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Citation: Chin. Phys. B, 2023, 32 (**10**): 100301. DOI: 10.1088/1674-1056/acdc11
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Geometric discord of tripartite quantum systems

Chunhe Xiong(熊春河)[1,2,†], Wentao Qi(齐文韬)[3], Maoke Miao(缪茂可)[4], and Minghui Wu(吴明晖)[2]

[1] *Interdisciplinary Center for Quantum Information, School of Physics, Zhejiang University, Hangzhou* 310027, *China*
[2] *School of Computer and Computing Science, Hangzhou City University, Hangzhou* 310015, *China*
[3] *School of Mathematical Sciences, Zhejiang University, Hangzhou* 310027, *China*
[4] *School of information and electrical engineering, Hangzhou City University, Hangzhou* 310015, *China*

(Received 19 April 2023; revised manuscript received 25 May 2023; accepted manuscript online 7 June 2023)

We study the quantification of geometric discord for tripartite quantum systems. Firstly, we obtain the analytic formula of geometric discord for tripartite pure states. It is already known that the geometric discord of pure states reduces to the geometric entanglement in bipartite systems, the results presented here show that this property is no longer true in tripartite systems. Furthermore, we provide an operational meaning for tripartite geometric discord by linking it to quantum state discrimination, that is, we prove that the geometric discord of tripartite states is equal to the minimum error probability to discriminate a set of quantum states with von Neumann measurement. Lastly, we calculate the geometric discord of three-qubit Bell diagonal states and then investigate the dynamic behavior of tripartite geometric discord under local decoherence. It is interesting that the frozen phenomenon exists for geometric discord in this scenario.

Keywords: geometric discord, tripartite quantum systems, quantum state discriminations, frozen discord

PACS: 03.65.Aa, 03.67.–a, 03.67.Mn, 03.65.Yz **DOI:** 10.1088/1674-1056/acdc11

1. introduction

Quantum correlation is not only a unique phenomenon but also a valuable resource of the quantum world. The characterization and quantification of quantum correlations lie at the very heart of exploring and exploiting quantum phenomena. As resources, quantum correlations such as entanglement,[1] non-locality,[2,3] discord,[4] and coherence,[5] offer remarkable advantages that make quantum information theory more powerful than classical theory.[6–13]

Quantum discord, proposed firstly by Olliver and Zurek,[14] and Henderson and Vedral,[15] is the quantum correlation that arises from the loss of information caused by quantum measurements. Since then, a lot of efforts have been made to generalize discord to tripartite and larger systems.[16–20] Recently, Radhakrishnan *et al.* generalized quantum discord to multipartite cases.[21] A feature of their formulation is that the definition of multipartite discord reduces to the standard definition of discord for bipartite correlated subsystems, and this has also led to research of multipartite quantum discord.[22–26]

Quantifying discord is not only the basic problem of quantum correlation theory, but also the premise of using quantum discord. After Datta gave a mathematical description of bipartite quantum states with zero discord,[27] a great deal of work began on the quantitative study of quantum discord from a geometric perspective, that is, this kind of discord is defined as the minimal distance between a state and the set of states with zero discord.[28–31]

In this paper, we consider the quantification of tripartite discord with geometric measure, which has been proven to be a nice measure to quantify entanglement,[32] discord,[29,30] and coherence.[33] For pure states, we obtain the analytic expression of tripartite geometric discord. It is already known that geometric discord of pure state reduces to the geometric entanglement in bipartite systems. However, our results show that it is no longer the case in tripartite systems.

Furthermore, we provide an operational meaning for geometric tripartite discord by linking it to quantum state discrimination, that is, we prove that the geometric discord of tripartite states is equal to the minimum error probability to discriminate a set of pure states with von Neumann measurement. This conclusion generalizes the main result in Ref. [29], where the authors first established the relationship in the bipartite quantum system. Moreover, we obtain the analytic formula of geometric discord for three-qubit Bell diagonal states.

Finally, we consider the dynamics of tripartite geometric discord under local decoherence. It is interesting that the frozen phenomenon exists in the geometric discord of three-qubit Bell diagonal states, since it has been shown that the original generalized discord of Bell diagonal states will always decay in this decoherence environment.[22]

The paper is organized as follows. We introduce and discuss the generalized geometric discord for tripartite systems in Section 2. We calculate the geometric discord of three-qubit Bell diagonal states and investigate the dynamic behavior in Section 3. Lastly, we present a conclusion in Section 4.

[†]Corresponding author. E-mail: xiongchunhe@zju.edu.cn

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2. Geometric tripartite discord

2.1. Geometric discord of tripartite system

Let us first start by reviewing the original definition of discord, which is defined as

$$\delta^{a:b}(\rho^{ab}) = \min_{\Pi^a} \left[I(\rho^{ab}) - J^{a:b}(\rho^{ab}) \right], \tag{1}$$

where the minimum is taken over all rank one projective measurements, and $I(\rho_{ab}) := S(\rho^a) + S(\rho^b) - S(\rho^{ab})$, $J^{a:b}(\rho^{ab}) := S(\rho^b) - \sum p_i S(\rho_i^b)$ with $S(\rho) = -\mathrm{tr}\rho\log\rho$ the von Neumann entropy of a state ρ. The probability to obtain outcome i is given by $p_i = \mathrm{tr}(\Pi_i^a \rho^{ab})$, and the corresponding post-measurement state of the subsystem b is given by $\rho_i^b = \mathrm{tr}_a(\Pi_i^a \rho^{ab})/p_i$.

For tripartite systems, two local measurements will be necessary in order to destroy all the correlations. In general, each local successive measurement is conditionally related to the previous measurement, then the two-partite measurement is written as

$$\Pi_{jk}^{ab} = \Pi_j^a \otimes \Pi_{k|j}^b,$$

where a, b, and c label the three subsystems, Π_j^a is a von Neumann projection operator on the subsystem a, $\Pi_{k|j}^b$ is a projector on subsystem b, conditioned on the measurement outcome on a. These states with zero discord of tripartite system have the following form:[21]

$$\sigma_{cc} = \sum_{jk} p_j^a p_{k|j}^b |\alpha_j\rangle_a\langle\alpha_j| \otimes |\beta_{k|j}\rangle_b\langle\beta_{k|j}| \otimes \rho_{k|j}^c, \tag{2}$$

where $\{|\alpha_j\rangle_a\}_j$ is a set of orthogonal basis, and for each fixed k, $\{|\beta_{k|j}\rangle_b\}_k$ is also a set of orthogonal basis. We call the quantum states with zero discord classically correlated and denote all of the classically correlated states of the tripartite system by $\mathcal{C}_{a:b:c}$.

With $\mathcal{C}_{a:b:c}$, the geometric discord of tripartite state is defined as

$$D_{\mathrm{g}}^{a:b:c}(\rho) := \min_{\sigma\in\mathcal{C}_{a:b:c}} \left(1 - F^2(\rho,\sigma)\right),$$

where $F(\rho,\sigma) := \mathrm{tr}\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}}$ is the fidelity between state ρ and σ.[34] Obviously, D_{g} is faithful in $\mathcal{C}_{a:b:c}$, invariant under local unitary transformations, and non-increasing under local operation in subsystem c. Because of these nice properties, the distance is also used to quantify quantum coherence.[33] Similarly, as a function of fidelity, the Bures distance has been used to quantify entanglement[35] and bipartite discord.[29,36] In particular, the Bures distance of discord is proved to be closely related to quantum state discrimination.[29]

2.2. Pure state case

Next, let us consider the quantification for pure states on the tripartite system.

Lemma 1 For tripartite pure state $|\psi^{abc}\rangle$, it can be decomposed as

$$|\psi^{abc}\rangle = \sum_{jk} \sqrt{\mu_{jk}} |\psi_j^a\rangle |\psi_{k|j}^b\rangle |\psi_{k|j}^c\rangle, \tag{3}$$

where $\mu_{jk} = \mu_j \mu_{k|j}$.

Proof Assuming that the Schmidt decomposition of $|\psi^{abc}\rangle$ between subsystem a and bc is $|\psi^{abc}\rangle = \sum_j \sqrt{\mu_j}|\psi_j^a\rangle|\psi_j^{bc}\rangle$, and for each $|\psi_j^{bc}\rangle$, the Schmidt decomposition between b and c is $|\psi_j^{bc}\rangle = \sum_k \sqrt{\mu_{k|j}}|\psi_{k|j}^b\rangle|\psi_{k|j}^c\rangle$, then each $|\psi^{abc}\rangle$ can be decomposed as

$$|\psi^{abc}\rangle = \sum_{jk} \sqrt{\mu_{jk}} |\psi_j^a\rangle |\psi_{k|j}^b\rangle |\psi_{k|j}^c\rangle,$$

where $\mu_{jk} = \mu_j \mu_{k|j}$.

With Lemma 1, we can derive the following result.

Theorem 2 For pure state $|\psi^{abc}\rangle$ with state decomposition as Eq. (3), then the geometric discord is given by

$$D_{\mathrm{g}}(|\psi^{abc}\rangle) = 1 - \sum_j \mu_j \mu_{\max}^j, \tag{4}$$

where each $\mu_{\max}^j$ is the maximum of $\{\mu_{k|j}\}$.

Proof See Appendix A.

In the bipartite system, it is well-known that geometric discord is equivalent to geometric entanglement on pure states. However, we find that it is not true for tripartite systems.

Example 1 Consider the symmetric state of three-qubit systems as follows:[32]

$$|S(3,1)\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle),$$

then the maximal entanglement eigenvalue $\Lambda_{\max} = 2/3$ and the entanglement is

$$E_{\mathrm{g}}(|S(3,1)\rangle) = 1 - \Lambda_{\max}^2 = \frac{5}{9}.$$

On the other hand, since the Schmidt decomposition between party a and party bc is

$$|S(3,1)\rangle = \sqrt{\frac{2}{3}}|0\rangle\left(\frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|10\rangle\right) + \sqrt{\frac{1}{3}}|1\rangle|00\rangle,$$

we have

$$D_{\mathrm{g}}(|S(3,1)\rangle) = 1 - \left(\frac{1}{3} + \frac{1}{3}\right) = \frac{1}{3} < \frac{5}{9} = E_{\mathrm{g}}(|S(3,1)\rangle).$$

We can conclude that there exists a pure state of tripartite systems whose geometric discord is strictly less than geometric entanglement.

2.3. Mixed state case

Now, let us consider the mixed-state case. For bipartite state, Spehner and Orszag linked the Bures distance of discord to quantum state discrimination.[29] Let us consider the case of tripartite systems.

Theorem 3 For mixed state $\rho \in D(\mathcal{H}_{abc})$, the geometric discord is equivalent to the minimal error to discriminate a set of quantum states with von Neumann measurement, that is,

$$D_{\mathrm{g}}(\rho) = \min_{|\alpha_i\beta_{j|i}\rangle} P_{\mathrm{e}}^{\text{opt v.N}}\{(q_{ij},\rho_{ij})\},$$

where the probability $q_{ij} = \langle\alpha_i\beta_{j|i}|\mathrm{tr}_c[\rho]|\alpha_i\beta_{j|i}\rangle$ and the corresponding state $\rho_{ij} = q_{ij}^{-1}\sqrt{\rho}|\alpha_i\beta_{j|i}\rangle\langle\alpha_i\beta_{j|i}|\otimes I_3\sqrt{\rho}$. The symbol $P_{\mathrm{e}}^{\text{opt v.N}}$ means the optimal error probability to discriminate the states with von Neumann measurement.

Proof Firstly, the classically correlated state $\sigma_{cc} \in \mathcal{C}_{a:b:c}$ has the following form:

$$\sigma_{cc} = \sum_{ijk} p_{ijk}|\alpha_i\rangle\langle\alpha_i|\otimes|\beta_{j|i}\rangle\langle\beta_{j|i}|\otimes|\gamma_{k|ij}\rangle\langle\gamma_{k|ij}|,$$

therefore, for any ρ, the fidelity between them is

$$\begin{aligned}
F(\rho,\sigma_{cc}) &= \max_U \mathrm{tr}|U\sqrt{\rho}\sqrt{\sigma_{cc}}| \\
&= \max_{|\Phi_{ijk}\rangle}|\sum_{ijk}\sqrt{p_{ijk}}\langle\Phi_{ijk}|\sqrt{\rho}|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle| \\
&= \max_{|\Phi_{ijk}\rangle}\sum_{ijk}\sqrt{p_{ijk}}\langle\Phi_{ijk}|\sqrt{\rho}|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle, \\
&\le \max_{|\Phi_{ijk}\rangle}\sqrt{\sum_{ijk}|\langle\Phi_{ijk}|\sqrt{\rho}|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle|^2},
\end{aligned}$$

where $|\Phi_{ijk}\rangle = U^\dagger|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle$ and the equality in the third line will hold if we choose the suitable phase factors of $|\Phi_{ijk}\rangle$ such that $\langle\Phi_{ijk}|\sqrt{\rho}|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle \ge 0$. The inequality follows from the Cauchy–Schwarz inequality and the equality holds when

$$p_{ijk} = \frac{|\langle\Phi_{ijk}|\sqrt{\rho}|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle|^2}{\sum_{ijk}|\langle\Phi_{ijk}|\sqrt{\rho}|\alpha_i\beta_{j|i}\gamma_{k|ij}\rangle|^2}.$$

Furthermore, one has

$$F^2(\rho,\mathcal{C}_{a:b:c}) = \max_{|\psi_{k|ij}\rangle}\max_{|\gamma_{k|ij}\rangle}\sum_{ijk}|\langle\psi_{k|ij}|\gamma_{k|ij}\rangle|^2, \tag{5}$$

where $|\psi_{k|ij}\rangle = \langle\alpha_i\beta_{j|i}|\sqrt{\rho}|\Phi_{ijk}\rangle \in \mathcal{H}_c$. We proceed to evaluate $|\psi_{k|ij}\rangle$ and $|\Phi_{ijk}\rangle$. Let us fix ij and consider the orthogonal family of projectors of $\mathcal{H}_a$ of rank n_1 defined by

$$\Pi_{ij} = \sum_k |\Phi_{ijk}\rangle\langle\Phi_{ijk}|. \tag{6}$$

By using the Cauchy–Schwarz inequality, for fixed ij one has

$$\begin{aligned}
&\max_{\psi_{k|ij}}\sum_k|\langle\psi_{k|ij}|\gamma_{k|ij}\rangle|^2 \le \sum_k||\psi_{k|ij}||^2 \\
=&\mathrm{tr}[\Pi_{ij}\sqrt{\rho}|\alpha_i\rangle\langle\alpha_i|\otimes|\beta_{j|i}\rangle\langle\beta_{j|i}|\otimes I_c\sqrt{\rho}].
\end{aligned} \tag{7}$$

Note that Eq. (7) will be equality if the vectors $|\psi_{k|ij}\rangle$ are orthogonal for different ij's and each of them can be decomposed into the sum of product states. First, we show that the vectors $|\psi_{k|ij}\rangle$ are orthogonal provided that the $|\Phi_{ijk}\rangle$ are chosen appropriately. Actually, for an arbitrary orthonormal basis $|\Phi_{ijk}\rangle$ of $\mathcal{H}_{abc}$, let us consider the Hermitian matrix $S^{(ij)}$ with coefficients given by the scalar products $S^{(ij)}_{k,l} = \langle\psi_{k|ij}|\psi_{l|ij}\rangle$. Since $S^{(ij)}$ is a Hermitian matrix, one can find a unitary matrix $V^{(ij)}$ such that $(V^{(ij)})^\dagger S^{(ij)}V^{(ij)}$ is orthogonal in the first r_{ij} rows, where r_{ij} is the rank of $S^{(ij)}$. Let $|\tilde{\Phi}_{ijk}\rangle = \sum_l V^{(ij)}_{l,k}|\Phi_{ijl}\rangle$. Then $|\tilde{\Phi}_{ijk}\rangle$ is an orthonormal basis of $\mathcal{H}$ and $\sum_k|\tilde{\Phi}_{ijk}\rangle\langle\tilde{\Phi}_{ijk}| = \Pi_{ij}$. Moreover, the vectors $|\tilde{\psi}_{k|ij}\rangle = \sum_l V^{(ij)}_{l,k}|\psi_{l|ij}\rangle$ form an orthogonal set.

As a result, one finds

$$\begin{aligned}
&F^2(\rho,\mathcal{C}_{a:b:c}) \\
=&\max_{\Pi_{ij}}\max_{|\alpha_i\rangle,|\beta_{j|i}\rangle}\sum_{ij}\mathrm{tr}[\Pi_{ij}\sqrt{\rho}|\alpha_i\beta_{j|i}\rangle\langle\alpha_i\beta_{j|i}|\otimes I_c\sqrt{\rho}] \\
=&\max_{|\alpha_i\rangle,|\beta_{j|i}\rangle} P_{\mathrm{s}}^{\text{opt v.N}}(\{q_{ij},\rho_{ij}\}),
\end{aligned}$$

where the probability $q_{ij} = \langle\alpha_i\beta_{j|i}|\mathrm{tr}_c[\rho]|\alpha_i\beta_{j|i}\rangle$ and the corresponding state $\rho_{ij} = q_{ij}^{-1}\sqrt{\rho}|\alpha_i\beta_{j|i}\rangle\langle\alpha_i\beta_{j|i}|\otimes I_c\sqrt{\rho}$.

Furthermore, the geometric discord is given by

$$D_{\mathrm{g}}(\rho) = 1 - \max_{|\alpha_i\beta_{j|i}\rangle} P_{\mathrm{s}}^{\text{opt v.N}}\{(q_{ij},\rho_{ij})\}.$$

Noting that, if ρ is invertible, then $\{\rho_{ij}\}_{ij}$ will be linearly independent.[29] In sequence, the result in Ref. [37] shows that the POVM maximizing the success probability $P_{\mathrm{s}}(\rho_{ij},q_{ij})$ is a von Neumann measurement with projectors, which implies

$$D_{\mathrm{g}}(\rho) = P_{\mathrm{e}}^{\text{opt v.N}}(\{q_{ij},\rho_{ij}\}) = P_{\mathrm{e}}^{\text{opt}}(\{q_{ij},\rho_{ij}\}).$$

3. Three qubit Bell diagonal states and dynamics behavior

3.1. Three qubit Bell diagonal states

Let us calculate the geometric discord of the three-qubit Bell diagonal state, that is,

$$\rho_{abc} = \frac{1}{8}\Big(I + \sum_j c_j\sigma_j\otimes\sigma_j\otimes\sigma_j\Big), \tag{8}$$

whose matrix form in computation basis is of the form (B2).

Let us first consider the geometric discord between subsystem a and bc. Based on the relationship between bipartite state discrimination and bipartite geometric discord,[29] one has

$$\max_{\sigma\in\mathcal{C}_{a:bc}} F^2(\rho_{abc},\sigma) = \max_{|\alpha_i\rangle} P_{\mathrm{s}}^{\text{opt v.N}}(\{p_i,\rho_i\}),$$

where $\rho_i = p_i^{-1}\sqrt{\rho_{abc}}(|\alpha_i\rangle_a\langle\alpha_i|\otimes I_{bc})\sqrt{\rho_{abc}}$ and $p_i = \langle\alpha_i|\rho_a|\alpha_i\rangle$. Since subsystem a is a qubit, then the ensemble

$\{p_i,\rho_i\}$ contains only two states and the corresponding quantum state discrimination task is easy to handle. Actually, denote the optimal orthogonal projectors by Π_1 and $\Pi_2 = I-\Pi_1$, then

$$P_{\rm s}^{\{\Pi_i\}}(\{p_i,\rho_i\}) = p_1{\rm tr}(\Pi_1\rho_1)+p_2{\rm tr}((I-\Pi_1)\rho_2)$$
$$= \frac{1}{2}(1-{\rm tr}\Lambda)+{\rm tr}(\Pi_1\Lambda),$$

where $\Lambda = p_1\rho_1 - p_2\rho_2$. By using the minimax principle,[38] the maximum of ${\rm tr}(\Pi_1\Lambda)$ over all projectors Π_1 of rank 4 is equal to the sum of the 4 highest eigenvalues $\lambda_1 \geq \cdots \geq \lambda_4$ of the Hermitian matrix Λ.

With the optimal probability of quantum state discrimination of two states, we can obtain

$$D_{\rm g}^{a:bc}(\rho_{abc}) = \frac{1}{2}\left(1-\sqrt{1-||c||^2+c_{\max}^2}\right),$$

where $c_{\max} := \max\{|c_1|,|c_2|,|c_3|\}$. Furthermore, since the closest classical correlated state of the above equation is actually in $\mathcal{C}_{a:b:c}$ (see Appendix B), it holds

$$D_{\rm g}^{a:b:c}(\rho_{abc}) = D_{\rm g}^{a:bc}(\rho_{abc}) = \frac{1}{2}\left(1-\sqrt{1-||c||^2+c_{\max}^2}\right),$$

for each three-qubit Bell diagonal state ρ_{abc}.

3.2. Dynamic of geometric discord under local channels

The frozen correlation is an interesting phenomenon of bipartite quantum discord under the noisy environment.[39] To verify if such phenomena still exists in three-qubit systems, we consider that each qubit of the states ρ_{abc} in Eq. (B1) under the phase flip channel, with the Kraus operators $K_0 = {\rm diag}(\sqrt{1-p/2},\sqrt{1-p/2})$ and $K_1 = {\rm diag}(\sqrt{p/2},-\sqrt{p/2})$, where $p = 1-\exp(-\gamma t)$, and γ is the phase damping rate.

For the initial state of Eq. (B1), the time evolution of the total system under the phase flip channel is given by

$$\rho_{abc}(t) = \frac{1}{8}\left(I_{abc}+\sum_j c_j(t)\sigma_j\otimes\sigma_j\otimes\sigma_j\right),$$

where $c_1(t) = c_1\exp(-3\gamma t)$, $c_2(t) = c_2\exp(-3\gamma t)$ and $c_3(t) = c_3$. Then there are several cases that are given as follows:

(i) If $|c_3| \geq \{|c_1|,|c_2|\}$, then $D_{\rm g}^{a:b:c}(\rho_{abc}(t)) = (1/2)(1-\sqrt{1-(c_1^2+c_2^2)\exp(-6\gamma t)})$ will decay to zero as t tends to infinity.

(ii) If $|c_2| \geq |c_1| \geq |c_3|$, then $D_{\rm g}^{a:b:c}(\rho_{abc}(t)) = (1/2)(1-\sqrt{1-c_3^2-c_1^2\exp(-6\gamma t)})$ when $t \leq (\ln|c_2|-\ln|c_3|)/(3\gamma)$, and the discord transform to $(1/2)(1-\sqrt{1-(c_1^2+c_2^2)\exp(-6\gamma t)})$ for $t > (\ln|c_2|-\ln|c_3|)/(3\gamma)$.

(iii) If $|c_2| \geq |c_3| \geq |c_1|$, then $D_{\rm g}^{a:b:c}(\rho_{abc}(t)) = (1/2)(1-\sqrt{1-c_3^2-c_1^2\exp(-6\gamma t)})$ when $t \leq (\ln|c_2|-\ln|c_3|)/3\gamma$, and the discord transform to $(1/2)(1-\sqrt{1-(c_1^2+c_2^2)\exp(-6\gamma t)})$ for $t > (\ln|c_2|-\ln|c_3|)/(3\gamma)$.

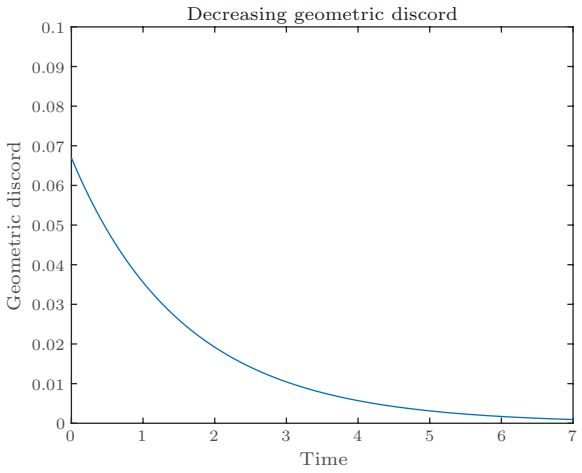


Fig. 1. The case of $c_1 = 0.3$, $c_2 = 0.4$, $c_3 = 0.8$, and $\gamma = 0.1$.

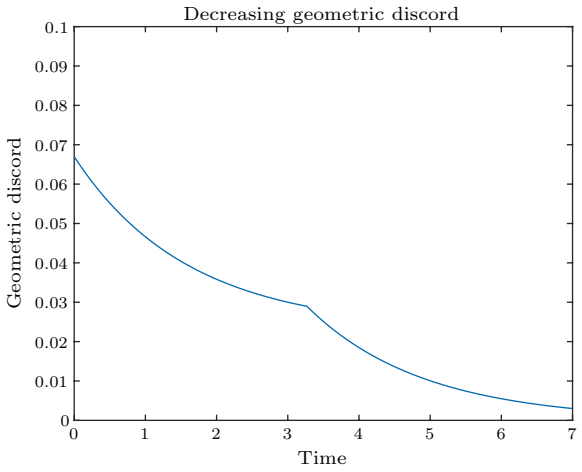


Fig. 2. The case of $c_1 = 0.4$, $c_2 = 0.8$, $c_3 = 0.3$, and $\gamma = 0.1$.

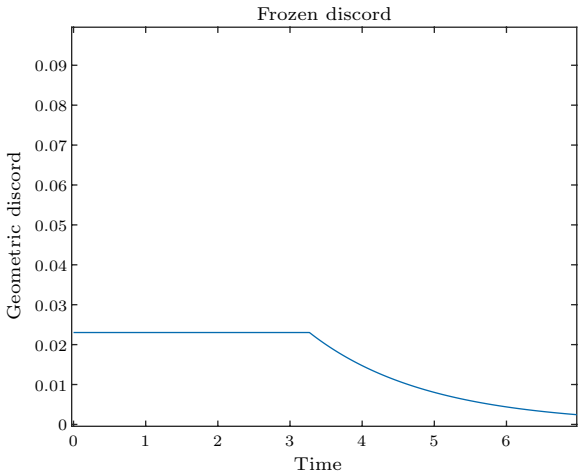


Fig. 3. The case of $c_1 = 0$, $c_2 = 0.8$, $c_3 = 0.3$, and $\gamma = 0.1$.

Example 2 Let $\gamma = 0.1$. For case i with $c_1 = 0.3$, $c_2 = 0.4$, $c_3 = 0.8$, the geometric discord decay to zero as t grows (see Fig. 1). For case ii with $c_1 = 0.4, c_2 = 0.8, c_3 = 0.3$, the geometric discord decay to zero as t grows and the speed increases when $t \geq \frac{\ln|c_2|-\ln|c_3|}{3\gamma}$ (see Fig. 2). For case iii with $c_1 = 0$, $c_2 = 0.8$, $c_3 = 0.3$, the geometric discord do not suffer from decay until $t \leq \frac{\ln|c_2|-\ln|c_3|}{3\gamma}$, which indicates that frozen

phenomenon exists for geometric discord on tripartite systems (see Fig. 3). This is not the case for original generalized discord revealed in Ref. [22].

4. Conclusion

In summary, we have obtained the analytic formula for geometric discord of tripartite systems and found that the geometric discord of pure state is not equal to the geometric entanglement for symmetric state of three-qubit systems, which implies that quantum discord and entanglement have a more complicated relationship in multipartite systems.

Furthermore, we provide an operational meaning for geometric discord of tripartite systems by linking it to quantum state discrimination, and calculate the geometric discord for generalized Bell diagonal states of three-qubit systems.

Lastly, we investigate the dynamic behavior of geometric discord of three-qubit systems under local decoherence and show that the frozen phenomenon exists for geometric discord of three-qubit systems.

Acknowledgments

Project supported by the National Natural Science Foundation of China (Grant No. 12201555) and China Postdoctoral Science Foundation (Grant No. 2021M702864).

Appendix A: Proof of Theorem 2

Proof Denote the classically correlated state

$$\sigma_{cc}=\sum_{jkl}p_{jkl}|\alpha_j\beta_{k|j}\gamma_{l|jk}\rangle_{abc}\langle\alpha_j\beta_{k|j}\gamma_{l|jk}|,$$

where $p_{jkl}\geq 0$ and $\sum p_{jkl}=1$. Moreover, $|\alpha_j\rangle$ is an orthogonal basis of $\mathcal{H}_a$, and for fixed j, $|\beta_{k|j}\rangle$ is an orthogonal basis of $\mathcal{H}_b$, and $|\alpha_j\beta_{k|j}\gamma_{l|jk}\rangle$ is an orthogonal basis of $\mathcal{H}_c$ for each jk. Then, the square of fidelity between $|\psi^{abc}\rangle$ and σ_{cc} is

$$\begin{aligned}&\max_{\sigma_{cc}\in\mathcal{C}_{a:b:c}}F^2(|\psi^{abc}\rangle\langle\psi^{abc}|,\sigma_{cc})\\&=\langle\psi^{abc}|\sigma_{cc}|\psi^{abc}\rangle\\&=\max_{p_{jkl},|\alpha_j\beta_{k|j}\gamma_{l|jk}\rangle}\sum_{jkl}p_{jkl}|\langle\alpha_j\beta_{k|j}\gamma_{l|jk}|\psi^{abc}\rangle|^2\\&\leq\max_{||\alpha||=||\beta||=||\gamma||=1}|\langle\alpha\otimes\beta\otimes\gamma|\psi^{abc}\rangle|^2,\end{aligned}$$

where the inequality follows from the fact that $\sum p_{jkl}=1$. Actually, denote $\mu^j_{\max}=\max\{\mu_{k|j}\}$ for each j, then

$$\begin{aligned}&|\langle\alpha\otimes\beta\otimes\gamma|\psi^{abc}\rangle|\\=&|\sum_{jk}\sqrt{\mu_j\mu_{k|j}}\langle\alpha|\psi^a_j\rangle\langle\beta|\psi^b_{k|j}\rangle\langle\gamma|\psi^c_{k|j}\rangle|\\\leq&\sum_j\sqrt{\mu_j}|\langle\alpha|\psi^a_j\rangle|\sum_k\sqrt{\mu_{k|j}}|\langle\beta|\psi^b_{k|j}\rangle\langle\gamma|\psi^c_{k|j}\rangle|\\\leq&\sum_j\sqrt{\mu_j}|\langle\alpha|\psi^a_j\rangle|\sqrt{\mu^j_{\max}}\sum_k|\langle\beta|\psi^b_{k|j}\rangle\langle\gamma|\psi^c_{k|j}\rangle|\\\leq&\sum_j\sqrt{\mu_j\mu^j_{\max}}|\langle\alpha|\psi^a_j\rangle|\sqrt{\sum_k|\langle\beta|\psi^b_{k|j}\rangle|^2}\sqrt{\sum_k|\langle\gamma|\psi^c_{k|j}\rangle|^2}\\\leq&\sqrt{\sum_j\mu_j\mu^j_{\max}}\sqrt{\sum_j|\langle\alpha|\psi^a_j\rangle|^2}=\sqrt{\sum_j\mu_j\mu^j_{\max}},\end{aligned}$$

where the last two inequalities follow the Cauchy–Schwartz inequality. Denote the Schmidt vector of each $\mu^j_{\max}$ by $|\psi^b_{\max|j}\rangle|\psi^c_{\max|j}\rangle$, then the closest classical correlated state is a pure state

$$|\phi\rangle^\star_{cc}=\sum_i\frac{\sqrt{\mu_i\mu^i_{\max}}}{\sqrt{\sum_j\mu_j\mu^j_{\max}}}|\psi^a_i\rangle|\psi^b_{\max|i}\rangle|\psi^c_{\max|i}\rangle.$$

Appendix B: Geometric discord of three-qubit Bell diagonal states

Let us calculate the geometric discord of the three-qubit Bell diagonal state, that is,

$$\rho_{abc}=\frac{1}{8}\Big(I+\sum_j c_j\sigma_j\otimes\sigma_j\otimes\sigma_j\Big),\tag{B1}$$

whose matrix form in computation basis is

$$\rho_{abc}=\frac{1}{8}\begin{pmatrix}1+c_3&0&0&0&0&0&0&c_1+\mathrm{i}c_2\\0&1-c_3&0&0&0&0&c_1-\mathrm{i}c_2&0\\0&0&1-c_3&0&0&c_1-\mathrm{i}c_2&0&0\\0&0&0&1+c_3&c_1+\mathrm{i}c_2&0&0&0\\0&0&0&c_1-\mathrm{i}c_2&1-c_3&0&0&0\\0&0&c_1+\mathrm{i}c_2&0&0&1+c_3&0&0\\0&c_1+\mathrm{i}c_2&0&0&0&0&1+c_3&0\\c_1-\mathrm{i}c_2&0&0&0&0&0&0&1-c_3\end{pmatrix},\tag{B2}$$

and the eigenvalues are $\lambda_{1(2)}=\frac{1}{8}(1\mp||c||)$. Moreover, the inverse of the above state is $\rho^{-1}_{abc}=\frac{8}{1-||c||^2}(I-\sum_j c_j\sigma_j\otimes\sigma_j\otimes\sigma_j)$.

As a result, if $||c||=1$, ρ_{abc} reduces to a pure state, and the geometric discord is given by Eq. (4). If $||c||\neq 1$, then we have $\rho_{abc}>0$ and

$$D_{\mathrm{g}}(\rho_{abc})=\max_{|\alpha_i\rangle}P^{\mathrm{opt}\ vN}_{\mathrm{e}}(\{\rho_i,q_i\})=\max_{|\alpha_i\rangle}P^{\mathrm{opt}}_{\mathrm{e}}(\{\rho_i,q_i\}).$$

Let us first consider the geometric discord between subsystems a and bc. Denote $|\alpha_{1(2)}\rangle\langle\alpha_{1(2)}| = (1/2)(I \pm \boldsymbol{u}\boldsymbol{\sigma})$, then

$$\begin{aligned} P_{\rm s}^{\{\Pi_i\}}(\{\rho_i, q_i\}) &= q_1 {\rm tr}(\Pi_1\rho_1) + q_2 {\rm tr}(\Pi_2\rho_2) \\ &= \frac{1}{2}(1 - {\rm tr}[\Lambda]) + {\rm tr}(\Pi_1\Lambda), \end{aligned}$$

where $\Lambda = \sqrt{\rho_{abc}}(|\alpha_1\rangle\langle\alpha_1| - |\alpha_2\rangle\langle\alpha_2|)\sqrt{\rho_{abc}}$. Based on the min-max principle,[38] the maximum of ${\rm tr}(\Pi_1\Lambda)$ over all projectors Π_1 of rank 4 is equal to the sum of the 4 highest eigenvalues $\lambda_1 \geq \cdots \geq \lambda_4$ of the Hermitian matrix Λ.

For general $|\alpha_{1(2)}\rangle$, one has $\Lambda_u = \sqrt{\rho_{abc}}(\boldsymbol{u}\boldsymbol{\sigma} \otimes I_4)\sqrt{\rho_{abc}}$, and the matrix form of $\Gamma_u = \rho_{abc}\sum_i u_i\sigma_i \otimes I_4$ is

$$\frac{1}{8}\begin{pmatrix} (1+c_3)u_3 & 0 & 0 & \xi\eta & (1+c_3)\eta^* & 0 & 0 & -\xi u_3 \\ 0 & (1-c_3)u_3 & \xi^*\eta & 0 & 0 & (1-c_3)\eta^* & -\xi^* u_3 & 0 \\ 0 & \xi^*\eta & (1-c_3)u_3 & 0 & 0 & -\xi^* u_3 & (1-c_3)\eta^* & 0 \\ \xi\eta & 0 & 0 & (1+c_3)u_3 & -\xi u_3 & 0 & 0 & (1+c_3)\eta^* \\ (1-c_3)\eta & 0 & 0 & \xi^* u_3 & -(1-c_3)u_3 & 0 & 0 & \xi^*\eta^* \\ 0 & (1+c_3)\eta & \xi u_3 & 0 & 0 & -(1+c_3)u_3 & \xi\eta^* & 0 \\ 0 & \xi u_3 & (1+c_3)\eta & 0 & 0 & \xi\eta^* & -(1+c_3)u_3 & 0 \\ \xi^* u_3 & 0 & 0 & (1-c_3)\eta & \xi^*\eta^* & 0 & 0 & -(1-c_3)u_3 \end{pmatrix},$$

where $\xi = c_1 + {\rm i}c_2$, $\eta = u_1 + {\rm i}u_2$. The eigenvalues of both Λ_u and Γ_u are the same, that is,

$$\begin{aligned} \lambda_{1(2)} &= \frac{1}{8}\big[-c_1u_1 - c_2u_2 - c_3u_3 \\ &\quad \pm \sqrt{(c_1u_1 + c_2u_2 + c_3u_3)^2 + 1 - ||c||^2}\big], \\ \lambda_{3(4)} &= \frac{1}{8}\big[-c_1u_1 + c_2u_2 + c_3u_3 \\ &\quad \pm \sqrt{(-c_1u_1 + c_2u_2 + c_3u_3)^2 + 1 - ||c||^2}\big], \\ \lambda_{5(6)} &= \frac{1}{8}\big[c_1u_1 - c_2u_2 + c_3u_3 \\ &\quad \pm \sqrt{(c_1u_1 - c_2u_2 + c_3u_3)^2 + 1 - ||c||^2}\big], \\ \lambda_{7(8)} &= \frac{1}{8}\big[c_1u_1 + c_2u_2 - c_3u_3 \\ &\quad \pm \sqrt{(c_1u_1 + c_2u_2 - c_3u_3)^2 + 1 - ||c||^2}\big]. \end{aligned}$$

Therefore, the fidelity between ρ_{abc} and classically correlated states on the bipartite system a and bc is

$$\begin{aligned} F^2(\rho_{abc}, \mathcal{C}_{a:bc}) = \frac{1}{2} + \frac{1}{8}\Big(&\sqrt{\Big(\sum_j c_j u_j\Big)^2 + 1 - ||c||^2} \\ &+ \sum_i \sqrt{\Big(\sum_j c_j u_j - 2c_i u_i\Big)^2 + 1 - ||c||^2}\Big). \end{aligned}$$

From Appendix C, one has

$$F^2(\rho_{abc}, \mathcal{C}_{a:bc}) = \frac{1}{2}(1 + \sqrt{1 - ||c||^2 + c_{\max}^2}),$$

where $c_{\max}$ has the maximal absolute value of $\{c_1, c_2, c_3\}$. As a result, the geometric discord between a and bc is

$$D_{\rm g}^{a:bc}(\rho) = \frac{1}{2}\Big(1 - \sqrt{1 - ||c||^2 + c_{\max}^2}\Big).$$

(i) Assume $c_{\max} = c_3$, then the optimal measurement is $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$. Furthermore, the eigenspaces of Γ_u are spanned by the following projections:

$$\begin{aligned} \Pi_{00} &= (1-t)|000\rangle\langle 000| + \frac{\xi}{2}|000\rangle\langle 111| \\ &\quad + \frac{\xi^*}{2}|111\rangle\langle 000| + t|111\rangle\langle 111|, \\ \Pi_{01} &= (1-t)|001\rangle\langle 001| + \frac{\xi^*}{2}|001\rangle\langle 110| \\ &\quad + \frac{\xi}{2}|110\rangle\langle 001| + t|110\rangle\langle 110|, \\ \Pi_{10} &= (1-t)|010\rangle\langle 010| + \frac{\xi^*}{2}|010\rangle\langle 101| \\ &\quad + \frac{\xi}{2}|101\rangle\langle 010| + t|101\rangle\langle 101|, \\ \Pi_{11} &= (1-t)|011\rangle\langle 011| + \frac{\xi}{2}|011\rangle\langle 100| \\ &\quad + \frac{\xi^*}{2}|100\rangle\langle 011| + t|100\rangle\langle 100|, \end{aligned}$$

where $t = \frac{c_1^2 + c_2^2}{2(1+\sqrt{1-c_1^2-c_2^2})}$ and $\xi = c_1 + {\rm i}c_2$, and the corresponding eigenspaces of Λ_u are $\hat{\Pi}_i = \frac{\sqrt{\rho}^{-1}\Pi_i\sqrt{\rho}^{-1}}{{\rm tr}[\rho^{-1}\Pi_i]}, i = 00, 01, 10, 11$. As a result, the optimal projection to discriminate $\{\rho_i, q_i\}$ is $\Psi_1^{\rm opt} = \sum_i \hat{\Pi}_i$ and $\Psi_2^{\rm opt} = I - \Psi_1$, and the closest classically correlated state of ρ_{abc} is[29]

$$\begin{aligned} \rho_{cc} &= \frac{1}{F^2(\rho)}\sum_i |\alpha_i\rangle^{\rm opt}\langle\alpha_i| \otimes \langle\alpha_i^{\rm opt}|\sqrt{\rho}\Psi_i^{\rm opt}\sqrt{\rho_{abc}}|\alpha_i^{\rm opt}\rangle \\ &= \frac{1}{F^2(\rho_{abc})}(|0\rangle\langle 0| \otimes \langle 0|\Psi_1^{\rm opt}|0\rangle + |1\rangle\langle 1| \otimes \langle 1|\Psi_2^{\rm opt}|1\rangle) \\ &= \frac{1}{F^2(\rho_{abc})}\Big[|0\rangle\langle 0| \otimes \langle 0|\sum_i \frac{\Pi_i}{{\rm tr}[\rho_{abc}^{-1}\Pi_i]}|0\rangle \\ &\quad + |1\rangle\langle 1| \otimes \langle 1|\Big(\rho_{abc} - \sum_i \frac{\Pi_i}{{\rm tr}[\rho_{abc}^{-1}\Pi_i]}\Big)|1\rangle\Big]. \end{aligned}$$

Denote $\pi_i = 1/{\rm tr}[\rho_{abc}^{-1}\Pi_i]$ and $\tau_{00} = \pi_{11}$, $\tau_{01} = \pi_{10}$, $\tau_{10} = \pi_{01}$, $\tau_{11} = \pi_{00}$, then one has

$$\rho_{cc} = \frac{1}{F^2(\rho_{abc})}\Big[|0\rangle\langle 0| \otimes \sum_i \pi_i|i\rangle\langle i| + |1\rangle\langle 1| \otimes (\langle 1|\rho_{abc}|1\rangle$$

$$-\sum_j \tau_j |j\rangle\langle j|)\Big],$$

where $i,j=00,01,10,11$. Since $\langle 1|\rho_{abc}|1\rangle=\frac{1}{8}(I\otimes I-c_3\sigma_3\otimes\sigma_3)$ is a diagonal state, then the closest correlated state ρ_{cc} is also a diagonal state, which means $\rho_{cc}\in\mathcal{C}_{a:b:c}$. In other words, for this kind of state,

$$D_{\rm g}^{a:b:c}(\rho)=D_{\rm g}^{a:bc}(\rho)=\frac{1}{2}\Big(1-\sqrt{1-c_1^2-c_2^2}\Big).$$

(ii) If $c_{\max}=c_1$, it can be verified that the unitary matrix $U=(1/2)(-I+{\rm i}\sigma)$ satisfies $U^\dagger\sigma_1U=\sigma_3$, $U^\dagger\sigma_2U=\sigma_1$, $U^\dagger\sigma_3U=\sigma_2$, therefore,

$$\begin{aligned}\rho'_{abc}:=&U_a^\dagger\otimes U_b^\dagger\otimes U_c^\dagger\rho_{abc}U_a\otimes U_b\otimes U_c\\=&\frac{1}{8}\Big(I+\sum_j c'_j\sigma_j\otimes\sigma_j\otimes\sigma_j\Big).\end{aligned}$$

Then, $c'_3=c_1$ is the maximal, and the local-unitary invariance of geometric discord implies

$$D_{\rm g}^{a:b:c}(\rho)=D_{\rm g}^{a:bc}(\rho)=\frac{1}{2}\Big(1-\sqrt{1-c_2^2-c_3^2}\Big).$$

(iii) If $c_{\max}=c_2$, it can be verified that the unitary matrix $U=(1/2)(I+{\rm i}\sigma)$ satisfies $U^\dagger\sigma_1U=\sigma_2$, $U^\dagger\sigma_2U=\sigma_3$, $U^\dagger\sigma_3U=\sigma_1$, therefore,

$$D_{\rm g}^{a:b:c}(\rho_{abc})=D_{\rm g}^{a:bc}(\rho_{abc})=\frac{1}{2}\Big(1-\sqrt{1-c_1^2-c_3^2}\Big).$$

(iv) If the maximal $c_{\max}$ is not unique, for example, $|c_1|=|c_2|>|c_3|$, then there are infinite optimal projections with $|\alpha_0\rangle=(1/2)(I+sc_1\sigma_1+(1-s)c_2\sigma_2)$, $s\in[0,1]$. As a result, the closest classically correlated state is not unique. Based on the above discussion, it also holds

$$\begin{aligned}D_{\rm g}^{a:b:c}(\rho_{abc})=&D_{\rm g}^{a:bc}(\rho_{abc})\\=&\frac{1}{2}\Big(1-\sqrt{1-||c||^2+c_{\max}^2}\Big).\end{aligned}\tag{B3}$$

Appendix C: Proof of the inequality

Let $f=f_1+f_2+f_3+f_4$ with

$$\begin{aligned}f_1&=\sqrt{(c_1u_1+c_2u_2+c_3u_3)^2+1-||c||^2},\\f_2&=\sqrt{(-c_1u_1+c_2u_2+c_3u_3)^2+1-||c||^2},\\f_3&=\sqrt{(c_1u_1-c_2u_2+c_3u_3)^2+1-||c||^2},\\f_4&=\sqrt{(c_1u_1+c_2u_2-c_3u_3)^2+1-||c||^2},\end{aligned}$$

the problem is to maximal f by choosing $\sum_i u_i^2=1$, where $\sum_i c_i^2\le 1$. By the Cauchy–Schwartz inequality, $g+h\le\sqrt{2(g^2+h^2)}$ for real numbers g and h, and the equality holds for $g=h$. As a result, we can obtain

$$f\le\sqrt{2}\Big(\sqrt{f_1^2+f_2^2}+\sqrt{f_3^2+f_4^2}\Big)\le 2\sqrt{f_1^2+f_2^2+f_3^2+f_4^2},$$

the equality holds for $f_1=f_2=f_3=f_4$, which means that

$$\begin{aligned}c_1u_1(c_2u_2+c_3u_3)=c_1u_1(c_2u_2-c_3u_3)=0,\\c_2u_2(c_1u_1+c_3u_3)=c_2u_2(c_1u_1-c_3u_3)=0,\\c_3u_3(c_1u_1+c_2u_2)=c_3u_3(c_1u_1-c_2u_2)=0.\end{aligned}$$

In conclusion, $f=4f_1=4\sqrt{1-||c||^2+c_{\max}^2}$, where $c_{\max}=\max\{|c_1|,|c_2|,|c_3|\}$.

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