From entanglement to discord: A perspective based on partial transposition

Liang-Liang Sun [*], Xiang Zhou, and Sixia Yu [†]
Department of Modern Physics and National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China

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Here, we show that partial transposition, which is initially introduced to study entanglement, can also inspire many results on quantum discord, including (I) a discord criterion of a spectrum invariant under partial transposition, stating that one state must contain discord if its spectrum is changed by the action of partial transposition, and (II) an approach to estimate the geometric quantum discord and the one-way deficit based on the change of the spectrum. To compare with entanglement theory, we also lower bound the geometric quantum entanglement and the entanglement of relative entropy. Thus, on one hand, we illustrate an approach to specify and estimate discord based on partial transposition. On the other hand, we show that, entanglement and discord, two basic notions of nonclassical correlations, can be placed on the same ground such that their interplay and distinction can be illustrated within a universal framework.

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I. INTRODUCTION

One distinctive feature of quantum theory is that quantum systems can demonstrate various forms of nonclassical correlations, which often find applications in quantum information science [1–4]. Entanglement was the first such notion to be known and then appreciated as a key resource in many quantum information tasks, such as quantum teleportation [5], cryptography [6], quantum algorithms [7–9], and metrology [10]. Entanglement was even believed to be responsible for why quantum resources can outperform classical ones. This belief started to change when quantum discord was discovered, which goes beyond entanglement and exists in a wide range of quantum states that may be separable. As entanglement, discord can also demonstrate quantum advantages in diversified tasks, such as mixed-state quantum computing [11,12], bounding distributed entanglement [13], remote state preparation [14], and quantum state merging [15,16]. Although it is known that entanglement must demonstrate quantum discord, the specification and quantification of these two basic properties are commonly seen as distinct subjects and follow different lines of research. One interesting question is whether or not these two properties can be characterized and quantified within a universal framework [17].

Much focus has been placed on entanglement and many powerful tools have been introduced [1,18]. One may concern whether these tools can be borrowed to specify and estimate the relatively less studied discord. For this purpose, we consider the primary tool of detecting entanglement, namely, the positive partial transpose (PPT) criterion [19,20], with which one state is certified to be entangled if its partially transposed density matrix presents a negative eigenvalue. This criterion also induces one computable entanglement quantifier, referred to as negativity [21,22], as the sum of negative eigenvalues in absolute values. Although the tool of PPT was related to discord, e.g., in $(2 \times n)$-dimensional system, all discord-free states belong to a subclass of PPT states, called strong PPT states [23], quantum discord is mainly detected with a discord witness [24,25]. To quantify discord, quite a few measures have been introduced [3,4]. Unfortunately, most of them are hard to compute. One exception is the geometric quantum discord (GQD) [26–28], which can be equivalently defined as the minimal disturbance under a projective measurement performed on one party, and thus can be computed via an optimization on the measurement [27–31].

In this paper, we show that many results on quantum discord can be inspired by the map of partial transposition. We first illustrate that the spectrum of discord-free states is invariant (up to relabeling of indices) under partial transposition. Therefore, the change of the spectrum indicates the presence of discord. We refer to this criterion as the spectrum invariant under partial transposition (SIPT) in contrast to the PPT in entanglement theory. Quantitatively, we find that the spectrum change implies a lower bound on the GQD and a discordlike quantity of a one-way deficit. For the sake of comparing discord and entanglement, we also provide lower bounds for the geometric quantum entanglement and the entanglement of relative entropy. Thus, a perspective based on partial transposition is provided, in which entanglement is specified and estimated based on the negative eigenvalues presented under the map, and in contrast, discord is specified and estimated based on the change of the spectrum.

II. PRELIMINARIES

Let us first briefly review some basic notions. One quantum state ρ_{AB} is said to be entangled if it cannot be written as the

[*]sun18@ustc.edu.cn
[†]yusixia@ustc.edu.cn

mixture of product states, namely,

$$\rho_{AB} = \sum_i f_i \cdot \rho_{i,A} \otimes \rho_{i,B}. \tag{1}$$

One can expand a general bipartite state in $N \otimes M$-dimensional Hilbert space, entangled or separable, in a chosen product basis as

$$\rho_{AB} = \sum_{i,j}^{N} \sum_{k,l}^{M} \rho_{ij,kl} |i\rangle\langle j|_A \cdot |k\rangle\langle l|_B. \tag{2}$$

Henceforth we shall omit the subscripts A, B where not introducing ambiguity. Given this decomposition, performing a partial transposition on Alice's side leads to

$$\rho^{\Gamma_A} = \sum_{i,j}^{N} \sum_{k,l}^{M} \rho_{ij,kl} |j\rangle\langle i| \cdot |k\rangle\langle l|. \tag{3}$$

The density matrix of any separable state is positive, and one state is certified to be entangled if it violates the PPT criterion. The PPT criterion also induces an entanglement quantifier of negativity as the sum of the negative spectrum in the absolute value as

$$\mathcal{N} := \frac{\|\rho^{\Gamma_A}\|_{\mathrm{tr}} - 1}{2}, \tag{4}$$

where $\|A\|_{\mathrm{tr}} = \mathrm{Tr}\sqrt{AA^{\dagger}}$.

Quantum discord (QD) is a typical quantum correlation referring to the phenomenon where a composite quantum system contains more information than the subsystems taken separably. By definition, one discord-free state ρ can be written in the form of

$$\rho = \sum_i f_i \cdot |i\rangle\langle i| \otimes \rho_i, \tag{5}$$

where $\{|i\rangle\}$ is one set of orthogonal bases. It is clear that an entangled state must contain discord, however, it is not necessary for the converse.

III. THE CRITERION OF SPECTRUM INVARIANT PARTIAL TRANSPOSITION

The partially transposed matrix depends on the party and basis on which it is performed. However, the spectrum of the partially transposed state is independent on them. We specify the spectrum of ρ by $\lambda^{\downarrow}(\rho)$, shortened as $\lambda^{\downarrow}$, where the elements are arranged in descending order, namely, $\lambda^{\downarrow} = (\lambda_1^{\downarrow}, \lambda_2^{\downarrow}, \ldots, \lambda_{M\cdot N}^{\downarrow})$ with $\lambda_i^{\downarrow} \geqslant \lambda_{i+1}^{\downarrow}, \forall i$. The fact that $\lambda^{\downarrow}(\rho^{\Gamma_A}) = \lambda^{\downarrow}(\rho^{\Gamma_B})$ can be illustrated via $\lambda^{\downarrow}(\rho^{\Gamma_A}) = \lambda^{\downarrow}([\rho^{\Gamma_A}]^{\Gamma}) = \lambda^{\downarrow}(\rho^{\Gamma_B})$, where Γ specifies the usual transposition acting on the joint system, which does not alter the state's spectrum. The different choices of the basis to perform a partial transposition can be captured with a local unitary operation U_A acting on Alice's side. The basis-independence feature can be illustrated as $\lambda^{\downarrow}[(\mathrm{U}_A\,\rho\,\mathrm{U}_A^{\dagger})^{\Gamma_A}] = \lambda^{\downarrow}[(\mathrm{U}_A\,\rho\,\mathrm{U}_A^{\dagger})^{\Gamma_B}] = \lambda^{\downarrow}[\mathrm{U}_A(\rho^{\Gamma_B})\,\mathrm{U}_A^{\dagger}] = \lambda^{\downarrow}[\rho^{\Gamma_B}] = \lambda^{\downarrow}[\rho^{\Gamma_A}]$. Therefore, the spectrum of the partially transposed state is determined solely by state ρ.

Considering a discord-free state $\rho = \sum_i f_i \cdot |i\rangle\langle i|_A \otimes \rho_{i,B}$, one can perform partial transposition with respect to the basis $\{|i\rangle_A\}$ without losing any generality. Clearly, the state is invariant under the operation. An immediate consequence is our criterion of SIPT.

Theorem 1. The spectrum of a discord-free state ρ is invariant under partial transposition:

$$\lambda^{\downarrow}(\rho) = \lambda^{\downarrow}(\rho^{\Gamma_A}). \tag{6}$$

Thus, from the perspective of partial transposition, a change of the spectrum under the map indicates a nontrivial discord. To certify quantum entanglement, the change needs to be large enough to ensure the presence of a negative spectrum.

To verify discord via Theorem 1, one can compute the spectrum of ρ and ρ^{Γ_A}, then make a statement after comparing them, or alteratively, by using the method based on the moments of matrix defined as $\Pi_n(\rho) := \mathrm{Tr}(\rho^n)$, noting that

$$\Pi_n(\rho) = \Pi_n(\rho^{\Gamma_A}), \forall n, \text{ if } \lambda^{\downarrow}(\rho) = \lambda^{\downarrow}(\rho^{\Gamma_A}). \tag{7}$$

Such a justification begins with the third moment as $\Pi_1(\rho) = \Pi_1(\rho^{\Gamma_A})$ and $\Pi_2(\rho) = \Pi_2(\rho^{\Gamma_A})$ are trivially satisfied, which is due to the fact that partial transposition is trace preserving and $\Pi_2(\rho) = \Pi_2(\rho^{\Gamma_A})$ is trivially satisfied. To deal with a state ρ of a $M \otimes N$-dimensional system, a sufficient judgment of Eq. (7) stops at most in the $(M \cdot N + 2)$th moment.

It is interesting to ask a question whether SIPT provides a sufficient and necessary justification of discord. Unfortunately, it is not the case as there are states containing discord while the spectrum is invariant under partial transposition, such as the X state having equal antidiagonal terms [32]. This is similar to the case in entanglement theory, where there are bound entangled states standing positivity under partial transposition, for which the PPT criterion fails.

IV. QUANTITATIVE ESTIMATION OF DISCORD AND DISCORDLIKE QUANTITY

Motivated by the fact that the negative spectrum of a partially transposed state can be used to quantify entanglement, we consider how the spectrum change under partial transposition quantitatively relates to quantum discord.

A. Lower bounds of GQD

GQD is defined as the minimum Hilbert-Schmidt distance or 2-norm between the state of interest ρ and the set of discord-free states specified by $\mathcal{D}$ [26–28],

$$D_{\mathrm{HS}}(\rho) = \min_{\varrho \in \mathcal{D}} \|\rho - \varrho\|_2^2. \tag{8}$$

For later use, we define the set of positive and normalized spectra as Ω: If a spectrum $r \in \Omega$, its elements are positive $r_i \geqslant 0, \forall i$ and normalized $\sum_i r_i = 1$. Clearly, if ϱ is a zero-discord state, i.e., $\varrho \in \mathcal{D}$, the spectrum of its partial transpose $\lambda^{\Gamma_A}(\varrho) \in \Omega$.

As preparation for estimating D_{HS}, we first provide an estimate of the quantity $\min_{r\in\Omega} \|\lambda'^{\downarrow} - r^{\downarrow}\|_2^2$ with $\lambda'^{\downarrow}$ specifying the spectrum of ρ^{Γ_A}, which is trivial if $\lambda'^{\downarrow} \in \Omega$. Otherwise, we have the following:

Lemma 1. An analytic lower bound on $\min_{r\in\Omega} \|\lambda'^{\downarrow} - r^{\downarrow}\|_2^2$ specified by $\mathfrak{L}(\lambda'^{\downarrow})$ is given as (see the Appendix for the proof)

$$\mathfrak{L}(\lambda'^{\downarrow}) := \min_{r\in\Omega} \|\lambda'^{\downarrow} - r^{\downarrow}\|_2^2 = \|\lambda'_{(\bar{n})}\|_2^2 + n\tau^2, \tag{9}$$

where $\lambda'^{\downarrow}$ is partitioned into two parts, namely, $\lambda'^{\downarrow} = \lambda'^{\downarrow}_{(n)} \bigcup \lambda'^{\downarrow}_{(\bar{n})}$ with $\lambda'^{\downarrow}_{(n)} = \{\lambda'^{\downarrow}_1, \dots, \lambda'^{\downarrow}_n\}$ and $\lambda'^{\downarrow}_{(\bar{n})} = \{\lambda'^{\downarrow}_{n+1}, \dots, \lambda'^{\downarrow}_{MN}\}$ with n specifying the minimal number such that $\tau := \frac{\sum_{i=1}^{n}\lambda'^{\downarrow}_i - 1}{n} \geqslant \lambda'^{\downarrow}_{n+1}$ and MN are the number of eigenvalues. The r achieving the minimum is $\{\lambda'^{\downarrow}_1 - \tau, \dots, \lambda'^{\downarrow}_n - \tau\} \bigcup \{0, \dots, 0\}$.

We then have the following:

Theorem 2. The GQD is lower bounded as

$$D_{\rm HS} \geqslant L^{\mathcal{D}} := \max\left\{L^D_{\rm PPT}, L^D_{\rm SIPT}\right\}, \tag{10}$$

where $L^D_{\rm SIPT} = \frac{\|\lambda^{\downarrow} - \lambda'^{\downarrow}\|_2^2}{4} + \mathfrak{L}(\frac{\lambda'^{\downarrow} + \lambda^{\downarrow}}{2})$ and $L^D_{\rm PPT} = \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-}$, λ specifies the spectrum of ρ, and $\mathcal{N}$ is negativity defined in Eq.(4).

By this theorem, one can estimate the GQD by the change of the spectrum of the partially transposed state or the negativity.

We first derive the lower bound specified by $L^D_{\rm SIPT}(\rho)$ on $D_{\rm HS}$ from the violation of the SIPT criterion, namely, using the change of the spectrum under partial transposition of the quantum state as

$$D_{\rm HS}(\rho) \geqslant \frac{\|\lambda^{\downarrow} - \lambda'^{\downarrow}\|_2^2}{4} + \mathfrak{L}\left(\frac{\lambda'^{\downarrow} + \lambda^{\downarrow}}{2}\right) := L^D_{\rm SIPT}(\rho). \tag{11}$$

We specify the closest free-discord state of ρ by $\rho_{\min}$ and its spectrum by $\lambda^{\downarrow}_{\min}$,

$$\begin{aligned}
2D_{\rm HS}(\rho) &= \|\rho - \rho_{\min}\|_2^2 + \left\|\rho^{\Gamma_A} - \rho^{\Gamma_A}_{\min}\right\|_2^2 \\
&\geqslant \|\lambda^{\downarrow} - \lambda^{\downarrow}_{\min}\|_2^2 + \|\lambda'^{\downarrow} - \lambda^{\downarrow}_{\min}\|_2^2 \\
&= \sum_i \left[\lambda^{\downarrow 2}_i + \lambda'^{\downarrow 2}_i + 2\lambda^{\downarrow 2}_{i,\min} - 2(\lambda^{\downarrow}_i + \lambda'^{\downarrow}_i)\lambda^{\downarrow}_{i,\min}\right] \\
&= \frac{\|\lambda^{\downarrow} - \lambda'^{\downarrow}\|_2^2}{2} + 2\left\|\frac{\lambda'^{\downarrow} + \lambda^{\downarrow}}{2} - \lambda^{\downarrow}_{\min}\right\|_2^2 \\
&\geqslant \frac{\|\lambda^{\downarrow} - \lambda'^{\downarrow}\|_2^2}{2} + 2\min_{r^{\downarrow}\in\Omega}\left\|\frac{\lambda'^{\downarrow} + \lambda^{\downarrow}}{2} - r^{\downarrow}\right\|_2^2 \\
&= \frac{\|\lambda^{\downarrow} - \lambda'^{\downarrow}\|_2^2}{2} + 2\mathfrak{L}\left(\frac{\lambda'^{\downarrow} + \lambda^{\downarrow}}{2}\right) \\
&:= 2L^D_{\rm SIPT}(\rho).
\end{aligned} \tag{12}$$

The first equality is due to 2-norm being invariant under partial transposition as it only involves the sum of the square modulus of matrix elements which is invariant under partial transposition. This observation implies $\|\rho - \varrho\|_2^2 = \|\rho^{\Gamma_A} - \varrho^{\Gamma_A}\|_2^2$. The first inequality follows from where, for any two states ρ and ϱ, it holds $\|\rho - \varrho\|_2^2 \geqslant \|\lambda^{\downarrow}(\rho) - \lambda^{\downarrow}(\varrho)\|_2^2$ [33]. The last equality is due to Lemma 1.

GQD is often related to the negativity of entanglement [34,35]. We can also provide a lower on GQD in terms of negativity (see the Appendix),

$$D_{\rm HS} \geqslant \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-} := L'^D_{\rm PPT}, \tag{13}$$

where we have specified the numbers of positive and negative elements of λ' by N_+ and N_-, respectively. The proof follows as

$$\begin{aligned}
D_{\rm HS} &= \min_{\varrho\in\mathcal{D}} \|\rho - \varrho\|_2^2 = \left\|\rho^{\Gamma_A} - \varrho^{\Gamma_A}_{\min}\right\|_2^2 \\
&\geqslant \|\lambda'^{\downarrow} - \lambda^{\downarrow}_{\min}\|_2^2 \\
&\geqslant \min_{r^{\downarrow}} \|\lambda'^{\downarrow} - r^{\downarrow}\|_2^2 \\
&= \mathfrak{L}(\lambda') := L'^D_{\rm PPT}, \qquad (14) \\
&\geqslant \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-} := L^D_{\rm PPT}. \qquad (15)
\end{aligned}$$

Equation (14) is due to the above Lemma, and the proof for Eq. (15) is left for the Appendix. Here, two inequivalent lower bounds, namely, $L^D_{\rm PPT} := \mathfrak{L}(\lambda')$ and $L^D_{\rm PPT} := \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-}$, are provided, which are nontrivial only if state ρ violates the PPT criterion, namely, $\mathcal{N} > 0$. $L^D_{\rm PPT}$ can be compared with the lower bound based on the entanglement witness reported in Refs. [34,35],

$$D_{\rm HS} \geqslant \frac{4\mathcal{N}^2}{d^2 - d} := L^D_{\rm WIT}, \tag{16}$$

where $d := \min\{M, N\}$. The $L^D_{\rm PPT}$ can be larger than $L^D_{\rm WIT}$, for instance, in the case where N_- is smaller than $\frac{d^2-d}{4}$. This is possible as there are entangled states having only one negative eigenvalue for any dimensional system while $\frac{d^2-d}{4} > 1$ when $d \geqslant 3$. It is worth stressing that some states may violate SIPT but do not violate PPT (for instance, bound entangled states), for which $L^D_{\rm SIPT}(\rho)$ is nonzero. One two-qutrit bound entangled state [36,37] is analyzed in the Appendix.

B. Comparison with previous results

To compare our lower bounds obtained above with known results, let us consider the Werner and isotropic states. For a $(d \times d)$-dimensional system, the Werner state reads

$$\rho_W = \frac{d - z}{d^3 - d} I_{AB} + \frac{dz - 1}{d^3 - d} F_{AB}, \quad z \in [-1, 1] \tag{17}$$

with $F_{AB} = \sum_{ij} |i\rangle\langle j| \otimes |j\rangle\langle i|$ the swapping operator. The negativity for the Werner state is

$$\mathcal{N}_W = \max\left\{0, -\frac{z}{d}\right\}, \tag{18}$$

so that it is entangled for $-1 < z < 0$. The exact value of GQD has been calculated to be [28,30]

$$D_{\rm HS}(\rho_W) = \frac{(dz - 1)^2}{d(d - 1)(d + 1)^2}. \tag{19}$$

The previous estimation of GQD, namely, Eq. (16), reads

$$L^D_{\rm WIT}(\rho_W) = \frac{4\mathcal{N}_W^2}{d^2 - d}.$$

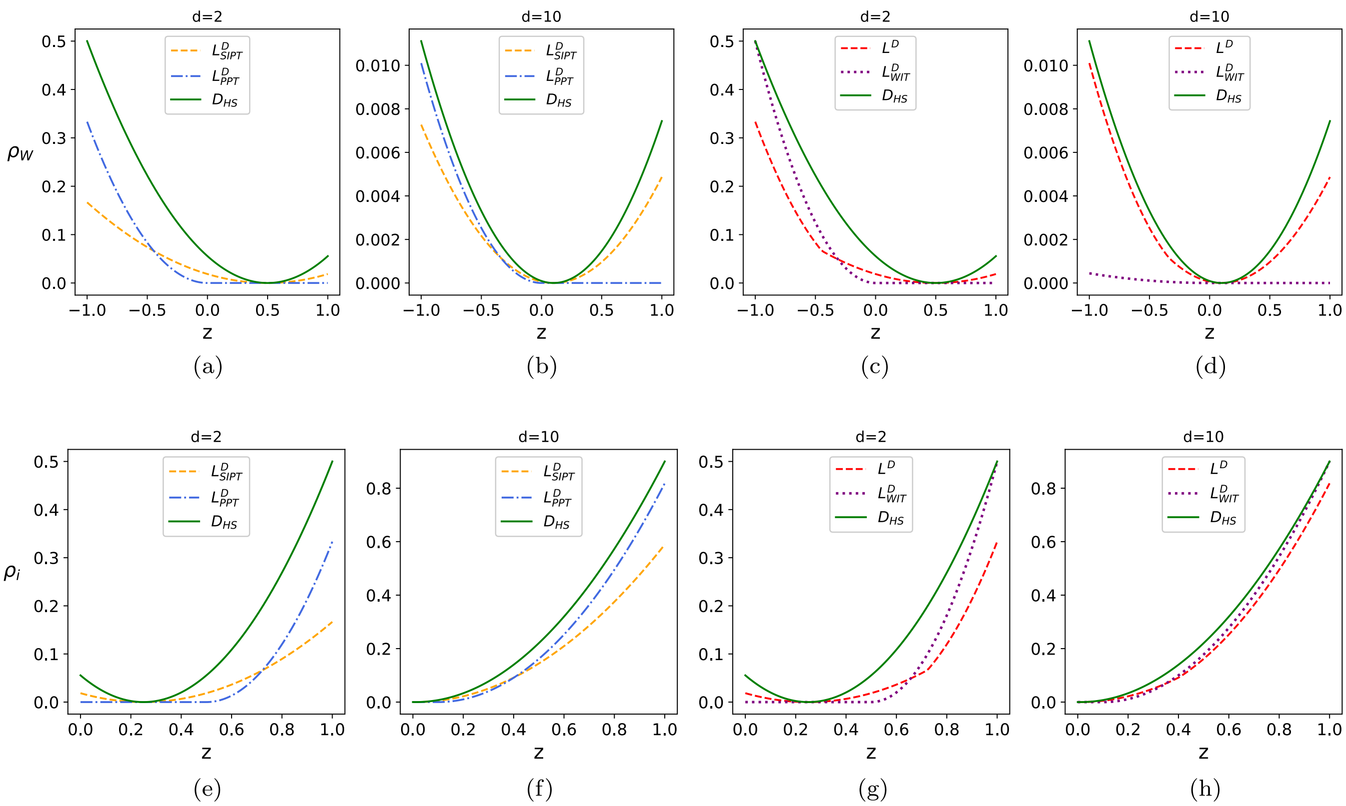

FIG. 1. Comparing the lower bounds on GQD of the Werner and isotropic states: In the first row, we compare our two lower bounds, namely, L^D_{PPT} and L^D_{SIPT}, with the exact value denoted by D_{HS} in (a) and (d) respectively for the cases of $d=2$ and $d=10$, and compare $L^D := \max\{L^D_{\mathrm{PPT}}, L^D_{\mathrm{SIPT}}\}$ with the previous result L^D_{WIT} and exact value in (c) and (d). The second row is for the comparisons when considering isotropic states.

Our bound is given by

$$L^D(\rho_W) = \max\left\{L^D_{\mathrm{SIPT}}(\rho_W), L^D_{\mathrm{PPT}}(\rho_W)\right\}$$

with (see the Appendix)

$$L^D_{\mathrm{SIPT}}(\rho_W) = \frac{1}{2}D_{\mathrm{HS}} + \begin{cases} 0, & -\frac{1}{d+2} \leqslant z, \\ \frac{[(d+2)z+1]^2}{4(d-1)(d+1)^3}, & z < -\frac{1}{d+2}, \end{cases}$$

$$L^D_{\mathrm{PPT}}(\rho_W) = \frac{d^2\mathcal{N}_W^2}{d^2-1}.$$

These two lower bounds are plotted in two diagrams in the top left-hand side in Fig. 1 for two dimensions $d = 2, 10$, together with the exact value. For comparison, we also plot our best lower bound, the previous bound Eq. (16) from the witness, and the exact value in the top right-hand side of Fig. 1.

For another example, we consider the $(d \times d)$-dimensional isotropic state

$$\rho_i = \frac{1-z}{d^2-1}I_{AB} + \frac{d^2z-1}{d^2-1}|\Psi\rangle\langle\Psi|, \quad z \in [0, 1], \tag{20}$$

where $|\Psi\rangle = \sum_i \frac{1}{\sqrt{d}}|ii\rangle$ is a maximally entangled state. As its negativity is

$$\mathcal{N}_i = \max\left\{0, \frac{dz-1}{2}\right\}, \tag{21}$$

the isotropic state ρ_i is entangled when $\frac{1}{d} < z \leqslant 1$. We also have the exact value of its GQD, which reads [28,30]

$$D_{\mathrm{HS}}(\rho_i) = \frac{(d^2z-1)^2}{d(d-1)(d+1)^2}. \tag{22}$$

With details given in the Appendix, our bounds in this case are

$$L^D_{\mathrm{SIPT}}(\rho_i) = \frac{1}{2}D_{\mathrm{HS}}(\rho_i) + \begin{cases} 0, & \text{otherwise}, \\ \frac{[2d+1-d(d+2)z]^2}{4(d-1)(d+1)^3}, & \frac{2d+1}{d(d+2)} < z, \end{cases}$$

$$L^D_{\mathrm{PPT}}(\rho_i) = \frac{4\mathcal{N}_i^2}{d^2-1}.$$

These bounds are plotted in two diagrams in the bottom left-hand side of Fig. 1 corresponding to $d = 2, 10$, together with the exact value. The comparison with known results is shown in the two diagrams in the bottom right-hand side of Fig. 1.

From a numerical comparison we see that for those states violating SIPT but not violating PPT, the lower bound L^D_{SIPT} is nontrivial while the other two lower bounds, namely, L^D_{PPT} and L^D_{WIT}, are trivial, as shown in Figs. 1(b) and 1(d) for $z > 0$. When the state violates the criterion of PPT, namely, $\mathcal{N} > 0$, L^D_{PPT} could be larger than L^D_{SIPT} [shown in Fig. 1(a) for $z < 0$ and Fig. 1(e)] and L_{WIT} [shown in Figs. 1(b) and 1(d)].

In the following, we show that such a lower bound also induces the estimate of another discordlike quantity, namely, the one-way deficit.

C. Lower-bound one-way deficit

A quantum work deficit [4,38] is introduced to capture the connection between thermodynamics and information and defined as the additional extractable information, or work from a bipartite quantum state when the two parties are in the same place as compared to the cases when they are in distant locations. Denoting the dephasing operation on Bob's side as $\{\Pi_B^i\}$ and $\varrho_{AB} = \sum_i \mathrm{I} \otimes \Pi_B^i \rho_{AB} \mathrm{I} \otimes \Pi_B^i$, the one-way deficit reads

$$\mathcal{WD}_B := \min_{\{\Pi_B^i\}} S(\rho_{AB} \| \varrho_{AB}), \tag{23}$$

where $S(\rho\|\varrho) := \mathrm{Tr}(\rho \ln \rho - \rho \ln \varrho)$ and the minimization is taken over all projective measurements performed on Bob's side. Clearly, ϱ_{AB} is a discord-free state for any $\{\Pi_B^i\}$. We thus have

$$\begin{aligned}\min_{\{\Pi_B^i\}} S(\rho_{AB}\|\varrho_{AB}) &\geqslant \min_{\varrho\in\Omega} S(\rho_{AB}\|\varrho) = S(\rho_{AB}\|\varrho_{\mathrm{min,re}}) \\ &\geqslant \frac{\|\rho - \varrho_{\mathrm{min,re}}\|_{\mathrm{tr}}^2}{2\ln 2} \geqslant \min_{\varrho'\in\Omega} \frac{\|\rho - \varrho'\|_{\mathrm{tr}}^2}{2\ln 2} \\ &= \frac{\|\rho - \varrho_{\mathrm{min,tr}}\|_{\mathrm{tr}}^2}{2\ln 2} \geqslant \frac{\|\rho - \varrho_{\mathrm{min,tr}}\|_{2}^2}{2\ln 2} \\ &\geqslant \frac{L^{\mathcal{D}}}{2\ln 2},\end{aligned} \tag{24}$$

where $\varrho_{\mathrm{min,re}}$ specifies the closest discord-free state of ρ with respect to the relative entropy, and $\rho_{\mathrm{min,tr}}$ specifies the closest state with respect to trace distance, and we have used the quantum Pinsker inequality $S(\rho\|\varrho) \geqslant \frac{1}{2\ln 2}\|\rho - \varrho\|_{\mathrm{tr}}^2$ in the second inequality and the norm inequality $\|\rho - \varrho\|_{\mathrm{tr}}^2 \geqslant 2\|\rho - \varrho\|_2^2$ [39] in the fourth inequality.

V. QUANTITATIVE ESTIMATION OF SOME ENTANGLEMENT MEASURES

Let us move to entanglement theory and estimate two entanglement measures that can be seen as the counterparts of the above ones in entanglement theory. The geometric geometric of entanglement is defined as the minimal Hilbert-Schmidt distance between the state of interest and the set of separable states specified by $\mathcal{S}$ [40] as

$$E_{\mathrm{HS}}(\rho) := \min_{\varrho\in\mathcal{S}} \|\rho - \varrho\|_2^2. \tag{25}$$

Note that separable states are PPT and 2-norm is invariant under partial transposition. By the same consideration in Eq. (14) as

$$\begin{aligned}E_{\mathrm{HS}}(\rho) &= \min_{\varrho\in\mathcal{S}} \|\rho^{\Gamma_A} - \varrho^{\Gamma_A}\|_2^2 \\ &\geqslant L^D_{\mathrm{PPT}} \geqslant \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-} \qquad (26) \\ &\geqslant \frac{4\mathcal{N}^2}{M\cdot N},\end{aligned} \tag{27}$$

we have used $N_- + N_+ \leqslant M \cdot N$ in the third inequality and the minimum is taken when $N_- = N_+ = \frac{M\cdot N}{2}$.

For a comparison to the one-way deficit, we now consider the relative entropy of entanglement. This measure serves as an upper bound for the entanglement of distillation, namely, the minimal number of singlets that are needed to build a single copy of the concerned state. By a similar derivation done in Eq. (24), we have

$$E_{\mathrm{re}} := \min_{\varrho\in\mathcal{S}} S(\rho\|\varrho) \geqslant \frac{L^D_{\mathrm{PPT}}}{2\ln 2}. \tag{28}$$

VI. CONCLUSION

Entanglement and discord are two typical quantum correlations that are generally studied separately. In this paper, we show that one can use the partial transposition, a primary tool of entanglement theory, to study discord, and many aspects of the two notions can be connected in a one-to-one correspondence. In contrast to the PPT in entanglement theory, we show that discord can be specified by the change of spectrum of the density matrix after partial transposition, which leads to a discord criterion of SIPT. Analogously to the entanglement measure of negativity, the change of the spectrum is shown to imply the estimation of the GQD and one-way deficit. We also estimate the geometric measure of quantum entanglement and the relative entropy of entanglement. In this way, we provide not only one perspective to investigate discord but also a hierarchical specification and quantitative estimation of entanglement and discord.

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APPENDIX

1. Proof of the Lemma

With λ' we specify the spectrum of the partially transposed state ρ, and $\lambda'^{\downarrow} = \lambda'^{\downarrow}_{(n)} \bigcup \lambda'^{\downarrow}_{(\bar{n})}$ with $\lambda'^{\downarrow}_{(n)} = \{\lambda'^{\downarrow}_1, \dots, \lambda'^{\downarrow}_n\}$ and $\lambda'^{\downarrow}_{(\bar{n})} = \{\lambda'^{\downarrow}_{n+1}, \dots, \lambda'^{\downarrow}_{N\cdot M}\}$ where the subscript n denotes where the spectrum is partitioned. N_+ and N_- denote the number of positive and nonpositive elements of λ'. With Ω we specify the set of positive and normalized spectra, namely, if $r \in \Omega$, $\sum_i r_i = 1$ and $r_i \geqslant 0$, and $\Omega_\delta \subseteq \Omega$, if $r \in \Omega_\delta$, $\sum_{i\leqslant N_+} r_i = \delta < 1$. For later use, with n_δ we specify the minimum number such that $\tau_\delta := \frac{\sum_{i=1}^{n_\delta} \lambda'^{\downarrow}_i - \delta}{n_\delta} \geqslant \lambda'^{\downarrow}_{n_\delta+1}$. The notion n in the main text is n_1 here defined and τ is τ_1. Two properties of n_δ and τ_δ are given as follows.

(1) $\tau_\delta < \lambda'^{\downarrow}_{n_\delta}$: Otherwise, $\tau_\delta \geqslant \lambda'^{\downarrow}_{n_\delta}$, we have $\frac{\sum_{i=1}^{n_\delta-1} \lambda'^{\downarrow}_i - \delta}{n_\delta - 1} = \frac{n_\delta \tau_\delta - \lambda'_{n_\delta}}{n_\delta - 1} \geqslant \frac{(n_\delta - 1)\tau_\delta}{n_\delta - 1} \geqslant \lambda'^{\downarrow}_{n_\delta}$, implying that n_δ is not the minimum number as $n'_\delta = n_\delta - 1$ also ensures that $\frac{\sum_{i=1}^{n'_\delta} \lambda'^{\downarrow}_i - \delta}{n'_\delta} \geqslant \lambda'^{\downarrow}_{n'_\delta+1}$.

(2) $n_\delta \leqslant n_1$ if $\delta < 1$: For $\delta < 1$, one has $\frac{\sum_{i=1}^{n_1} \lambda'^{\downarrow}_i - \delta}{n_1} > \frac{\sum_{i=1}^{n_1} \lambda'^{\downarrow}_i - 1}{n_1} \geqslant \lambda'^{\downarrow}_{n_1+1}$, and one may find $n_\delta < n_1$ such that $\frac{\sum_{i=1}^{n_\delta} \lambda'^{\downarrow}_i - \delta}{n_\delta} \geqslant \lambda'^{\downarrow}_{n_\delta+1}$.

The proof of the Lemma consists of two parts. First, we show that the minimum value

$$f(\delta) := \min_{r\in\Omega_\delta} \|\lambda'^{\downarrow}_{(N_+)} - r^{\downarrow}_{(N_+)}\|_2^2$$

is achieved if its first part $r^{\downarrow}_{(N_+)} = \{r^{\downarrow}_i = \lambda'^{\downarrow}_i - \tau_\delta, \forall i : \lambda'^{\downarrow}_i \geqslant \tau_\delta; r^{\downarrow}_i = 0, \forall i : 0 < \lambda'^{\downarrow}_i < \tau_\delta\}$, and $f(\delta) > f(1)$. The former can be proved by considering another $\gamma \in \Omega_\delta, \neq r$. As $(\lambda'^{\downarrow}_i - r^{\downarrow}_i)^2 = \lambda'^{\downarrow 2}_i - 2\int_0^{r^{\downarrow}_i}(\lambda'_i - x_i)dx_i$, we have

$$\begin{aligned}
\|\lambda'^{\downarrow}_{(N_+)} - r^{\downarrow}_{(N_+)}\|_2^2 - \|\lambda'^{\downarrow}_{(N_+)} - \gamma^{\downarrow}_{(N_+)}\|_2^2 &= -2\sum_{i\leqslant N_+}\int_0^{r^{\downarrow}_i}(\lambda'^{\downarrow}_i - x_i)dx_i + 2\sum_{i\leqslant N_+}\int_0^{\gamma^{\downarrow}_i}(\lambda'^{\downarrow}_i - x_i)dx_i \\
&= -2\sum_{i|\gamma^{\downarrow}_i<r^{\downarrow}_i\leqslant N_+}\int_{\gamma^{\downarrow}_i}^{r^{\downarrow}_i}(\lambda'^{\downarrow}_i - x_i)dx_i + 2\sum_{i|r^{\downarrow}_i<\gamma^{\downarrow}_i\leqslant N_+}\int_{r^{\downarrow}_i}^{\gamma^{\downarrow}_i}(\lambda'^{\downarrow}_i - x_i)dy_i \\
&\leqslant -2\tau_\delta\sum_{i|\gamma^{\downarrow}_i<r^{\downarrow}_i}(r^{\downarrow}_i - \gamma^{\downarrow}_i) + 2\tau_\delta\sum_{i|r^{\downarrow}_i<\gamma^{\downarrow}_i}(\gamma^{\downarrow}_i - r^{\downarrow}_i) = 0 \\
&= 2\tau_\delta\sum_i(\gamma^{\downarrow}_i - r^{\downarrow}_i) = 2\tau_\delta(\delta - \delta) = 0,
\end{aligned} \tag{A1}$$

where we have used when $x_i \in [\gamma^{\downarrow}_i, r^{\downarrow}_i]$ and $r^{\downarrow}_i > \gamma^{\downarrow}_i \geqslant 0$, we have $\lambda'^{\downarrow}_i - x_i \geqslant \lambda'^{\downarrow}_i - r^{\downarrow}_i = \tau_\delta$, and $x_i \in [r_i, \gamma_i]$ and $r^{\downarrow}_i < \gamma^{\downarrow}_i$, $\lambda'^{\downarrow}_i - x_i \leqslant \lambda'^{\downarrow}_i - r^{\downarrow}_i \leqslant \tau_\delta$. Thus one has

$$f(\delta) = \sum_{i=n_\delta+1}^{N_+}\lambda'^2_i + n_\delta\tau_\delta^2 \tag{A2}$$

and

$$f(1) = \sum_{i=n_1+1}^{N_+}\lambda'^2_i + n_1\tau^2. \tag{A3}$$

We now prove $f(\delta) > f(1)$. When $n_\delta = n_1$, $f(\delta) > f(1)$ follows from $\tau < \tau_\delta$.

When $n_1 > n_\delta$, we have $n_1 \geqslant n_\delta + 1$ and $\lambda'^{\downarrow}_{n_\delta} > \tau_\delta \geqslant \lambda'_{n_\delta+1} \geqslant \lambda'_{n_1} \geqslant \tau$ (by the properties 1 and 2), so we then have

$$f(\delta) - f(1) = \sum_{n_\delta}^{n_1}\left(\lambda'^2_i - \tau^2\right) + n_\delta\left(\tau_\delta^2 - \tau^2\right) > 0. \tag{A4}$$

Thus we have proved that $\min_\delta f(\delta) = f(1) = \sum_{i=n_1+1}^{N_+}\lambda'^2_i + n_1\tau^2$.

Second, we prove that

$$\|\lambda'_{(\bar{N}_+)} - r_{(\bar{N}_+)}\|_2^2 \geqslant \sum_{i\geqslant N_+}\lambda'^2_i = \|\lambda'_{(\bar{N}_+)}\|_2^2.$$

This is straightforward as $\lambda'^{\downarrow}_{i>N_+} \leqslant 0$ while $r^{\downarrow}_{i>N_+} \geqslant 0$. Then we have

$$\begin{aligned}
\|\lambda'^{\downarrow} - r^{\downarrow}\|_2^2 &= \|\lambda'^{\downarrow}_{(N_+)} - r^{\downarrow}_{(N_+)}\|_2^2 + \|\lambda'^{\downarrow}_{(\bar{N}_+)} - r^{\downarrow}_{(\bar{N}_+)}\|_2^2 \\
&\geqslant f(1) + \|\lambda'_{(\bar{N}_+)}\|_2^2 = \sum_{i=n_1+1}^{MN}\lambda'^2_i + n\tau^2.
\end{aligned} \tag{A5}$$

The last inequality is saturated when $r^{\downarrow} = \{r^{\downarrow}_i = \lambda'^{\downarrow}_i - \tau, \forall i : \lambda'^{\downarrow}_i > \tau_1; r^{\downarrow}_i = 0 \quad \forall i : \lambda'^{\downarrow}_i \leqslant \tau\}$.

2. Proof of $L_{\mathrm{PPT}} \geqslant \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-}$

Let $r^{\downarrow}$ achieving $\min_{r\in\Omega}\|\lambda'^{\downarrow} - r^{\downarrow}\|$ when $r^{\downarrow} = \{r^{\downarrow}_1, \ldots, r^{\downarrow}_{N_+}\}\bigcup\{0, \ldots, 0\}$, so we have

$$\begin{aligned}
\|\lambda'^{\downarrow} - r^{\downarrow}\|_2^2 &= \|\lambda'^{\downarrow}_{(N_+)} - \lambda^{\downarrow}_{(N_+)}\|_2^2 + \|\lambda'^{\downarrow}_{(\bar{N}_+)} - r^{\downarrow}_{(\bar{N}_+)}\|_2^2 \\
&\geqslant \frac{\mathcal{N}^2}{N_+} + \frac{\mathcal{N}^2}{N_-},
\end{aligned} \tag{A6}$$

where $\mathcal{N} = -\sum_{i>N_+}\lambda'^{\downarrow}_i$ specifies negativity. By the convexity of $\|\cdot\|_2^2$ and $\sum_{i\leqslant N_+}\lambda'^{\downarrow}_i - r^{\downarrow}_i = 1 + \mathcal{N} - 1 = \mathcal{N}$ and $\sum_{i>N_+}\lambda'^{\downarrow}_i - r^{\downarrow}_i = -\mathcal{N}$, one has $\|\lambda'^{\downarrow}_{(N_+)} - r^{\downarrow}_{(N_+)}\|_2^2 \geqslant \frac{\mathcal{N}^2}{N_+}$ with the inequality being saturated when $\lambda'^{\downarrow}_i - r^{\downarrow}_i = \frac{\mathcal{N}}{N_+}$ for $i \leqslant N_+$, and $\|\lambda'^{\downarrow}_{(\bar{N}_+)}\|_2^2 \geqslant \frac{\mathcal{N}^2}{N_-}$ with the inequality saturated when $\lambda'^{\downarrow}_i = \lambda'^{\downarrow}_{i+1} = \cdots = \lambda'^{\downarrow}_{MN} = -\frac{\mathcal{N}}{N_-}$ for $i > N_+$.

3. Lower bounds for the GQD of the Werner state

The eigenvalues of ρ_W are

$$\lambda_i \in \left\{\frac{1\pm z}{d(d\pm 1)}\right\}$$

with multiplicity

$$d_\pm = \frac{d(d\pm 1)}{2}$$

while the eigenvalues of the partial transpose $\rho_W^{\Gamma_A}$ are $\lambda'_i = \frac{d-z}{d(d^2-1)}$ with multiplicity d^2-1 or $\lambda'_i = \frac{z}{d}$. In the case of $z \geqslant \frac{1}{d+2}$ the average $\frac{\lambda^{\downarrow}_i + \lambda'^{\downarrow}_i}{2}$ is non-negative so that $\mathfrak{L}(\frac{\lambda'^{\downarrow}+\lambda^{\downarrow}}{2}) = 0$ from which it follows

$$L_{\mathrm{SIPT}} = \frac{||\lambda'^{\downarrow} - \lambda^{\downarrow}||^2}{4} = \frac{D_{\mathrm{HS}}(\rho_W)}{2}.$$

In the case $z < -\frac{1}{d+2}$ there is a single negative value $\lambda_- := \frac{1+(d+2)z}{2d(d+1)}$ in the sequence $\frac{\lambda'^{\downarrow}+\lambda^{\downarrow}}{2}$ and it holds $n = d^2 - 1$ and

$\tau = -\lambda_-/(d^2-1)$ giving rise to the lower bound

$$L_{\mathrm{SIPT}} = \frac{D_{\mathrm{HS}}}{2} + \frac{d^2\lambda_-^2}{d^2-1}.$$

4. SIPT works for bound entangled states

Here, we provide a family of two-qutrit states containing many bound entangled states (we refer to Ref. [37] for details) as

$$\rho = |\phi_3\rangle\langle\phi_3| + b\sum_{k=0}^{2}|k, k\oplus 1\rangle\langle k, k\oplus 1| + c\sum_{k=0}^{2}|k, k\oplus 2\rangle\langle k, k\oplus 2|, \tag{A7}$$

where $|\phi_3\rangle \equiv \frac{\sqrt{3}}{3}\sum_{i=0}^{2}|ii\rangle$ and with respect to the constraint $a + 3(b + c) = 1$. There are three distinct eigenvalues for ρ as

$$\lambda = \{a, b, c\}.$$

The transposition of ρ also has three distinct eigenvalues as

$$\lambda' = \left\{\frac{a}{3}, \frac{1}{6}\left[1 - a \pm \sqrt{4a^2 + 9(b-c)^2}\right]\right\}.$$

Notably, the spectrum of ρ is changed by partial transposition even if they are positive. Then the L_{SIPT}^{D} is nontrivial.

5. Lower bounds for the GQD of the isotropic state

The eigenvalues of ρ_i are

$$\lambda_i \in \left\{\frac{1-z}{d^2-1}, z\right\}$$

with multiplicity $\{d^2-1, 1\}$ while the eigenvalues of its partial transpose are

$$\lambda_i' \in \left\{\frac{1+dz}{d(d+1)}, \frac{1-dz}{d(d-1)}\right\}$$

with multiplicity $\{d_+, d_-\}$. As the smallest value in the sequence $\frac{\lambda'^{\downarrow}+\lambda^{\downarrow}}{2}$ is

$$\lambda^* = \frac{2d+1-d(d+2)z}{2d(d^2-1)},$$

so that in the case of

$$z \leqslant \frac{2d+1}{d(d+2)}$$

we have $\mathfrak{L}(\frac{\lambda'^{\downarrow}+\lambda^{\downarrow}}{2}) = 0$, so that

$$L_{\mathrm{SIPT}} = \frac{||\lambda'^{\downarrow} - \lambda^{\downarrow}||^2}{4} = \frac{D_{\mathrm{HS}}(\rho_i)}{2},$$

otherwise we have

$$L_{\mathrm{SIPT}} = \frac{D_{\mathrm{HS}}(\rho_i)}{2} + \frac{d^2 d_-}{d_+}\lambda^{*2},$$

giving the desired results.

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