Necessary and sufficient condition for saturating the upper bound of quantum discord

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We revisit the upper bound of quantum discord given by the von Neumann entropy of the measured subsystem. Using the Koashi-Winter relation, we obtain a trade-off between the amount of classical correlation and quantum discord in the tripartite pure states. The difference between the quantum discord and its upper bound is interpreted as a measure on the classical correlative capacity. Further, we give the explicit characterization of the quantum states saturating the upper bound of quantum discord, through the equality condition for the Araki-Lieb inequality. We also demonstrate that the saturating of the upper bound of quantum discord precludes any further correlation between the measured subsystem and the environment.

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I. INTRODUCTION

Recently, it has been recognized that entanglement does not depict all possible quantum correlations contained in a bipartite state. Based on the measurement on the subsystem in the bipartite system, quantum discord was proposed as a measure for the quantum correlation beyond entanglement [1–5]. Quantum discord was viewed as a figure of merit for characterizing the nonclassical resources in the deterministic quantum computation with one-qubit [6, 7]. It was also discussed that zero-discord of the initial system-environment states is a necessary and sufficient condition for completely positivity of reduced dynamical maps [8, 9]. At the same time, a necessary and sufficient condition for nonzero-discord was also given for any dimensional bipartite states [10]. Most recently, operational interpretations of quantum discord were proposed in [11, 12], where quantum discord was shown to be a quantitative measure about the performance in the quantum state merging [13]. Over the past decade, quantum discord has received a lot of attentions in Refs. [14–30], and also see the reviews [4, 5].

In general, quantum discord is upper bounded by the entropy of the measured subsystem [31–35], but it has remained an open question when this bound is saturated for general mixed states. For this question, some sufficient conditions were given in [33–36]. This motivates us to systematically investigate the upper bound of quantum discord and give a necessary and sufficient condition for saturating the upper bound of quantum discord. On the other hand, as an achievable upper bound of the quantum discord, the von Neumann entropy of a system can be considered as the quantum correlative capacity which tells us how strongly can this system be quantum correlated with others [34]. So we want to ask another question: what can the closeness between the quantum discord and the upper bound tell us?

It is interesting that there are monogamic relations between different measures on correlations [37]. In this paper, by purifying the bipartite systems and using the Koashi-Winter relation [37], we obtain a new monogamic relation: a system being quantum correlated with another one limits its possible classical correlation with a third system. For the bipartite systems, the total amount of quantum discord between two subsystems and the classical correlation between the measured subsystem and the environment cannot exceed the von Neumann entropy of the measured subsystem. We further prove that the necessary and sufficient condition for saturating the upper bound of quantum discord is equivalent to the equality condition for the Araki-Lieb inequality [38–41]. And we give the explicit characterization of the quantum states saturating the upper bound of quantum discord, through which we demonstrate that saturating the upper bound of quantum discord means that the measured subsystem cannot be further correlated with the environment. For a two-qubit system, quantum discord is strictly less than the von Neumann entropy of the measured qubit of two-qubit states other than when the two-qubit system in pure states.

This paper is organized as follows. In Sec. II, we give a brief review on quantum discord. In Sec. III we show that there is a trade-off between the quantum discord and the classical correlation, and then we prove a necessary and sufficient condition for the saturating of the upper bound of quantum discord. Section IV is the conclusion.

II. REVIEW OF QUANTUM DISCORD

First, we recall the concepts and properties of the quantum discord. Let Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be a bipartite quantum system. Let $\mathcal{D}(\mathcal{H})$ be a set of bounded, positive-semidefinite operators with unit trace on $\mathcal{H}$. Given a bipartite quantum state $\rho^{AB} \in \mathcal{D}(\mathcal{H})$, the von Neumann mutual information between the two subsystems $A$ and $B$ is defined as [41]

$$I(A : B) := S(A) + S(B) − S(AB),$$

where $S(X) := −\text{Tr} \rho^X \log_2 \rho^X$ is the von Neumann entropy, $\rho^X$ is a quantum state of system $X$ [41]. The
mutual information $I(A:B)$ is a measure of the total amount of correlations in the bipartite quantum state. Generally speaking, it was divided into quantum correlation and classical correlation [1, 3, 42].

The classical correlation was seen as the amount of information about the subsystem $A$ that can be obtained via performing a measurement on the other subsystem $B$. Then, the measure of the classical correlation [2] is defined by

$$J(A|B) := \max_{\{E^B_i\}} \left( S(A) - \sum_i p_i S(A|E^B_i) \right),$$

where $\{E^B_i\}$ is the positive operator valued measure (POVM) on $B$, $S(A|E^B_i)$ is the von Neumann entropy of the post-measurement states $\rho^A_i = \text{Tr}_B(E^B_i \rho^{AB})$ corresponds to outcome $i$ with the probability $p_i = \text{Tr}(E^B_i \rho^{AB})$. Therefore, quantum discord [1, 3] is defined by the difference of the quantum mutual information and the classical correlation

$$D(A|B) := I(A:B) - J(A|B).$$

Quantum discord is asymmetric with respect to $A$ and $B$, in general, $D(A|B) \neq D(B|A)$, and it is always non-negative [1, 3]. Quantum discord vanishes if and only if there exists an optimal choice of measurement $\{E^B_i\}$ on $B$ leaves the state $\rho^{AB}$ unperturbed [32]. The condition for zero-discord can be reduced to the equality condition using relative entropy [31, 44], and was also discussed in Refs [1, 10, 31]. For any bipartite pure state $|\psi\rangle^{AB}$, one checks that

$$D(B|A) = S(A) = S(B) = D(A|B).$$

III. THE UPPER BOUND OF QUANTUM DISCORD

A. A trade-off between quantum discord and classical correlation

For any general bipartite mixed state $\rho^{AB}$, we can always find a tripartite pure state $\rho^{ABE} = |\Psi\rangle^{ABE}\langle\Psi|$ such that $\rho^{AB} = \text{Tr}_E(\rho^{ABE})$, where $E$ represents the environment. Hereafter, we will consider this purification about general bipartite mixed state $\rho^{AB}$. The monogamic relation between the entanglement of formation and the classical correlation between the two subsystems is given by [37]

$$E_F(A:E) + J(A|B) = S(A),$$

where $E_F(A:E)$ is entanglement of formation (EoF), defined as $E_F(A:E) = \min\{p_i, |\psi_i\rangle\} \sum_i p_i \text{Tr}_E(|\psi_i\rangle\langle\psi_i|)$, where the minimum is taken over all pure ensembles $\{p_i, |\psi_i\rangle\}$ satisfying $\rho^{AE} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. This relation is universal for any tripartite pure states. Thus, we can give an other reorder version of Koashi-Winter relation,

$$E_F(E:A) + J(E|B) = S(E).$$

Due to the symmetric property of the EoF, i.e., $E_F(A:E) = E_F(E:A)$, we can eliminate the EoF by combining Eqs. (5a) and (5b), then we obtain

$$J(A|B) + J(E|B) = S(A) - S(E).$$

To be clearer, we substitute $D(A|B) = I(A:B) - J(A|B)$ into the above equation, and obtain a trade-off between the quantum discord and the classical correlation as follows

$$D(A|B) + J(E|B) = S(B).$$

This new monogamic relation tell us that the amount of quantum correlation between $A$ and $B$, plus the amount of classical correlation between $B$ and the complementary part $E$, must be equal to the entropy of the measured subsystem $B$. More importantly, based on this new monogamic equation, we can introduce

$$\tilde{J}(B/A) := S(B) - D(A|B),$$

which quantifies classically correlative capacity of $B$ with other systems except $A$. In other words, for general tripartite mixed states $\rho^{ABC}$, the classical correlation between $B$ and $C$ cannot be greater than $\tilde{J}(B/A)$. To be convinced, let us purify $\rho^{ABC}$ as $\rho^{ABC} = \text{Tr}_E(\rho^{ABE} |\Psi\rangle\langle\Psi|)$, then we have $J(C|B) = \tilde{J}(B/A)$ due to the monogamic relation [4]. Because the classical correlation is non-increasing under the local quantum operation [2], then we have

$$J(C|B) \leq J(C|E|B) = \tilde{J}(B/A),$$

which is equivalent to

$$D(A|B) + J(C|B) \leq S(B).$$

We emphasize that Eq. (10) is applicable for any tripartite state $\rho^{ABC}$ and the equality holds if and only if $\rho^{ABC}$ is pure. We can see that the total amount of the quantum discord between two subsystems and the classical correlation between the measured subsystem and the environment cannot exceed the von Neumann entropy of the measured subsystem.

B. The upper bound of quantum discord

The monogamic relation [4] directly supplies a general upper bound for the quantum discord, which was proved in Refs [31, 35]. In the following, we are going to determine which states saturate this bound. Combining the monogamic relation [4] with the equality condition for Araki-Lieb inequality, we have the following result.

**Theorem 1.** For the bipartite state $\rho^{AB}$, we have

$$D(A|B) \leq S(B)$$

with equality if and only if there exist a decomposition of $\mathcal{H}^A$ as $\mathcal{H}^A = \mathcal{H}^L \otimes \mathcal{H}^R$ such that

$$\rho^{AB} = \rho^{AL} \otimes |\psi\rangle^{AR}(\psi).$$


To prove this theorem, we first introduce a lemma as follows.

**Lemma 2.** Considering different correlations and entropy in the bipartite states, the following conditions are equivalent

1. \( D(A|B) = S(B) \);
2. \( S(A) - S(B) = S(AB) \);
3. \( E_F(A : B) = S(B) \).

If one of them is satisfied, then the others are satisfied.

**Proof.** The equivalence of these conditions can be proved by the trade-off relation \( \rho \) for the purification \( |\psi^{ABE}\rangle \). From Eq. (17), we can see that \( D(A|B) = S(B) \) is equivalent to \( J(E|B) = 0 \). It is known that the classical correlation vanishes if and only is the states are product states, see Refs. \[2, 42\]. So we have

\[
J(E|B) = 0 \iff \rho^{EB} = \rho^E \otimes \rho^B \quad (13)
\]

\[
\iff S(EB) = S(B) + S(E). \quad (14)
\]

For the tripartite pure states, we have \( S(A) = S(EB) \) and \( S(E) = S(AB) \). Thus Eq. (14) is equivalent to \( S(A) - S(B) = S(AB) \) and we obtain the equivalence between the first and second conditions. Meanwhile, the third condition is equivalent to \( J(B|E) = 0 \) due to the Koashi-Winter relation \( E_F(A : B) = S(B) - J(B|E) \). Again using the property of the classical correlation, we can see the third condition is equivalent to \( \rho^{EB} = \rho^E \otimes \rho^B \), and in turn equivalent to the first condition. \( \square \)

Form the above lemma, we will complete the proof of Theorem 3.

**Proof of Theorem 3** The inequality was recently given in \[31, 53\], and it is also a direct consequence of Eq. (17). Therefore, we obtain that quantum discord \( D(A|B) \) saturates the upper bound \( S(B) \) if and only if \( S(A) - S(B) = S(AB) \), which is the equality condition of the Araki-Lieb inequality \[40\].

\[
|S(A) - S(B)| \leq S(AB) \quad (15)
\]

when \( S(A) \geq S(B) \).

Recently, the quantum states saturated the Araki-Lieb inequality was explicitly given by Zhang and Wu \[34\], by using the explicit characterization of quantum states that saturates the strong subadditivity inequality \[44\] and the relation between the Araki-Lieb inequality and the strong subadditivity inequality \[41\]. From the result in Ref \[30\], we know that \( S(A) - S(B) = S(AB) \) if and only if there exist a decomposition \( \mathcal{H}^A = \mathcal{H}^A_L \otimes \mathcal{H}^A_R \) such that

\[
\rho^{AB} = \rho^{AL} \otimes |\varphi\rangle^{AR} \langle \varphi|. \quad (16)
\]

This completes this proof of Theorem 3. \( \square \)

![FIG. 1: Schematics diagram for the Theorem 1 and 3.](image)

In both subfigures, the right side of the solid line are the measured subsystems B. In (a), the quantum discord saturates the general upper bound given by the von Neumann entropy of the measured subsystem \( B \) if and only if there exists a decomposition of \( \mathcal{H}^A \) as \( \mathcal{H}^A_L \otimes \mathcal{H}^A_R \) such that \( \rho^{AB} = \rho^{AL} \otimes |\varphi\rangle^{AB} \langle \varphi| \); In (b), the quantum discord equals the von Neumann entropy of the unmeasured subsystem \( A \) if there exist a decomposition of \( \mathcal{H}^B \) as \( \mathcal{H}^B_L \otimes \mathcal{H}^B_R \) such that \( \rho^{AB} = |\psi\rangle^{AB} \langle \psi| \otimes \rho^{BR} \).

This result shows that quantum discord is equal to the measured system entropy if and only if the equality in the Araki-Lieb inequality holds. It is an interesting thing that the measured subsystem \( B \) cannot correlate with the environment \( E \) if the quantum discord between \( A \) and \( B \) is equal to the entropy of the measured subsystem. In other words, there must exists an isolated pure subsystem enclosing the measured subsystem in the Hilbert space \( \mathcal{H}^A \otimes \mathcal{H}^B \) when \( D(A|B) = S(B) \). One can also see that given the entropy of the measured subsystem, the maximal quantum discord between \( A \) and \( B \) will forbid system \( B \) from being correlated to other systems outside this composite system.

Due to the asymmetric property of quantum discord, one may ask whether or not Theorem 1 still holds if we consider \( S(A) \) instead of \( S(B) \). In fact, a conjecture about the von Neumann entropy and quantum discord was presented by Luo, Fu and Li in Ref. \[23\], namely

\[
D(A|B) \leq \min\{S(A), S(B)\}. \quad (17)
\]

Later, Li and Luo showed that the part \( D(A|B) \leq S(A) \) fails in general, but might be true for low-dimension systems \[34\].

We only have the following sufficient condition for the situation of \( D(A|B) = S(A) \).

**Theorem 3.** For the bipartite state \( \rho^{AB} \), we have

\[
D(A|B) = S(A), \quad (18)
\]

if the equality \( S(B) - S(A) = S(AB) \) is satisfied.

**Proof.** According to the equality condition for the Araki-Lieb inequality, \( S(B) - S(A) = S(AB) \) is equivalent to that there exists a decomposition \( \mathcal{H}^B = \mathcal{H}^B_L \otimes \mathcal{H}^B_R \) such that

\[
\rho^{AB} = |\psi\rangle^{AB} \langle \psi| \otimes \rho^{BR}. \quad (19)
\]
For this density matrix, we can get
\[ D(A|B) = D(A|B^L) = S(A), \]
where \( D(A|B^L) \) is the quantum discord for the pure state \( |\psi\rangle^{AB^L} \).

Besides, applying the Theorem\(^1\) and Lemma\(^2\) we can see that all the following quantities are equal:
\[ D(A|B) = D(B|A) = E_F(A : B) = S(A) = S(B^L) \]
for the quantum state \(^{19}\).

As an illustration, let us consider the following example
\[ \rho^{AB} = \frac{1}{4} \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}, \]

where \( \mathcal{H}_A = \mathbb{C}^2 \) and \( \mathcal{H}_B = \mathbb{C}^4 \). The reduced states can be obtained \( \rho^A = \frac{I_A}{2} \) and \( \rho^B = \frac{I_B}{2} \), where \( I^A \) and \( I^B \) are identity operators on \( \mathcal{H}_A \) and \( \mathcal{H}_B \), respectively. After some calculations one obtains
\[ S(AB) = 1, \ S(A) = 1, \ S(B) = 2. \]

Therefore, this state satisfies \( S(B) - S(A) = S(AB) \). On the other hand, one checks that \( \mathcal{H}_B = \mathcal{H}_{B^L} \otimes \mathcal{H}_{B^R} \) with \( \mathcal{H}_{B^L} = \mathcal{H}_{B^R} = \mathbb{C}^2 \). Then, \( \rho^{AB} \) is in the form of Eq. \(^{19}\) with \( \rho^{AB^L} = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \) and \( \rho^{B^R} = \frac{I^B}{2} \), where \( I^{B^R} \) is identity operator on \( \mathcal{H}_{B^R} \). With the result of Eq. \(^{21}\), we have
\[ D(A|B) = D(B|A) = E_F(A : B) = 1 \]
for this quantum state.

Through Theorem\(^1\) and Theorem\(^3\) we identify two conditions to witness the trapping of correlation within a pure-state subsystem, see Fig. 1. This opens a new way to investigate whether the correlation between A and B is essentially the correlation between smaller parts of them.

C. Arbitrary two-qubit states

Now, we will discuss the application of our results in two-qubit system. A two-dimension Hilbert space cannot be decomposed any more. The only possibility of \( |S(A) - S(B)| = S(AB) \) for two-qubit states is that \( \rho^{AB} \) is a pure state. Hence, its upper bound is not reachable except two-qubit pure state \(^{23}\), namely, we have
\[ D(B|A) < S(A), \ D(A|B) < S(B), \]
for any mixed two-qubit state.

IV. CONCLUSION

In this work, we have given a new monogamic relation between the quantum discord and the classical correlation in terms of the Koashi-Winter relations. Based on the equality conditions for the Araki-Lieb inequality, we have given a necessary and sufficient condition for the saturating of the upper bound of quantum discord. We have shown that the subsystem of the bipartite system can not correlated with the other system if the quantum discord of the bipartite system is equal to the entropy of the measured subsystem. We showed that there are some mixed states where quantum discord is equal to entanglement of formation. In particular, for two-qubit state, its upper bound is not reachable except pure state.

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