Quantum correlation via quantum coherence

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Abstract Quantum correlation includes quantum entanglement and quantum discord. Both entanglement and discord have a common necessary condition— —quantum coherence or quantum superposition. In this paper, we attempt to give an alternative understanding of how quantum correlation is related to quantum coherence. We divide the coherence of a quantum state into several classes and find the complete coincidence between geometric (symmetric and asymmetric) quantum discords and some particular classes of quantum coherence. We propose a revised measure for total coherence and find that this measure can lead to a symmetric version of geometric quantum correlation which is analytic for two qubits. In particular, this measure can also arrive at a monogamy equality on the distribution of quantum coherence. Finally, we also quantify a remaining type of quantum coherence and find that for two qubits it is directly connected with quantum nonlocality.

Keywords Quantum correlation \cdot quantum entanglement \cdot quantum coherence

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1 Introduction

Quantum coherence, or quantum superposition, is one of the most fundamental features of quantum world that are distinguished from the classical one. Associated with the tensor structure of the composite system, it directly leads to the formation of quantum entanglement which is usually treated as another key quantum mechanical feature and is so important that it has been recognized to be an important physical resource in quantum information processing (QIP). However, quantum coherence is only a necessary condition for the entanglement. In order to get a good understand of quantum entanglement, most including ourselves have been making efforts [1-13] to find out how to tell whether a state is entangled or not, or to what degree a given state is entangled, and to reveal the properties of entanglement measure of different types. Here we would like to ask the first question: how entanglement is related to quantum coherence?

Quantum entanglement is so familiar to us that it could be the first candidate when quantum correlation is mentioned. However, quantum entanglement does not cover all the quantumness of correlations. It has been shown that quantum discord can effectively quantify the quantum correlation [14-17]. It has been shown to have some similar properties to quantum entanglement, such as demonstrating the quantum advantage in some QIP, but it is beyond quantum entanglement because it can be present even in separable mixed states [18]. In the past few years, quantum discord has attracted many interests in the various fields [19-30], but the understanding of quantum discord remains limited. For example, the original quantum discord is an information-theoretic one that is only analytically calculated for some special states [26,27], even though the geometric quantum discord has the analytic expression for all two-qubit states [31]; Quantum discord is not symmetric if we exchange the two subsystems of the measured quantum state, which even shows completely opposite behavior; In particular, quantum discords in terms of different definitions are not consistent with each other for the ordering of some quantum states [20]. Recently, several attempts on the operational interpretation of quantum discord have been given to the information theoretic quantum discord which is related to the quantum state merging [32,33] and the relative-entropy-based quantum discord which is connected with distillable entanglement [34]. Thus we come up with the second natural question: How can we understand the geometric quantum discord from the most fundamental quantum mechanical feature--quantum coherence?

In this paper, we will answer the above two questions by studying the relation between geometric quantum discord, quantum entanglement and quantum coherence. We classify the quantum coherence into three classes based on some particular approaches, whilst some measure can be naturally given to the quantum coherence of different classes. We find that geometric quantum discord of each possible type (including the symmetric and asymmetric version) is just consistent with a special class of quantum coherence, which serves as the answer to our second question. We also suggest a new measure for the total quantum coherence. It can serve as a symmetric geometric quantum correlation and can be analytically calculated for the systems of two quits. In particular, the new symmetric quantum correlation for pure states is equivalent to the squared concurrence. Associated with the coherence of the subsystems, we find an interesting monogamy equation that shows how quantum coherence is distributed or how entanglement is generated similar to 3-tangle introduced in Ref. [35]. In addition, we quantify the third class of quantum coherence and find that for the systems of two qubits, this class of quantum coherence measure is directly connected with some quantum nonlocality, i.e., the violation of Clauser-Horne-Shimony-Holt (CHSH) inequality [36]. Thus for the system of two qubits, not only quantum entanglement and quantum discord but also quantum nonlocality in terms of CHSH inequality can be understood in the fundamental frame-—quantum coherence. Our main results are listed in detail in Sec. II which is organized as follows. We first divide quantum coherence into three class, then we prove each kind of geometric quantum discord is consistent with a kind of quantum coherence, and then we show that our suggesting measure for the total coherence can serve as a symmetric quantum correlation measure, prove its equivalence to the squared coherence for pure states and show how it is related to the distribution of quantum coherence. By using this distribution property, we also use a constructive way to show the analytic quantum discord for pure states. Finally, we find out that the third class of quantum coherence can be related with the violation of CHSH inequality for bipartite states of qubits.

2 Quantum coherence and quantum discord

2.1 Quantum coherence

Quantum coherence arises from quantum superposition, which is a necessary condition for quantum correlations. Generally speaking, a good definition of quantum coherence does not only depend on the state of the system ρ , but also depend on the alternatives under consideration which are usually attached to different eigenvalues of an observable A. Since the off-diagonal elements of ρ characterize interference, they are usually called *coherences* with respect to the basis in which ρ is written [37,38]. The measurements on the observables that do not commute with A can reveal the interference. Based on different viewpoints, a lot of quantum coherence measure can be defined with respect to the basis [39,40]. Here we will present a new coherence measure by which we can classify the coherence.

In order to explicitly present our classification of quantum coherence and the corresponding measure, we consider an $n_1 \otimes n_2$ density matrix

$$\rho = \sum_{i,k=0}^{n_1-1} \sum_{j,l=0}^{n_2-1} \rho_{ij,kl} |ij\rangle \langle kl|, \qquad (1)$$



Fig. 1 Illustration of the classification of quantum coherence. Each ellipse corresponds to one class of coherence. The overlap of the two ellipses corresponds a special type of coherence. "TOTAL" means the total coherence. "CHSH" means that Class *III* is connected with the violation of CHSH inequality, which is only satisfied by two qubits.

with $\rho_{ij,ij} > 0$, $\sum \rho_{ij,ij} = 1$ and $\text{tr}\rho^2 \leq 1$. As mentioned in our previous paper [41], the coherence can be measured by the contribution of the offdiagonal entries of ρ . Although it provided an explicit geometric meaning of coherence in a given basis, it is obviously basis-vector (local basis-vector included) dependent. However, is the characteristics of the off-diagonal entries in the coherence measure the same? The answer is no. Now let us consider a scheme of local operations and classical communication. Suppose Alice and Bob share a quantum state ρ given in Eq. (1). If Alice performs von Neumann measurement on her qubit in terms of the same basis of ρ and then informs Bob her measurement outcomes, Bob can obtain all the exact information about the off-diagonal entries of ρ that are related to his reduced density matrix at least in theory (for example, based on his local quantum state tomography [42,43]). The other off-diagonal entries of ρ can not be attainable. So these unattainable off-diagonal entries can be regarded as Class I. On the contrary, if Bob performs von Neumann measurements on his qubit first, there will also exist some entries that Alice can not attain. These Alice's unattainable entries can be regarded as Class II. It is obvious that Class I and Class IIhave an overlap, which corresponds to the the off-diagonal entries along the anti-diagonal line of ρ . The entries in the overlap can not be attained by either Alice or Bob. We call the overlap as Class III. Thus from the point of view of coherence, we have classified the quantum coherence into three classes. Why do we classify the quantum coherence with such a scheme? One can also understand it in a physical way. When one subsystem of ρ undergoes any a quantum channel [44], one can find that the entries in Class i, i = I, II have different decoherence rates from the rest, while the decoherence of the entries in

Class *III* will happen if either subsystem undergoes a quantum channel. These can be shown for two qubits more obviously under the phase-damping channel (pure decoherence [45]). This classification is something like the classification of tripartite mixed-state entanglement [46], where the different classes have overlaps.

2.2 Geometric quantum discord

Now in order to measure the degree of quantum coherence, we introduce quantum coherence measures for each class. For a given $(m \otimes n)$ -dimensional ρ with different bases considered, i.e. $\rho_{U_A \otimes U_B} = (U_A \otimes U_B) \rho \left(U_A^{\dagger} \otimes U_B^{\dagger} \right)$. In order to collect the contributions of Bob's unattainable off-diagonal entries (Class I) from $\rho_{U_A \otimes U_B}$, we can select the entries as

$$\Delta_{kk',ll'} = \langle kk' | \rho_{U_A \otimes U_B} | ll' \rangle, k \neq l$$
⁽²⁾

where $|k\rangle$, $|l\rangle$ and $|k'\rangle$, $|l'\rangle$ are the computational basis of the subsystem A and B, respectively. So the contribution to quantum coherence in the sense of squared l_2 norm of matrix $[\Delta_{kk',ll'}]$ is given by

$$C_{[A|B]}(\rho) = \sum_{k',l',(k\neq l)} |\Delta_{kk',ll'}|^2.$$
 (3)

Thus Alice and Bob can select a proper frame $(U_A \text{ and } U_B)$ such that $C_{[A|B]}(\rho)$ can be minimized after their operations. Similarly, for the coherence in Class II, we have $C_{[B|A]}(\rho)$ can be given by

$$C_{[B|A]}(\rho) = \sum_{k' \neq l', k, l} |\Delta_{kk', ll'}|^2,$$
(4)

In this way, we have the following definition.

Definition 1.- Quantum coherence of the Class I and Class II for ρ are measured, respectively, by

$$D_{[A|B]}(\rho) = \min_{U_A, U_B} C_{[A|B]}(\rho),$$
(5)

and

$$D_{[B|A]}(\rho) = \min_{U_A, U_B} C_{[B|A]}(\rho),$$
(6)

which describe the minimal quantum coherence with different frames taken into account.

With this definition, we can arrive at the following conclusion.

Theorem 1.- $D_{[A|B]}(\rho)$ and $D_{[B|A]}(\rho)$ are consistent with the geometric discord of ρ with measurements performed on the corresponding side.

Proof. Insert Eq. (2) and Eq. (3) into Eq. (5), we can arrive at

$$D_{[A|B]}(\rho) = \min \sum_{k',l',k\neq l} \langle kk' | \rho_{U_A \otimes U_B} | ll' \rangle \langle ll' | \rho_{U_A \otimes U_B} | kk' \rangle$$

$$= \min \left\{ \sum_{k',l',k,l} \langle kk' | \rho_{U_A \otimes U_B} | ll' \rangle \langle ll' | \rho_{U_A \otimes U_B} | kk' \rangle$$

$$- \sum_{k',l',k} \langle kk' | \rho_{U_A \otimes U_B} | kl' \rangle \langle kl' | \rho_{U_A \otimes U_B} | kk' \rangle \right\}$$

$$= Tr\rho^2 - \max_{\tilde{k}} Tr \sum_{\tilde{k}} \left(\left| \tilde{k} \right\rangle \langle \tilde{k} \right| \otimes 1_n \right) \rho \left(\left| \tilde{k} \right\rangle \langle \tilde{k} \right| \otimes 1_n \right) \rho$$

$$= \min_{\tilde{k}} \left\| \rho - \sum_{\tilde{k}} \left| \tilde{k} \right\rangle \langle \tilde{k} \right| \otimes \rho_{\tilde{k}\tilde{k}} \right\|^2, \qquad (7)$$

where $\left|\tilde{k}\right\rangle = U_A \left|k\right\rangle$ and $\rho_{\tilde{k}\tilde{k}} = \left(\left\langle\tilde{k}\right|\otimes 1_n\right)\rho\left(\left|\tilde{k}\right\rangle\otimes 1_n\right)$ with 1_n the n-dimensional identity. It is obvious that Eq. (7) is consistent with the definition of the geometric quantum discord [16], which means that the quantum coherence measure $D_{[A|B]}(\rho)$ is the geometric quantum discord.

Analogously, the quantum coherence measure of Class II can be written as

$$D_{[B|A]}(\rho) = \min_{U_A, U_B} C_{[B|A]}(\rho)$$
$$= \min_{\tilde{k}'} \left\| \rho - \sum_{\tilde{k}} \rho_{\tilde{k}'\tilde{k}'} \otimes \left| \tilde{k}' \right\rangle \left\langle \tilde{k}' \right| \right\|^2, \tag{8}$$

where $\left|\tilde{k}'\right\rangle = U_B \left|k'\right\rangle$ and $\rho_{\tilde{k}'\tilde{k}'} = \left(1_m \otimes \left\langle\tilde{k}'\right|\right) \rho\left(1_m \otimes \left|\tilde{k}'\right\rangle\right)$ with 1_m the mdimensional identity. It is obvious that Eq. (8) is also a geometric discord of the other side.

Both Eq. (7) and Eq. (8) show that geometric quantum discords actually quantify the quantum coherence. Since quantum coherence is local-basis dependent, quantum discord also depends on the local basis, which means it might be increased by local operations. Based on Ref. [31], one can find that for bipartite systems of qubits, $D_{[B|A]}(\rho)$ and $D_{[A|B]}(\rho)$ can be analytically solved. In fact, from the point of calculation of view, one can find that the direct starting with our definition can lead to a relatively simple procedure. For example, based on the proof of Theorem 1, Eq. (5) will arrive at

$$D_{[A|B]}(\rho) = Tr\rho^{2} - \max_{\tilde{k}} Tr \sum_{\tilde{k}} \left(\left| \tilde{k} \right\rangle \left\langle \tilde{k} \right| \otimes 1_{n} \right) \rho \left(\left| \tilde{k} \right\rangle \left\langle \tilde{k} \right| \otimes 1_{n} \right) \rho$$

$$= Tr\rho^{2} - \max_{\tilde{k}, i, j, i', j'} \frac{1}{16} \left[4 + 2x_{i}x_{j} \left\langle \tilde{k} \right| \sigma_{i} \left| \tilde{k} \right\rangle \left\langle \tilde{k} \right| \sigma_{j} \left| \tilde{k} \right\rangle$$

$$+ 2y_{i}y_{j}Tr \left\{ \sigma_{i}\sigma_{j} \right\} + T_{ij}T_{i'j'} \left\langle \tilde{k} \right| \sigma_{i} \left| \tilde{k} \right\rangle \left\langle \tilde{k} \right| \sigma_{i'} \left| \tilde{k} \right\rangle Tr \left\{ \sigma_{j}\sigma_{j'} \right\} \right]$$

$$= Tr\rho^{2} - \frac{1}{4} \left(1 + \left\| y \right\|^{2} \right)$$

$$- \max \sum_{i, j, i'} \frac{1}{4} \left[x_{i}x_{j} + T_{ii'}T_{ji'} \right] \left\langle \psi_{1}^{1} \right| \sigma_{j} \left| \psi_{1}^{1} \right\rangle \left\langle \psi_{1}^{1} \right| \sigma_{i} \left| \psi_{1}^{1} \right\rangle$$

$$= \frac{1}{4} (\left\| T \right\|^{2} + \left\| \mathbf{x} \right\|^{2} - \max \mathbf{p}_{1}^{t} M \mathbf{p}_{1}), \qquad (9)$$

and similarly, Eq. (6) will directly arrive at

$$D_{[B|A]}(\rho) = \frac{1}{4} \left(\|\mathbf{y}\|^2 + \|T\|^2 - \max \mathbf{p}_2^t N \mathbf{p}_2) \right), \tag{10}$$

where $M = \mathbf{x}\mathbf{x}^t + TT^t$, $N = \mathbf{y}\mathbf{y}^t + T^tT$, and $\mathbf{x}, \mathbf{y}, T$ are the Bloch vectors and tensor obtained from the Bloch representation of ρ , the superscript t means transpose. In addition, σ_k in above equations denote the Pauli matrices, $\left|\tilde{k}\right\rangle$ is defined the same as that in Eq. (7), $\left|\psi_i^j\right\rangle$ denotes the *i*th orthonormal vector of the complete set $\left|\tilde{k}\right\rangle$ of *j*th subsystem and \mathbf{p}_j is the Bloch vector of $\left|\psi_1^1\right\rangle$. Thus, we can easily find that $D_{[A|B]}(\rho) = \frac{1}{4}\left(\|\mathbf{x}\|^2 + \|T\|^2 - \lambda_{1\max}\right)$ and $D_{[B|A]}(\rho) = \frac{1}{4}\left(\|\mathbf{y}\|^2 + \|T\|^2 - \lambda_{2\max}\right)$ with $\lambda_{1\max}$, $\lambda_{2\max}$ the maximal eigenvalue of $\mathbf{x}\mathbf{x}^t + TT^t$ and $\mathbf{y}\mathbf{y}^t + T^tT$, respectively. These results also provide a demonstration of the consistency of quantum discord and our coherence measure in two-qubit systems.

2.3 Symmetric quantum correlation

We have considered the partial contribution of quantum coherence which shows the coincidence between geometric quantum discord and quantum coherence measure. Now we turn to addressing the contribution of all the coherence of a density matrix ρ . A natural method to extracting the coherence is to collect all the off-diagonal elements by

$$\tilde{C}_{Total}(\rho) = \sum_{(kk') \neq (ll')} \left| \langle kk' | \rho_{U_A \otimes U_B} | ll' \rangle \right|^2.$$
(11)

Definition 2.- The measure of the total coherence can be defined as

$$\tilde{D}(\rho) = \min_{U_A, U_B} \tilde{C}_{Total}(\rho).$$
(12)

From this definition, one can arrive at the following rigorous conclusion.

Theorem 2.- $\dot{D}(\rho)$ is consistent with the geometric discord of ρ with twoside measurements.

Proof.

$$D(\rho)$$

$$= \min\left(\sum_{kk'll'} \left|\langle kk' \right| \rho_{U_A \otimes U_B} \left| ll' \rangle \right|^2 - \sum_{(kk')=(ll')} \left|\langle kk' \right| \rho_{U_A \otimes U_B} \left| ll' \rangle \right|^2\right)$$

$$= \min\left(Tr\rho_{U_A \otimes U_B}^2 - \sum_{kl} \left|\langle kl \right| \rho_{U_A \otimes U_B} \left| kl \rangle \right|^2\right)$$

$$= \min\left\|\rho - \sum_{kl} \left(\Pi_k \otimes \Pi_l\right) \rho \left(\Pi_k \otimes \Pi_l\right)\right\|^2, \qquad (13)$$

with $\Pi_i = U_{A/B} |i\rangle \langle i| U_{A/B}^{\dagger}$ the projector on A/B qubit in some basis $U_{A/B} |i\rangle$. It is obvious that Eq. (13) is actually the geometric discord with two-side measurements or the symmetric quantum discord.

It has been shown that $D(\rho)$ is completely consistent with the geometric discord with two-side measurements, but it is hard to analytically calculated even for a general two-qubit mixed state. This can be seen from the recent analysis given in Ref. [47]. In order to obtain an analytic expression at least for the two-qubit case, we would like to extract all the coherence with the following approach:

$$C_{Total}(\rho) = C_{[A|B]}(\rho) + C_{[B|A]}(\rho), \qquad (14)$$

which means that we have considered the contribution of the doubled coherence corresponding to the anti-diagonal entries. This is in fact completely valid from the measure point of view, because this does not influence the nature of coherence, but the relative value of the coherence. In addition, We can easily prove that $D(\rho)$ given in the following equation has an interesting property that will be shown by the corollary in the next subsection. Therefore, we would like to introduction the below definition.

Definition 3.- The total quantum coherence can also be alternatively defined by

$$D(\rho) = \min_{U_A, U_B} C_{Total}(\rho).$$
(15)

Similarly, in this definition, we also consider the possible minimal value of the contribution of anti-diagonal entries. $D(\rho)$ in this definition can be easily calculated by the following theorem.

Theorem 3. - The total quantum coherence measure $D(\rho)$ is given by

$$D(\rho) = D_{[A|B]}(\rho) + D_{[B|A]}(\rho), \tag{16}$$

which can grasp the symmetric quantum correlation.

Proof. Substitute Eq. (3) and Eq. (4) into Eq. (16), one will obtain that

$$D(\rho) = -\max_{\tilde{k}\tilde{k}'} \left[Tr \sum_{\tilde{k}\tilde{k}'} \left(\left| \tilde{k} \right\rangle \left\langle \tilde{k} \right| \otimes 1_n \right) \rho \left(\left| \tilde{k} \right\rangle \left\langle \tilde{k} \right| \otimes 1_n \right) \rho + Tr \sum_{\tilde{k}'} \left(1_m \otimes \left| \tilde{k}' \right\rangle \left\langle \tilde{k}' \right| \right) \rho \left(1_m \otimes \left| \tilde{k}' \right\rangle \left\langle \tilde{k}' \right| \right) \rho \right] + 2Tr\rho^2.$$
(17)

It is obvious that $|\tilde{k}\rangle$ and $|\tilde{k}'\rangle$ are independent. Thus $C_{[A|B]}(\rho)$ and $C_{[B|A]}(\rho)$ can be optimized separately. Therefore, we have

$$D(\rho) = \min_{U_A, U_B} C_{[A|B]}(\rho) + \min_{U_A, U_B} C_{[B|A]}(\rho)$$
(18)

$$= D_{[A|B]}(\rho) + D_{[B|A]}(\rho), \tag{19}$$

which happens to be the sum of the two classes of quantum coherence $D_{[A|B]}(\rho)$ and $D_{[B|A]}(\rho)$.

Now we prove that $D(\rho)$ can grasp the symmetric quantum correlation. It is obvious that $D(\rho)$ does not depend on the exchange of A and B. If $D(\rho) = 0$, it means that there exist U'_A and U'_B such that $\rho_{U'_A \otimes U'_B}$ is a diagonal matrix. In the same basis, the reduced matrices are also diagonal. That is, the density matrix ρ have a diagonal form in the product of its marginal bases [33,34]. So $\rho_{U'_A \otimes U'_B}$ has no quantum correlation. If a density matrix ρ is classical correlated, then it must have a diagonal form in the product of its marginal bases. Therefore, based on our definition of $D(\rho)$, we must be able to find such U'_A and U'_B that $\rho_{U'_A \otimes U'_B}$ has no off-diagonal elements in the basis. That is, $D(\rho)$ vanishes. Hence, $D(\rho)$ does not only measure the total coherence, but also it can serve as a symmetric measure of quantum correlation. The proof is completed.

2.4 Concurrence by the monogamy

As mentioned above, the introduction of the new measure of the total coherence lies in its intriguing properties. Now we will first show how this measure is connected with the bipartite concurrence of pure states. Let $\rho_{AB} = |\psi\rangle_{AB} \langle \psi|$ be an $(m \otimes n)$ - dimensional bipartite pure state, $\rho_A = \text{Tr}_B \rho_{AB}$ and $\rho_B = \text{Tr}_B \rho_{AB}$. Suppose $|\psi\rangle_{AB} = \sum_{ij} a_{ij} |ij\rangle$ in the computational basis, then we can obtain the concurrence of this state [48,49] is

$$\mathcal{C}\left(\left|\psi\right\rangle_{AB}\right) = 2\sqrt{\sum_{i < j, k < l} \left|a_{ik}a_{jl} - a_{il}a_{jk}\right|^2}.$$
(20)

Thus one will obtain the following theorem.

Theorem 4.-The concurrence of the state $|\psi\rangle_{AB}$ and the total coherence as well as the local coherence have the following monogamy relation:

$$\mathcal{C}^{2}(|\psi\rangle_{AB}) = \mathcal{D}(\rho_{AB}) - \mathcal{D}(\rho_{A}) - \mathcal{D}(\rho_{B}), \qquad (21)$$

with $\mathcal{D}(\cdot) = C_{Total}(\cdot)$ for convenience. *Proof.* Based on the definition of $C_{Total}(\rho_{AB})$, we have

$$\mathcal{D}(\rho_{AB}) = C_{[A|B]}(\rho_{AB}) + C_{[B|A]}(\rho_{AB})$$

$$= 2 \sum_{(ij)<(kl)} |a_{ij}a_{kl}^*|^2 + 2 \sum_{i< k, j\neq l} |a_{ij}a_{kl}^*|^2$$

$$= 2 \sum_{k,(j

$$+ 4 \sum_{i< k, j\neq l} |a_{ij}a_{kl}^*|^2, \qquad (22)$$$$

and

$$\mathcal{D}(\rho_A) + \mathcal{D}(\rho_B)$$

$$= 2 \sum_{i < j} \left| \sum_k a_{ik} a_{jk}^* \right|^2 + 2 \sum_{i < j} \left| \sum_k a_{ki} a_{kj}^* \right|^2$$

$$= 2 \sum_{(i < j), k} \left| a_{ik} a_{jk}^* \right|^2 + 2 \sum_{(i < j), k} \left| a_{ki} a_{kj}^* \right|^2$$

$$+ 2 \sum_{i < j, k \neq l} a_{ik} a_{jk}^* a_{il}^* a_{jl} + 2 \sum_{i < j, k \neq l} a_{ki} a_{kj}^* a_{li}^* a_{lj}.$$

Therefore

$$\mathcal{D}(\rho_{AB}) - \mathcal{D}(\rho_{A}) - \mathcal{D}(\rho_{B})$$

$$= 4 \sum_{i < k, j \neq l} |a_{ij}a_{kl}^{*}|^{2} - 2 \sum_{i < j, k \neq l} a_{ik}a_{jk}^{*}a_{il}^{*}a_{jl}$$

$$-2 \sum_{i < j, k \neq l} a_{ki}a_{kj}^{*}a_{li}^{*}a_{lj}$$

$$= \left(4 \sum_{i < j, k < l} a_{ik}a_{jl}^{*}a_{ik}^{*}a_{jl} - 2 \sum_{i < j, k < l} a_{ik}a_{jk}^{*}a_{il}^{*}a_{jl}\right)$$

$$-2 \sum_{i < j, k < l} a_{ki}a_{kj}^{*}a_{li}^{*}a_{lj}\right) + \left(4 \sum_{i < j, k > l} a_{ik}a_{jl}^{*}a_{ik}^{*}a_{jl}\right)$$

$$-2 \sum_{i < j, k < l} a_{ik}a_{jk}^{*}a_{il}^{*}a_{lj} - 2 \sum_{i < j, k > l} a_{ki}a_{kj}^{*}a_{ik}^{*}a_{jl}\right)$$

$$= 4 \sum_{i < j, k < l} |a_{ik}a_{jl} - a_{il}a_{jk}|^{2}, \qquad (23)$$

which is just consistent with $\mathcal{C}^2(|\psi\rangle_{AB})$. The proof is finished.

From Theorem 4, one can easily find that Eq. (21) has the similar form as the monogamy relation between the bipartite concurrence and the 3-tangle [35]. It directly demonstrates the distribution of coherence and provides some limitation on the coherence of the subsystem in some given basis. It also gives us an alternative understanding of pure-state entanglement. Actually, Theorem 4 can also be generalized to the mixed state, which is given by the following corollary.

Corollary 1. For a mixed state ρ_{AB} , the monogamy relation given in theorem 3 can become the following inequality,

$$\mathcal{C}^{2}(\rho_{AB}) \leq \min_{\{p_{i}, |\varphi_{i}\rangle_{AB}\}} \sum p_{i} \mathcal{D}(|\varphi_{i}\rangle_{AB}) - \mathcal{D}(\rho_{A}) - \mathcal{D}(\rho_{B}).$$
(24)

Proof. Let $\rho_{AB} = \sum_{i} p_i |\varphi_i\rangle_{AB} \langle \varphi_i|$ be the decomposition of ρ_{AB} that achieves the optimal average as $\min_{\{p_i, |\varphi_i\rangle_{AB}\}} \sum_{i} p_i \mathcal{D}(|\varphi_i\rangle_{AB})$. For each pure state $|\varphi_i\rangle_{AB}$, one can always use theorem 3 and obtain the corresponding monogamy equation. Add all the monogamy equations, we will arrive at

$$\sum p_i \mathcal{C}^2 \left(|\varphi_i\rangle_{AB} \right) = \sum p_i \left[\mathcal{D}(|\varphi_i\rangle_{AB}) - \mathcal{D}(\rho_A^i) - \mathcal{D}(\rho_B^i) \right]$$
(25)

with $\rho_A^i = Tr_B |\varphi_i\rangle_{AB} \langle \varphi_i |$ and $\rho_B^i = Tr_A |\varphi_i\rangle_{AB} \langle \varphi_i |$. Since $\rho_{A/B} = \sum_i p_i \rho_{A/B}^i$ and $\mathcal{D}(\rho_A^i) = \sum_{j \neq k} \left| \left(\rho_A^i \right)_{jk} \right|^2$, based on the convexity of $\mathcal{D}(\rho_A^i)$ we have

$$\sum p_i \mathcal{C}^2 \left(|\varphi_i\rangle_{AB} \right) \le \sum p_i \mathcal{D}(|\varphi_i\rangle_{AB}) - \mathcal{D}(\rho_A) - \mathcal{D}(\rho_B).$$
(26)

Because the concurrence $\mathcal{C}(|\varphi_i\rangle_{AB})$ is also a convex function, it follows that

$$\sum p_i \mathcal{C}^2 \left(|\varphi_i\rangle_{AB} \right) \ge \left[\sum p_i \mathcal{C} \left(|\varphi_i\rangle_{AB} \right) \right]^2 \ge \mathcal{C}^2 \left(\rho_{AB} \right).$$
(27)

Eq. (26) and Eq. (27) show that the proposition is right, which completes the proof. $\hfill\blacksquare$

Again Eq. (24) is similar to that of the monogamy relation for the mixed state given in Ref. [35]. Eq. (24) shows that the squared concurrence plus the local coherence will be never larger than the average total coherence. In fact, from our theorem 3, one can easily find the exact value of geometric discord and our suggested symmetric quantum correlation measure without any optimization procedure, which is also one of the reasons why we consider the doubled anti-diagonal entries in the definition of the symmetric correlation measure.

Corollary 2.- For a bipartite pure state $\rho = |\phi\rangle \langle \phi|$ defined in arbitrary $(m \otimes n)$ dimension, the geometric discord and the symmetric quantum correlations can be given by the concurrence as

$$D(\rho) = \mathcal{C}^2(\rho) \tag{28}$$

$$D_{[A|B]}(\rho) = D_{[B|A]}(\rho) = \frac{1}{2}C^2(\rho).$$
(29)

Proof. Since ρ is a pure state, theorem 3 holds for ρ . That is,

$$C^{2}(\rho) = \mathcal{D}(\rho) - \mathcal{D}(\rho_{A}) - \mathcal{D}(\rho_{B}), \qquad (30)$$

with $\rho_A = Tr_B\rho$, $\rho_B = Tr_A\rho$, $\mathcal{D}(\rho_A) = \sum_{i \neq j} |\rho_{Aij}|^2$ and $\mathcal{D}(\rho_B) = \sum_{i \neq j} |\rho_{Bij}|^2$. It is obvious that Eq. (30) is independent of the basis. So we can select U_A and U_B such that $U_A\rho_A U_A^{\dagger}$ and $U_B\rho_B U_B^{\dagger}$ are diagonal, thus we have

$$\mathcal{D}(U_A \rho_A U_A^{\dagger}) = \mathcal{D}(U_B \rho_B U_B^{\dagger}) = 0.$$
(31)

It easily turns out

$$D(\rho_{AB}) = \min_{U_A \otimes U_B} \mathcal{D}(\rho_{AB(U_A \otimes U_B)}) \le \mathcal{C}^2(\rho_{AB}).$$
(32)

On the contrary, select U'_A and U'_B such that the optimization $\min_{U_A \otimes U_B} \mathcal{D}(\rho_{AB(U_A \otimes U_B)})$ is attained, i.e.

$$D(\rho_{AB}) = \mathcal{D}(\rho_{AB}(U'_A \otimes U'_B)).$$
(33)

However, $\mathcal{D}(\rho_A)$ and $\mathcal{D}(\rho_B)$ could be non-zero, so from Eq. (30), one will arrive at

$$D(\rho_{AB}) \geqslant \mathcal{C}^2(\rho_{AB}). \tag{34}$$

Eq. (32) and Eq. (34) show $D(\rho_{AB}) = C^2(\rho_{AB})$.

Next we will turn to the proof of Eq. (29). Since $D_{[A|B]}(\rho)$ and $D_{[B|A]}(\rho)$ are invariant under local unitary operations, we would like to consider the state ρ after the Schmidt decomposition. In this case, ρ can be written by

$$\rho = \sum_{i,j=0}^{\min\{m,n\}} \sigma_i \sigma_j |ii\rangle \langle jj|, \qquad (35)$$

with σ_i the Schmidt coefficients. Based on the definitions of $D_{[A|B]}(\rho)$ and $D_{[B|A]}(\rho)$ given in Eq. (3) and Eq. (4), respectively, that is,

$$D_{[A|B]}(\rho) = \sum_{(\alpha \neq \gamma), \beta, \delta,} \sum_{i,j=0}^{\min\{m,n\}} \left| \sigma_i \sigma_j \left\langle \alpha \beta \right| ii \right\rangle \left\langle jj \right| \left| \gamma \delta \right\rangle \right|^2$$
(36)

and

$$D_{[B|A]}(\rho) = \sum_{(\beta \neq \delta), \alpha, \gamma,} \sum_{i,j=0}^{\min\{m,n\}} |\sigma_i \sigma_j \langle \alpha \beta | ii \rangle \langle jj | \gamma \delta \rangle|^2, \qquad (37)$$

where $|\alpha\rangle$, $|\beta\rangle$, $|\gamma\rangle$ and $|\delta\rangle$ are the optimal local orthonormal basis in their corresponding subspace such that the optimization of $D_{[A|B]}(\rho)$ and $D_{[B|A]}(\rho)$ is achieved. From the two Eqs. (36) and (37), one can easily find that $D_{[A|B]}(\rho)$ will become $D_{[B|A]}(\rho)$ and vice versa, if we exchange their subspace. Thus we have $D_{[A|B]}(\rho) = D_{[B|A]}(\rho)$. According to Eq. (28) and Theorem 2, it is natural that Eq. (29) hold. The proof is finished.

and

2.5 Possible connection with nonlocality: violation of CHSH inequality for two qubits

In this part, for the integrity we will quantify the third class of quantum coherence which corresponds to the overlap of quantum coherence in Class I and Class II. From our classification, we can find that the quantum coherence of Class III does not depend on the exchange of subsystems A and B. In the same way as the quantification of quantum coherence of Class I and Class II, we can extract all the anti-diagonal entries of ρ within all possible local frames as

$$\tilde{\Delta}_{kk',ll'} = \langle kk' | \rho_{U_A \otimes U_B} | ll' \rangle, \begin{cases} k+l=m-1\\ k'+l'=n-1 \end{cases}.$$
(38)

Thus the contribution of anti-diagonal entries can be described as

$$v(\rho) = \sum_{\substack{k+l=m-1\\k'+l'=n-1}} \left| \tilde{\Delta}_{kk',ll'} \right|^2.$$
(39)

Similarly to the previous definitions, considering all the potential U_A and U_B , we will arrive at a new definition.

Definition 4.- The third class of coherence can be measured by

$$V(\rho) = \min_{U_A, U_B} v(\rho).$$
(40)

A dual measure of coherence can also be defined as

$$\tilde{V}(\rho) = \max_{U_A, U_B} v(\rho).$$
(41)

In fact, what $V(\rho)$ and $\tilde{V}(\rho)$ characterize for a general state except the coherence defined by us has been unknown yet. This is also why we consider the contribution of the anti-diagonal entries by introducing both the maximum and the minimum. Of course, a simple result can be seen for the pure states of two qubits. That is, $V(\rho) = 0$ means that the two-qubit pure state is separable. In fact, for the system of two qubits, one can further find that both $V(\rho)$ and $\tilde{V}(\rho)$ are closely related to the violation of the remarkable CHSH inequality. In this sense, we would like to make the following conjecture.

Conjecture.- At least one of $V(\rho)$ and $\tilde{V}(\rho)$ could be related to the nonlocality subject to some Bell theory.

Next we will show how $V(\rho)$ and $\tilde{V}(\rho)$ are connected with the violation of CHSH inequality for two qubits. Substitute the Bloch representation of ρ_{AB}

into Eq. (39), it follows that

$$v(\rho) = \frac{1}{4} \sum_{i,j=1}^{3} T_{ij} T_{ij} - \frac{1}{4} \sum_{i,k,l=1}^{3} T_{ik} T_{il} \langle \psi_{1}^{2} | \sigma_{k} | \psi_{1}^{2} \rangle$$

$$\times \langle \psi_{1}^{2} | \sigma_{l} | \psi_{1}^{2} \rangle - \frac{1}{4} \sum_{i,j,k=1}^{3} T_{ik} T_{jk} \langle \psi_{1}^{1} | \sigma_{i} | \psi_{1}^{1} \rangle \langle \psi_{1}^{1} | \sigma_{j} | \psi_{1}^{1} \rangle$$

$$+ \frac{1}{4} \sum_{i,j,k,l=1}^{3} T_{ik} T_{jl} \langle \psi_{1}^{1} | \sigma_{j} | \psi_{1}^{1} \rangle \langle \psi_{1}^{1} | \sigma_{i} | \psi_{1}^{1} \rangle$$

$$\times \langle \psi_{1}^{2} | \sigma_{k} | \psi_{1}^{2} \rangle \langle \psi_{1}^{2} | \sigma_{l} | \psi_{1}^{2} \rangle$$

$$= \frac{1}{4} (||T||^{2} - \mathbf{p}_{1}^{t} T T^{t} \mathbf{p}_{1} - \mathbf{p}_{2}^{t} T^{t} T \mathbf{p}_{2} + \mathbf{p}_{1}^{t} T \mathbf{p}_{2} \mathbf{p}_{2}^{t} T^{t} \mathbf{p}_{1}), \qquad (42)$$

where $|\psi_i^j\rangle$ similar to that in Eq. (9) means the *i*th orthonormal vector subject to *j*th subsystem, σ_i denote the Pauli matrices and \mathbf{p}_j is the Bloch vector of $|\psi_1^j\rangle$. Thus we can obtain the rigorous expressions as follows.

Theorem 5.-For a bipartite state of qubits,

$$V(\rho) = \frac{1}{4}\sigma_{\min} \tag{43}$$

and

$$\tilde{V}(\rho) = \frac{1}{4} (\|T\|^2 - \sigma_{\min}),$$
(44)

where σ_{\min} is the minimal eigenvalue of TT^t .

Proof. In order to give an analytic optimization of Eq. (42), we would like to turn to a simple basis, since Eq. (42) is not changed under local unitary transformations. Consider the singular value decomposition of T as $T = U\Lambda V$, then U and V are orthogonal matrix and $\Lambda = diag[\sigma_1, \sigma_2, \sigma_3]$ with

$$\sigma_1 \ge \sigma_2 \ge \sigma_3 \ge 0,\tag{45}$$

since T is a real matrix. Thus U and V that could appear in Eq. (42) can be absorbed by \mathbf{p}_1 and \mathbf{p}_2 and for the habit, we let $\mathbf{p}_1 = [x_1, x_2, x_3]^t$ and $\mathbf{p}_2 = [y_1, y_2, y_3]^t$ which should be distinguished from the expressions given in Eq. (9) and Eq. (10). Thus the optimizations defined in Eq. (40) and Eq. (41) are changed into

$$V(\rho) = \min_{U_A, U_B} v(\rho) = \frac{1}{4} (\|T\|^2 - \max L)$$
(46)

$$\tilde{V}(\rho) = \max_{U_A, U_B} v(\rho) = \frac{1}{4} (\|T\|^2 - \min L)$$
(47)

with

$$L(x_i, y_i) = \sum_{i=1}^{3} \sigma_i^2 \left(x_i^2 + y_i^2 \right) - \left(\sum_{i=1}^{3} \sigma_i x_i y_i \right)^2.$$
(48)

Now we would like to first calculate the minimum of L. Based on Cauchy-Schwarz inequality, we can easily find that

$$L \ge \sum_{i=1}^{3} \sigma_{i}^{2} \left(x_{i}^{2} + y_{i}^{2} \right) - \sum_{i=1}^{3} \sigma_{i}^{2} x_{i}^{2}$$
$$= \sum_{i=1}^{3} \sigma_{i}^{2} y_{i}^{2} \ge \sigma_{3}^{2} = \sigma_{\min}.$$
(49)

It is obvious that the inequality (49) can be saturated if $\mathbf{p}_1 = \mathbf{p}_2 = [0, 0, 1]^t$ based on Eq. (45). So we have that Eq. (44) is satisfied.

Now we prove Eq. (43). Based on the Lagrange multiplier method, the Lagrange function of Eq. (48) can be given by

$$\Phi(x_i, y_i, \lambda, \mu) = L(x_i, y_i) + \lambda \left(\sum_{i=1}^3 x_i^2 - 1\right) + \mu \left(\sum_{i=1}^3 y_i^2 - 1\right),$$
(50)

with λ, μ the Lagrange multipliers. Derivatives on the parameters of $\Phi(x_i, y_i, \lambda, \mu)$ can be given by

$$\begin{cases} \frac{\partial \Phi}{\partial x_i} = 2\left(\sigma_i^2 + \lambda\right) x_i + 2A\sigma_i y_i = 0\\ \frac{\partial \Phi}{\partial y_i} = 2\left(\sigma_i^2 + \mu\right) y_i + 2A\sigma_i x_i = 0 \end{cases},$$
(51)

with

$$A = \sum_{i=1}^{3} \sigma_i x_i y_i.$$
(52)

The Eq. (51) has non-zero solution requires that there exists at least an i such that

$$\det\left[\begin{pmatrix} \sigma_i^2 + \lambda & A\sigma_i \\ A\sigma_i & \sigma_i^2 + \mu \end{pmatrix}\right] = 0.$$
(53)

First of all, we suppose $\sigma_1 > \sigma_2 > \sigma_3 > 0$. It is not difficult to find that if there exists a single i = k such that Eq. (53) holds, one can easily find $x_k = y_k = 1$, and the others are zero. The extremes of L in this case are σ_k^2 . If Eq. (53) holds for all i = 1, 2, 3, one will find that Eq. (51) has no solution. So the remaining is that two equations in Eq. (53) hold, and one does not hold. Satisfying this condition, there exists three possibilities. However, it proves that the procedure of the calculations are similar and their solutions also have the similar form. Without loss of generality, we set Eq. (53) is only satisfied for i = 1, 2, which directly implies

$$x_3 = y_3 = 0. (54)$$

In particular, we can get an equation group from Eq. (53) as

$$\begin{cases} \left(\sigma_1^2 + \lambda\right) \left(\sigma_1^2 + \mu\right) - \sigma_1^2 A^2 = 0\\ \left(\sigma_2^2 + \lambda\right) \left(\sigma_2^2 + \mu\right) - \sigma_2^2 A^2 = 0 \end{cases}$$
(55)

A direct simplification will lead to

$$\lambda \mu = \sigma_1^2 \sigma_2^2, \tag{56}$$

and

$$A^{2} = \frac{\left(\sigma_{1}^{2} + \lambda\right)\left(\sigma_{1}^{2} + \mu\right)}{\sigma_{1}^{2}}.$$
(57)

In addition, based on Eq. (51), one can also find that

$$y_i = \sqrt{\frac{\sigma_i + \lambda}{\sigma_i + \mu}} x_i, i = 1, 2.$$
(58)

Substitute Eqs. (56-58) into Eq. (51), we will obtain that

$$x_1^2 = \frac{\left(\sigma_2^2 + \lambda\right)\sigma_1^2}{\lambda(\sigma_1^2 - \sigma_2^2)}.$$
(59)

Insert Eqs. (56-59) into Eq. (48), L can be rewritten as

$$L_{12} = \sigma_1^2 \left(x_1^2 + y_1^2 \right) + \sigma_2^2 \left(x_2^2 + y_2^2 \right) - A^2$$

$$= 2\sigma_2^2 + \left(\sigma_1^2 - \sigma_2^2 \right) \left(x_1^2 + y_1^2 \right)$$

$$- \frac{\left(\sigma_1^2 + \lambda \right) \left(\sigma_1^2 + \mu \right)}{\sigma_1^2}$$

$$= \sigma_2^2 - \sigma_1^2 - \frac{\lambda^2 + \sigma_1^2 \sigma_2^2}{\lambda}$$

$$+ \frac{\left[\sigma_1^2 \left(\lambda + \sigma_2^2 \right) + \lambda \left(\lambda + \sigma_1^2 \right) \right] \sigma_1^2 (\lambda + \sigma_2^2)}{\sigma_1^2 \lambda (\lambda + \sigma_2^2)}$$

$$= \sigma_1^2 + \sigma_2^2, \qquad (60)$$

which provides an extreme. Similarly, if we assume Eq. (53) holds for any i = k, l, one will always obtain

$$L_{kl} = \sigma_k^2 + \sigma_l^2. \tag{61}$$

Actually, one can easily check that the cases that there exist some "=" hold in $\sigma_1 \ge \sigma_2 \ge \sigma_3$, are completely covered by the above calculation. We won't repeat the similar calculations. Compare the solutions given in Eqs. (60,61), one will obtain that the maximum is obviously provided by Eq. (60). Substitute this solution into Eq. (46), we arrive at Eq. (43). The proof is completed.

From this theorem, we can directly find the connection with the violation of CHSH inequality.

Corollary 3.-If ρ is a bipartite quantum state of qubits,

$$\tilde{V}(\rho) > \frac{1}{4} \tag{62}$$

or

$$V(\rho) < \frac{1}{4} \left(\|T\|^2 - 1 \right)$$
 (63)

is equivalent to the violation of CHSH inequality.

Proof. From Eq. (47), it follows that $4\tilde{V}(\rho) = \sigma_1^2 + \sigma_2^2$, where σ_i^2 denote the eigenvalues of TT^t in decreasing order. In Ref. [50], it was explicitly reported that if $\sigma_1^2 + \sigma_2^2 > 1$, the state will violate the CHSH inequality. So in our case, one can easily conclude that if $\tilde{V}(\rho) > \frac{1}{4}$, the state ρ will violate CHSH inequality. In addition, it is obvious that

$$V(\rho) + \tilde{V}(\rho) = \frac{1}{4} \|T\|^2, \qquad (64)$$

from which one can find that ρ violate CHSH inequality means $V(\rho) < \frac{1}{4} \left(\|T\|^2 - 1 \right)$. This is the end of the proof.

Before the end of this section, we would like to emphasize that, even though we have found a very interesting connection between the violation of CHSH inequality and some special quantum coherence (anti-diagonal entries of density matrices), we have not yet made sure whether this kind of connection is suitable for the high dimensional bipartite quantum states.

3 Conclusion and discussion

We have shown the complete coincidence between geometric quantum discords and different classes of quantum coherence in terms of the classification of quantum coherence. The coincidence provides an alternative understanding of the asymmetric and symmetric geometric quantum discords based on the fundamental quantum mechanical feature— quantum coherence. Furthermore, a recommended total quantum coherence measure has led to a new symmetric geometric quantum discord. It has been shown that this kind of total quantum coherence can be used to construct the monogamy relation between the quantum coherence and quantum concurrence which can also been understood as some interpretation of the origin of entanglement. What's more, it is also shown that the coherence of Class *III* can be directly connected with the violation of CHSH inequality for two qubits.

In fact, there are many interesting questions for the future. 1) Is the quantum coherence of Class *III* connected with the violation of CHSH inequality in high dimension or some special nonlocality? 2) Replacing the minimization in Eq. (5), Eq. (6), Eq. (12) and Eq. (16) by the maximization ones similar to Eq. (44), one can obtain a different definition of quantum coherence measure. Can the new definition be connected with other interesting issues, such as entanglement, nonlocality, correlations and so on? 3) How can we quantify the quantum coherence of multipartite quantum states in the same manner and do the different quantum coherence measure correspond to different multipartite geometric quantum discords either?

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