance between $\rho_X$ and the set of A-classical X-state provide a upper bound for Bures GQD for general X-states $\rho_X$, namely
\[ \min_{\sigma_{A-cl} \in \mathcal{C}_A} d_B(\rho_X, \sigma_{A-cl})^2 \leq \min_{\sigma_{A-cl} \in \mathcal{C}_A} d_B(\rho_X, \sigma_{A-cl})^2 \]
where $C_A$ is the set of all A-classical X states. Obviously, this inequality become to equality for these states which has X-state CCS. In addition, the GQD can be indeed a upper bound for some case. For example, a X-state with $a = b = \frac{1}{3}$, $|x| = |y| = c = d = \frac{2}{3}$, then
\[ g = -\frac{4}{9}, \Delta = -\frac{1}{3}, m_{\text{opt}} = \sqrt{\frac{3}{10}}, \]
\[ \lambda_1(0) = \frac{1}{\sqrt{6}}, \lambda_1(1) = \frac{\sqrt{2} + 1}{6}, \lambda_1(m_{\text{opt}}) = \sqrt{\frac{5}{24}} \]
The fact, $\lambda_1(m_{\text{opt}}) > \lambda_1(0) > \lambda_1(1)$, indicates that the right side of Eq.(30) is a strict upper bound for Bures GQD for this state. In other words, the optimal measurement for two-qubit X-states is not always (0, 0, 1) and $(\cos \psi, \sin \psi, 0)$.

IV. CONCLUSION

How can we meaningfully quantify quantum correlations in arbitrary quantum states? This question lie at the very heart in quantum correlation theory. Not like the quantum coherence theory [33, 34]developed recently which has a easier quantifying, the quantification for quantum discord with a good measure is a hard nut to crack. In this paper, we evaluate the Bures-GQD for two-qubit X-states with the method developed
in [20, 21]. For X-states with $a = d, b = c$, we derive the explicit expression for both quantum and classical correlation in the perspective of geometric, and determine the corresponding closest zero-discord states and zero-correlation states (product states). This may help to understand decoherence processes and peculiar feature of quantum correlations during dynamics evolutions. For general X-states, on one hand, we calculate the Bures-GQD for these states which has a unique CCS based on the fact that the unique CCS for X-state must be also a X-state. On the other hand, a explicit expression for Bures-GQD is given for these states whose corresponding characteristic polynomial (31) has only two non-zero roots. In addition, we provide a upper bound for the Bures-GQD of general X-states based on the minimal Bures distance between the X-state and the set of X-state closest A-classical states.

This generalize results previously available only for a three-parameter subset of such states. There we maximize the fidelity with the help of the result from quantum state discrimination, it would be of interest to explore another method to calculate the maximum of fidelity which will be helpful for QSD task, vice versa.

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