

Analytical progress on symmetric geometric discord: Measurement-based upper boundsAdam Miranowicz,^{1,*} Paweł Horodecki,^{2,3} Ravindra W. Chhajlany,¹ Jan Tuziemski,^{2,3} and Jan Sperling⁴¹*Faculty of Physics, Adam Mickiewicz University, PL-61-614 Poznań, Poland*²*Faculty of Applied Physics and Mathematics, Technical University of Gdańsk, PL-80-952 Gdańsk, Poland*³*National Quantum Information Centre of Gdańsk, PL-81-824 Sopot, Poland*⁴*Arbeitsgruppe Quantenoptik, Institut für Physik, Universität Rostock, D-18051 Rostock, Germany*

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Quantum correlations may be measured by means of the distance from the state to the subclass of states Ω having well-defined classical properties. In particular, a geometric measure of asymmetric discord [Dakić *et al.*, *Phys. Rev. Lett.* **105**, 190502 (2010)] was recently defined as the Hilbert-Schmidt distance from a given two-qubit state to the closest classical-quantum (CQ) correlated state. We analyze a geometric measure of symmetric discord defined as the Hilbert-Schmidt distance from a given state to the closest classical-classical (CC) correlated state. The optimal member of Ω is just a specially measured original state for both the CQ and CC discords. This implies that this measure is equal to the quantum deficit of postmeasurement purity. We discuss some general relations between the CC discords and explain why an analytical formula for the CC discord, contrary to the CQ discord, can hardly be found even for a general two-qubit state. Instead of such an exact formula, we find simple analytical-measurement-based upper bounds for the CC discord which, as we show, are tight and faithful in the case of two qubits and may serve as independent indicators of two-party quantum correlations. In particular, we propose an adaptive upper bound, which corresponds to the optimal states induced by single-party measurements: optimal measurement on one of the parties determines an optimal measurement on the other party. We discuss how to refine the adaptive upper bound by nonoptimal single-party measurements and by an iterative procedure which usually rapidly converges to the CC discord. We also raise the question of optimality of the symmetric measurements realizing the CC discord on symmetric states and give a partial answer for the qubit case.

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I. INTRODUCTION

Entanglement is a fundamental type of quantum correlation that has come to be seen as an important resource in quantum information (see, e.g., Ref. [1]). However, quantum mechanics supports other types of quantum correlations in composite systems, distinct from entanglement, such as so-called quantum discord [2,3], whose characterization is the topic of much current research (see the review in Ref. [4] and references therein). Quantum discord is an information-theoretic measure of correlations where quantum correlations are identified in terms of the difference of two classically equivalent definitions of mutual information [2,3] in a composite system. A different possible perspective on the quantumness of correlations is captured in terms of quantum deficit functions [5], i.e., differences between certain properties of a state before and after classical-type measurements are performed on it. One such important property is the optimal thermodynamic work that can be extracted from a state in scenarios of classical (local) measurement complemented by zero-, one-, and two-way classical communication between measuring parties [5] (a state is classical if the deficit is 0). While the two-way scenario is rather involved, the zero- and one-way quantum work deficits are simply equal to the so-called relative entropy of quantumness [6,7]—the minimal entropic “distance” measure to specific classes of classical-type states.

Distance measures to sets of states with only classical correlations are promising and, conceptually, simple ways

of identifying quantum correlations. Recently, e.g., Dakić *et al.* [8] introduced a geometric measure of discord of a state as its minimal Hilbert-Schmidt distance metric to the set of states with null quantum discord [these states are one-side classical, or so-called classical-quantum (CQ) states of the form $\rho = \sum_i p_i P_i \otimes \rho_i$, where P_i 's are orthogonal projections with rank 1 and ρ_i 's are quantum states].

A natural, symmetric measure of quantum correlations can be obtained by constraining to a set of fully classical states, i.e., classical-classical (CC) states, which are diagonal in some product basis [9]. The optimization process required in the evaluation of (general) quantum correlation measures renders their calculation challenging. Here, we shall build on an equivalence between geometric measures of quantum discord and quantum deficits of purity to provide tight and faithful upper bounds on the symmetric geometric discord.

While, in general, geometric discord does not satisfy monotonicity properties (see Ref. [10]), which are usually expected for measures of quantum correlations, it may serve as a good lower bound for the relative entropy of discord [6,7] (remarkably different from the relative entropy of dissonance [7]). Moreover, geometric discord can be an indicator of quantum correlations.

The paper is organized as follows. In Sec. II, we provide some basic definitions and theorems for the discords in relation to quantum deficit. In Sec. III, we present our main result—the measurement-based upper bounds on the CC discord. In Sec. IV, we give explicit formulas for the upper bounds in the case of two qubits. In Sec. V, we present an analytical comparison of the discords and upper bounds for some classes of states. In Sec. VI, we present a few methods with

*miran@amu.edu.pl

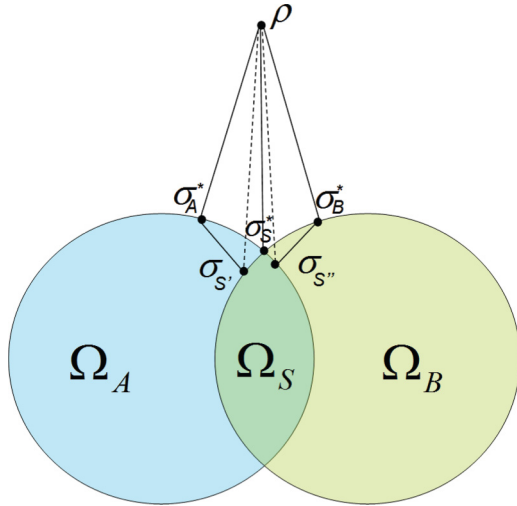


FIG. 1. (Color online) Venn-type diagram showing the sets of the CC ($\Omega_S = \Omega_{AB}$), CQ (Ω_A), and QC (Ω_B) states together with the closest states σ_i^* ($i = S, A, B$) according to the CC (D_S), CQ (D_A), and QC (D_B) geometric discords, respectively. States $\sigma_{S'}$ and $\sigma_{S''}$, which correspond to the adaptive upper bound $D_S^{(aub)}$, are the closest CC states for σ_A^* and σ_B^* , respectively. This is an intuitive graph, but more precisely, the point σ_A^* (σ_B^*) should be on the line between ρ and $\sigma_{S'}$ ($\sigma_{S''}$).

examples for optimization of the upper bounds. We conclude in Sec. VII.

II. BACKGROUND

We start by recalling the quantum zero-way and one-way work deficit [6]. Let the sets of states Ω_A , Ω_B , and Ω_S correspond to CQ, quantum-classical (QC), and CC states, respectively (see Fig. 1). Note that the set $\Omega_S \equiv \Omega_{AB} = \Omega_A \cap \Omega_B$ is obviously in the intersection of the other two sets, and any element of the intersection is in the set. Let $\tilde{\mathcal{M}}_X$ correspond to all von Neumann's measurements that are associated with the set Ω_X ($X = A, B, S$) in the following natural way, $\tilde{\mathcal{M}}_A = \mathcal{M}_A \otimes I_B$, $\tilde{\mathcal{M}}_B = I_A \otimes \mathcal{M}_B$, and $\tilde{\mathcal{M}}_S = \mathcal{M}_A \otimes \mathcal{M}_B$, where \mathcal{M}_A , \mathcal{M}_B are just local von Neumann's measurements performed by Alice and Bob in some orthonormal basis. We define the corresponding one-way ($X = A$ or B) and zero-way ($X = S$) quantum work deficits as

$$\Delta_X(\rho) = \min_{\tilde{\mathcal{M}}_X} S[\tilde{\mathcal{M}}_X(\rho)] - S(\rho), \quad (1)$$

where $S(\cdot)$ is the von Neumann entropy. The relative entropy of quantumness [6,7] is

$$D_X^R(\rho) = \min_{\sigma \in \Omega_X} S(\rho || \sigma). \quad (2)$$

There is an observation (see Sec. VID in Ref. [6]) that links the above quantities.

Observation 1. For any quantum state it holds that $\Delta_X(\rho) = D_X^R(\rho)$. Furthermore,

$$D_X^R(\rho) = \min_{\tilde{\mathcal{M}}_X} S(\rho || \tilde{\mathcal{M}}_X(\rho)), \quad (3)$$

which means that the optimal state σ_X^* , saturating the minimum in Eq. (2), comes from the optimal measurement in Eq. (1) of the examined state $\tilde{\mathcal{M}}_X^*(\rho) = \sigma_X^*$. A proof of Observation 1 is given in Appendix A.

Lemma 1. For any function f , any Hermitian operators F and G , and any von Neumann's measurement operation \mathcal{M} , we have $\text{tr}[Ff(\mathcal{M}(G))] = \text{tr}[\mathcal{M}(F)f(\mathcal{M}(G))]$. See Appendix A for a proof of this lemma.

Geometric discord as a purity deficit. Geometric measures of the discord of a state are also similarly completely determined by optimal measurements on it, as noted by Luo and Fu [11] and elucidated in the review by Modi *et al.* [4]. We formulate this property as follows.

Observation 2. Let $\sigma_X^* \in \Omega_X$ be an optimal state saturating the minimum for quantum geometric discord [8],

$$D_X(\rho) = \min_{\sigma \in \Omega_X} \|\rho - \sigma\|^2, \quad (4)$$

defined by the norm $\|A\| = \sqrt{\text{tr}(A^\dagger A)}$. Then it is realized by some optimal measurement $\tilde{\mathcal{M}}_X^*$ on ρ , i.e., $\sigma_X^* = \tilde{\mathcal{M}}_X^*(\rho)$, and satisfies the Pythagorean formula:

$$D_X(\rho) = \|\rho - \sigma_X^*\|^2 = \|\rho\|^2 - \|\sigma_X^*\|^2. \quad (5)$$

Thus, $\tilde{\mathcal{M}}_X^*$ maximizes the postmeasurement purity $\max_{\tilde{\mathcal{M}}_X} \text{tr}[(\tilde{\mathcal{M}}_X(\rho))^2]$, leading to the alternative formula:

$$\begin{aligned} D_X(\rho) &= \min_{\tilde{\mathcal{M}}_X} \|\rho - \tilde{\mathcal{M}}_X(\rho)\|^2 \\ &= \text{tr}(\rho^2) - \max_{\tilde{\mathcal{M}}_X} \text{tr}[(\tilde{\mathcal{M}}_X(\rho))^2]. \end{aligned} \quad (6)$$

See Appendix A for a proof of this observation. Note that choosing $X = A$ corresponds to one-side or asymmetric (CQ) geometric discord [8], while $X = S$ corresponds to the symmetric (CC) version [9]. The last form of Eq. (6) for geometric discord highlights an immediate analogy to the original deficit of Eq. (1) upon replacing the original von Neumann entropy $S(\rho) \equiv S_{\alpha=1}(\rho)$ with the Tsallis entropy $S_\alpha(\rho) = -\frac{1}{\alpha-1} \text{tr}(\rho^\alpha)$ (for $\alpha = 2$). We shall refer to the left-hand-side of Eq. (6) as a purity deficit, which is a special case of entropy-based deficits $\Delta_X^{\alpha,T} := \min_{\tilde{\mathcal{M}}_X} S_\alpha[\tilde{\mathcal{M}}_X(\rho)] - S_\alpha(\rho)$. For completeness, we provide a proof of Observation 2 in Appendix A (see Ref. [11] and Secs. II G and III B2 in Ref. [4] for alternate proofs).

Simple consequences. Observation 2 leads us to:

Lemma 2. For both the geometric discords D_X and the quantum discords D_X^R based on relative entropy, the following hold: (i) The CQ and QC discords bound the CC discord from below, $D_S(\rho) \geq \max[D_A(\rho), D_B(\rho)]$. (ii) We have simple implications $D_A(\rho) = 0 \Rightarrow D_S(\rho) = D_B(\rho)$ and $D_B(\rho) = 0 \Rightarrow D_S(\rho) = D_A(\rho)$, with the optimal measurement $\tilde{\mathcal{M}}_S^*$ being a product of the measurement realizing the respective CQ or QC discord and the one that commutes with the initially classical subsystem. (iii) $D_S(\rho) = 0 \Leftrightarrow D_A(\rho) = D_B(\rho) = 0$.

See Appendix A for a proof of this lemma.

III. MEASUREMENT-BASED UPPER BOUNDS ON THE CC DISCORD

We now turn to the main result of this paper. The explicit calculation of the geometric CC discord is, in general, difficult, as it involves optimization over all measurements of the

required form given by Eq. (6). In particular, the CC discord involves optimization over two sides of the states and so involves twice as many parameters as the CQ case. For the case of CQ-type discord, certain lower bounds have been found [11,12]. On the other hand, we show here that the measurement-based formula Eq. (6) can be fruitfully used to construct useful upper bounds on the CC discord. The conclusions of the present paragraph are valid for the geometric and relative entropy discords and for quantum deficit based on any quantum entropy S_α .

Let us recall that one refers to a bound as (i) *tight* if it coincides with the bounded quantity on some nontrivial subclass of states and (ii) *faithful* iff it vanishes on any state for which the bounded quantity vanishes.

A. Nonadaptive upper bound

An arbitrary measurement over two sides of the state is, by definition, an upper bound on discords:

$$D_S^{\sigma=\mathcal{M}_S(\rho)}(\rho) = S_\alpha(\sigma) - S_\alpha(\rho) = S_\alpha[\mathcal{M}_S(\rho)] - S_\alpha(\rho) \geq D_S(\rho), \quad (7)$$

where $\alpha \in [0, \infty]$. For ease of notation, let $\mathcal{M}_{X,\rho}^*$ denote the optimal measurement leading to the discord D_X of state ρ . The product of the two (CQ and QC) optimal measurements on state ρ leads to the first interesting bound, which we shall call the *simple product* (or *nonadaptive*) *bound*, for which the measurement-induced state is

$$\tilde{\sigma} = [\mathcal{M}_{A,\rho}^* \otimes \mathcal{M}_{B,\rho}^*](\rho) \quad (8)$$

in Eq. (7). This is one of the simplest kinds of bounds motivated by asking how the CC and CQ discords (or optimal measurements) are related. Indeed, we have noted in Lemma 2 that this type of bound trivially coincides with the CC discord in the special case where one of the CQ discords is null.

B. Adaptive upper bound

One can further introduce refined bounds that are *adaptive*, i.e., measurement on one of the parties is performed on the optimal state corresponding to the other party, as below:

$$\tilde{\sigma}' = [\mathcal{M}_{A,\rho}^* \otimes \mathcal{M}_{B,\mathcal{M}_{A,\rho}^*(\rho)}^*](\rho), \quad (9)$$

$$\tilde{\sigma}'' = [\mathcal{M}_{A,\mathcal{M}_{B,\rho}^*(\rho)}^* \otimes \mathcal{M}_{B,\rho}^*](\rho). \quad (10)$$

Note that part ii of Lemma 2 immediately leads to the following.

Fact 1. The bounds, (7), based on measurements, given by Eqs. (8)–(10), are faithful, so they may serve as independent indicators of two-side quantum correlations.

C. Iterative procedure for the adaptive upper bound

The adaptive form of Eqs. (9) and (10) allows for an iterative procedure that may be helpful in refining upper bound on the CC discord. Indeed, let X and X' be two opposite subsystems [i.e., $(X, X') = (A, B)$ or $(X, X') = (B, A)$]. Consider the following procedure.

Step 1. Choose the initial subsystem $X = X_0$ (either A or B), and initial measurement $\mathcal{M}_X = \mathcal{M}_{X_0}^*$.

Step 2. Iterate the following steps.

Step 2.1. Given input measurement \mathcal{M}_X on X calculate the output, i.e., optimal measurement $\mathcal{M}_{X',\mathcal{M}_X(\rho)}^*$ on the second system X' .

Step 2.2. Put X' in place of X and the output $\mathcal{M}_{X',\mathcal{M}_X(\rho)}^*$ as the input for Step 2.1; calculate its output again.

Step 2.3. Calculate the bound on the discord, given by Eq. (7), with the help of the measurement \mathcal{M}_S being the tensor product of the input-output pairs of measurements on X and X' presented in Steps 2.1 and 2.2; take the minimum of the two.

Step 2.4. Take the minimum of the output of Step 2.3 of two subsequent rounds.

Step 3. Stop the procedure if the outcome of Step 2.4 does not change.

IV. TWO-QUBIT CASE REVISITED

We now consider the case of the CC discord of two qubit states. The standard Bloch representation of any two-qubit state is

$$\rho = \frac{1}{4} \left(I \otimes I + \vec{x} \cdot \vec{\sigma} \otimes I + I \otimes \vec{y} \cdot \vec{\sigma} + \sum_{i,j=1}^3 T_{ij} \sigma_i \otimes \sigma_j \right) \equiv f(\vec{x}, \vec{y}, T) \equiv f(|x\rangle, |y\rangle, T), \quad (11)$$

where $\vec{\sigma} = [\sigma_1, \sigma_2, \sigma_3]$ is a vector of three Pauli matrices, T is the correlation matrix with elements $T_{ij} = \text{tr}[\rho(\sigma_i \otimes \sigma_j)]$, and $\vec{x} = [x_1, x_2, x_3]^T \equiv |x\rangle$ and $\vec{y} = [y_1, y_2, y_3]^T \equiv |y\rangle$ are the (column) local Bloch vectors with components $x_i = \text{tr}[\rho(\sigma_i \otimes I)]$ and $y_i = \text{tr}[\rho(I \otimes \sigma_i)]$.

A. CC vs CQ discords

We state the following simple

Fact 2. Any two-qubit state $\rho = f(|x\rangle, |y\rangle, T)$ is mapped into

$$\sigma_{(\hat{n})_A}(\rho) = f(|\hat{n}\rangle\langle\hat{n}|_x, |y\rangle, |\hat{n}\rangle\langle\hat{n}|_T), \quad (12)$$

$$\sigma_{(\hat{m})_B}(\rho) = f(|x\rangle, |\hat{m}\rangle\langle\hat{m}|_y, T|\hat{m}\rangle\langle\hat{m}|), \quad (13)$$

$$\sigma_{(\hat{n}, \hat{m})_S}(\rho) = f(|\hat{n}\rangle\langle\hat{n}|_x, |\hat{m}\rangle\langle\hat{m}|_y, |\hat{n}\rangle\langle\hat{n}|_T|\hat{m}\rangle\langle\hat{m}|) \quad (14)$$

by the measurement of (i) $\hat{n}\vec{\sigma}$ on the left qubits, (ii) $\hat{m}\vec{\sigma}$ on the right qubits, and (iii) $\hat{n}\vec{\sigma}$ and $\hat{m}\vec{\sigma}$ on the left and right qubits, respectively.

This follows from Lemma 1 and the fact that the diagonal of $\hat{n}\vec{\sigma}$ vanishes in the eigenbasis of any $\hat{n}'\vec{\sigma}$ with $\hat{n}' \perp \hat{n}$.

Observation 2 and Fact 2 directly lead to the analytical formula (see Ref. [8]) for the CQ discord D_A as follows:

$$\begin{aligned} D_A(\rho) &= \|\rho\|^2 - \|\sigma_A^*\|^2 \\ &= \text{tr}(\rho^2) - \max_{\hat{k}} (\text{tr}[\sigma_{(\hat{k})_A}(\rho)]^2) \\ &= \frac{1}{4} (\|\vec{x}\|^2 + \|T\|^2 - \max_{\hat{k}} [\hat{k}(|x\rangle\langle x| + TT^T)|\hat{k}\rangle]) \\ &= \frac{1}{4} (\|\vec{x}\|^2 + \|T\|^2 - k_x) = \frac{1}{4} (\text{tr}K_x - k_x), \end{aligned} \quad (15)$$

where \hat{k}_x is the largest eigenvalue of matrix $K_x = |x\rangle\langle x| + TT^T$. For clarity, we also write

$$\begin{aligned} 4\|\rho\|^2 &= 1 + \|\vec{x}\|^2 + \|\vec{y}\|^2 + \|T\|^2 \\ &\equiv 1 + \langle x|x\rangle + \langle y|y\rangle + \text{tr}(TT^T). \end{aligned} \quad (16)$$

However, Observation 2 yields more, *viz.*, the eigenvector $|\hat{k}_x\rangle$ corresponding to the eigenvalue k_x defines the optimal measurement of party A on ρ producing the closest CQ state σ , which (via Fact 2) is

$$\sigma_A^* = f(\langle \hat{k}_x | x \rangle |\hat{k}_x\rangle, |y\rangle, |\hat{k}_x\rangle \langle \hat{k}_x | T). \quad (17)$$

Analogously, one obtains $D_B(\rho) = \frac{1}{4}(\text{tr}K_y - k_y) = \frac{1}{4}(\|\vec{y}\|^2 + \|T\|^2 - k_y)$, where k_y is the largest eigenvalue of matrix $K_y = |y\rangle\langle y| + T^T T$ with eigenvector $|\hat{k}_y\rangle$. The closest QC state is

$$\sigma_B^* = f(|x\rangle, \langle \hat{k}_y | y \rangle |\hat{k}_y\rangle, T |\hat{k}_y\rangle \langle \hat{k}_y |). \quad (18)$$

Observation 2 also delivers the two-qubit CC discord,

$$D_S(\rho) = \|\rho\|^2 - \|\sigma_S^*\|^2, \quad (19)$$

where the norm of $\sigma_S^* = f(|x_S^*\rangle, |y_S^*\rangle, T_S^*)$ can be given in terms of some functions minimized solely over unit vectors $|\hat{x}_S\rangle$ (or, equivalently, $|\hat{y}_S\rangle$) as given in Appendix B. This is identical to the single Bloch-sphere optima obtained in Ref. [9].

B. Quest for symmetry of the optimal measurement for symmetric states

There is a general question whether the states symmetric under swapping subsystems always allow for a symmetric optimal measurement in the formula for the CC discord D_S . Here, we provide some partial results on this problem. Namely, there is a practical observation:

Theorem 1. Consider the two-qubit symmetric states ρ , i.e., the ones satisfying $\rho_{AB} = \rho_{BA}$ or, equivalently,

$$T = T^T, \quad (20)$$

$$|x\rangle = |y\rangle. \quad (21)$$

If the matrix T satisfies either $T \geq 0$ or $(-T) \geq 0$, then the optimal CC state σ_S^* and the corresponding measurement are symmetric, i.e., the optimal measurement basis is defined by some $|\hat{x}_S^*\rangle = |\hat{y}_S^*\rangle$.

Proof. Clearly, since $D_S(\rho) = \text{tr}(\rho^2) - \max_{\hat{x}_S, \hat{y}_S} \text{Tr}[\sigma_{(\hat{x}_S, \hat{y}_S)AB}(\rho)^2]$, we may write it in the form

$$D_S(\rho) = \text{tr}(\rho^2) - \frac{1}{4} \left[1 + \max_{\hat{x}_S, \hat{y}_S} u(\hat{x}_S, \hat{y}_S) \right], \quad (22)$$

where the function u is defined as

$$u(\hat{x}_S, \hat{y}_S) \equiv \langle \hat{x}_S | T | \hat{y}_S \rangle^2 + \langle \hat{x}_S | x \rangle^2 + \langle \hat{y}_S | y \rangle^2. \quad (23)$$

Following Theorem 1, it is not difficult to see that, by the symmetry of the initial state ρ , one has $|x\rangle = |y\rangle$. Now for $T > 0$ (all eigenvalues strictly positive) one defines the new scalar product $(x_S, y_S)_T = \langle \sqrt{T}x | \sqrt{T}y \rangle$, which defines also the norm $\|\vec{x}_S\|_T = \sqrt{(x_S, x_S)_T}$. Now, since $\|\vec{x}_S - \vec{y}_S\|_T^2 \geq 0$, for any pair of unit vectors $|\hat{x}_S\rangle$ and $|\hat{y}_S\rangle$ one has $\frac{1}{2}[u(\hat{x}_S, \hat{x}_S) + u(\hat{y}_S, \hat{y}_S)] \geq u(\hat{x}_S, \hat{y}_S)$, which means that the maximum in Eq. (22) is achieved by a symmetric pair ($|\hat{x}_S^*\rangle = |\hat{y}_S^*\rangle$). The proof for $(-T) > 0$ goes along the same lines. For the cases when $T \geq 0$ or $(-T) \geq 0$, i.e., where 0 eigenvalues are allowed, the statement follows from the continuity argument since here the argument realizing the maximum is continuous in parameters of the state.

We conjecture that in the case of the symmetric two-qubit states any minimum can be reached by symmetric measurement. We have performed both analytical and numerical

searches and found no counterexample to this hypothesis so far. However, for higher dimensions it may not be true since, as we know, there are numerous properties that break there.

C. Adaptive and nonadaptive upper bounds

We now turn to the upper bound for the CC discord. Using the adaptively measured states, given by Eqs. (9) and (10), we obtain the following upper bound from Eq. (7) for $\alpha = 2$.

Theorem. For an arbitrary two-qubit state the adaptive upper bound $D_S^{(\text{aub})}(\rho)$ for the CC discord can be given by

$$D_S^{(\text{aub})}(\rho) = \min_{i=S', S''} \|\rho - \sigma_i\|^2 = \|\rho\|^2 - \max_i \|\sigma_i\|^2, \quad (24)$$

where the CC states $\sigma_{S'}$ and $\sigma_{S''}$ are

$$\begin{aligned} \sigma_{S'} &= f(|x_{S'}\rangle, |y_{S'}\rangle, T_{S'}) = \sigma_{(\hat{k}_x, \hat{l}_y)_{S'}}(\rho) \\ &= f(\langle \hat{k}_x | x \rangle |\hat{k}_x\rangle, \langle \hat{l}_y | y \rangle |\hat{l}_y\rangle, |\hat{k}_x\rangle \langle \hat{k}_x | T | \hat{l}_y\rangle \langle \hat{l}_y |), \end{aligned} \quad (25)$$

$$\begin{aligned} \sigma_{S''} &= f(|x_{S''}\rangle, |y_{S''}\rangle, T_{S''}) = \sigma_{(\hat{l}_x, \hat{k}_y)_{S''}}(\rho) \\ &= f(\langle \hat{l}_x | x \rangle |\hat{l}_x\rangle, \langle \hat{k}_y | y \rangle |\hat{k}_y\rangle, \langle \hat{l}_x | T | \hat{k}_y\rangle \langle \hat{k}_y |), \end{aligned} \quad (26)$$

where $|\hat{k}_x\rangle$, $|\hat{k}_y\rangle$, $|\hat{l}_x\rangle$, and $|\hat{l}_y\rangle$ are the eigenvectors corresponding to the maximum eigenvalue of

$$K_x = \vec{x}\vec{x}^T + T T^T \equiv |x\rangle\langle x| + T T^T, \quad (27)$$

$$K_y = |y\rangle\langle y| + T^T T, \quad (28)$$

$$L_x = |x\rangle\langle x| + T |\hat{k}_y\rangle \langle \hat{k}_y | T^T, \quad (29)$$

$$L_y = |y\rangle\langle y| + T^T |\hat{k}_x\rangle \langle \hat{k}_x | T, \quad (30)$$

respectively. Note that $\sigma_{S'}$ in general differs from the σ_S^* used in Eq. (19). Explicitly, the norms are given by

$$\begin{aligned} \|\sigma_{S'}\|^2 &= \frac{1}{4}(1 + \|\vec{x}_{S'}\|^2 + \|\vec{y}_{S'}\|^2 + \|T_{S'}\|^2) \\ &= \frac{1}{4}(1 + \langle \hat{k}_x | x \rangle^2 + \langle \hat{l}_y | y \rangle^2 + \langle \hat{k}_x | T | \hat{l}_y \rangle^2), \end{aligned} \quad (31)$$

$$\begin{aligned} \|\sigma_{S''}\|^2 &= \frac{1}{4}(1 + \|\vec{x}_{S''}\|^2 + \|\vec{y}_{S''}\|^2 + \|T_{S''}\|^2) \\ &= \frac{1}{4}(1 + \langle \hat{l}_x | x \rangle^2 + \langle \hat{k}_y | y \rangle^2 + \langle \hat{l}_x | T | \hat{k}_y \rangle^2). \end{aligned} \quad (32)$$

Note that the measurement on direction $|\hat{l}_{x(y)}\rangle$ corresponds to the adaptive measurement $M_{A(B), \rho}^*$, since the correlation matrix of the optimally measured state on A (B) is, according to Eq. (17) [Eq. (18)], given by $|\hat{k}_x\rangle \langle \hat{k}_x | T (T |\hat{k}_y\rangle \langle \hat{k}_y |)$. Intuitively, the adaptive upper bound $D_S^{(\text{aub})}(\rho)$ can also be found by applying the following relation between the three discords valid for an arbitrary two-qubit state: If $D_A(\rho) = 0$, then $D_S(\rho) = D_B(\rho)$, and analogously, if $D_B(\rho) = 0$, then $D_S(\rho) = D_A(\rho)$ as given by Lemma 2. The bound can be constructed as follows (see Fig. 1):

$$D_S^{(\text{aub})}(\rho) = \min(D_{S'}, D_{S''}), \quad (33)$$

where

$$D_{S'} = \|\rho - \sigma_A^*\|^2 + \|\sigma_A^* - \sigma_{S'}\|^2 = \|\rho\|^2 - \|\sigma_{S'}\|^2, \quad (34)$$

$$D_{S''} = \|\rho - \sigma_B^*\|^2 + \|\sigma_B^* - \sigma_{S''}\|^2 = \|\rho\|^2 - \|\sigma_{S''}\|^2,$$

and $\sigma_{S'}$ and $\sigma_{S''}$, given by Eqs. (25) and (26), were calculated from the repeated application of Eqs. (17) and (18). It is also worth noting that

$$D_S^{(\text{aub})}(\rho) = 0 \Leftrightarrow D_S(\rho) = 0 \Leftrightarrow D_A(\rho) = D_B(\rho) = 0. \quad (35)$$

So, in particular, it means that $D_S^{(\text{aub})}(\rho)$ is nonzero iff ρ is not a CC state, and thus it may serve as an indicator of quantum correlations itself.

The nonadaptive upper bound (i.e., product bound) for a two-qubit state ρ can be given by

$$D_S^{(\text{nub})}(\rho) = \|\rho\|^2 - \|\sigma_{S_0}\|^2, \quad (36)$$

where

$$\sigma_{S_0} = f(\langle \hat{k}_x | x \rangle | \hat{k}_x \rangle, \langle \hat{k}_y | y \rangle | \hat{k}_y \rangle, | \hat{k}_x \rangle \langle \hat{k}_x | T | \hat{k}_y \rangle \langle \hat{k}_y |), \quad (37)$$

for which

$$\|\sigma_{S_0}\|^2 = \frac{1}{4}(1 + \langle \hat{k}_x | x \rangle^2 + \langle \hat{k}_y | y \rangle^2 + \langle \hat{k}_x | T | \hat{k}_y \rangle^2). \quad (38)$$

We have the following inequalities:

$$\max(D_A, D_B) \leq D_S \leq D_S^{(\text{aub})} \leq D_S^{(\text{nub})}, \quad (39)$$

where the last inequality can be immediately concluded by comparing Eqs. (31) and (32) with Eq. (38).

We note here that the adaptive bound, given by Eq. (24), is very effective. Indeed, the largest gap to the exact value $\Delta = D_S^{(\text{aub})}(\rho) - D_S(\rho)$, observed by us numerically, is just a few percent, and it is usually of the order 10^{-4} or 10^{-5} for randomly generated rank 4 states. Interestingly, we have also observed that it is exactly 0 for almost all classes of states for which there are known analytical expressions for D_S .

V. DISCORDS AND UPPER BOUNDS FOR SOME CLASSES OF STATES

A. Examples of a simple relation between discords and their upper bounds

Here, we present some examples of analytical calculation of the CQ and CC discords and the adaptive upper bound to show their relations.

Example 1. For (a) pure states, (b) Bell diagonal states, and, also, (c) states with both marginals vanishing, i.e., $|x\rangle = |y\rangle = 0$, it holds that

$$D_A = D_B = D_S = D_S^{(\text{aub})}. \quad (40)$$

For these states, D_S can be easily found by showing explicitly that the lower bound $D_A = D_B$ is equal to the upper bound $D_S^{(\text{aub})}$.

Example 2. For states with a maximally mixed single marginal, e.g., $|x\rangle = 0$ (and analogously for $|y\rangle = 0$), we have

$$\begin{aligned} 4\|\sigma_S^*\|^2 &= 1 + \underbrace{\langle x | \hat{x}_S^* \rangle^2}_{=0} + \langle y | \hat{y}_S^* \rangle^2 + \langle \hat{x}_S^* | T | \hat{y}_S^* \rangle^2 \\ &= 1 + \langle y | \hat{y}_S^* \rangle^2 + \langle \hat{x}_S^* | [T | \hat{y}_S^* \rangle \langle \hat{y}_S^* | T^T] | \hat{x}_S^* \rangle. \end{aligned} \quad (41)$$

Since $|\hat{x}_S^*\rangle$ maximizes $\|\sigma_S\|^2$, then it holds that

$$|\hat{x}_S^*\rangle = \frac{T |\hat{y}_S^*\rangle}{\sqrt{\langle \hat{y}_S^* | T^T T | \hat{y}_S^* \rangle}}. \quad (42)$$

Thus, we obtain

$$\begin{aligned} 4\|\sigma_S^*\|^2 &= 1 + \langle y | \hat{y}_S^* \rangle^2 + \left[\langle \hat{y}_S^* | T^T \left(\frac{T |\hat{y}_S^*\rangle}{\sqrt{\langle \hat{y}_S^* | T^T T | \hat{y}_S^* \rangle}} \right) \right]^2 \\ &= 1 + \langle y | \hat{y}_S^* \rangle^2 + \langle \hat{y}_S^* | T^T T | \hat{y}_S^* \rangle \\ &= 1 + \langle \hat{y}_S^* | (|y\rangle \langle y| + T^T T) | \hat{y}_S^* \rangle \\ &= 1 + \max[\text{eig}(|y\rangle \langle y| + T^T T)], \end{aligned} \quad (43)$$

so finally,

$$D_S = \frac{1}{4} \{ \langle y | y \rangle + \|T\|^2 - \max[\text{eig}(|y\rangle \langle y| + T^T T)] \}, \quad (44)$$

which is equal to the QC discord D_B and the adaptive upper bound $D_S^{(\text{aub})}$, which follows from a simple direct calculation. By performing an analogous derivation for $|y\rangle = 0$, we conclude that

$$\begin{aligned} |x\rangle = 0 &\Rightarrow D_A \leq D_B = D_S = D_S^{(\text{aub})}, \\ |y\rangle = 0 &\Rightarrow D_B \leq D_A = D_S = D_S^{(\text{aub})}. \end{aligned} \quad (45)$$

B. Example of a nontrivial relation between discords and their upper bounds

Here, we give an example of a nontrivial relation between CC, CQ, and QC discords and their tight upper bounds as shown in Figs. 2 and 3. Specifically, we study mixtures of Bell's state $|\Psi_\phi\rangle = [|01\rangle + \exp(i\phi)|10\rangle]/\sqrt{2}$ and $|00\rangle$ (i.e., state separable and orthogonal to $|\Psi_\phi\rangle$) as defined by Refs. [1,13]

$$\rho(p, \phi) = p|\Psi_\phi\rangle \langle \Psi_\phi| + (1-p)|00\rangle \langle 00| \quad (46)$$

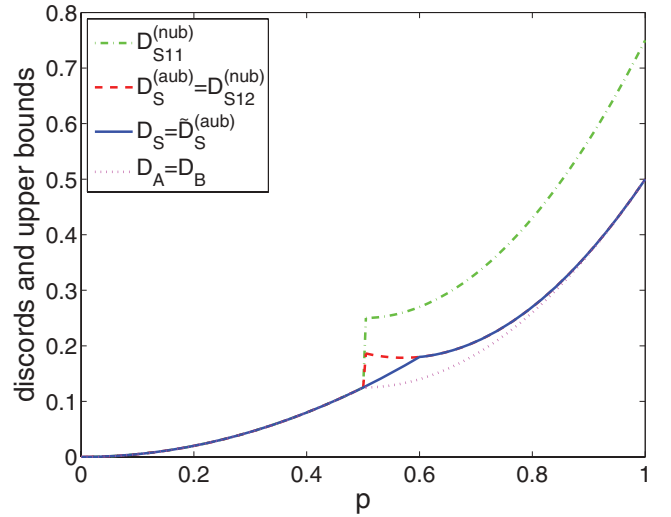


FIG. 2. (Color online) Geometric discords and their tight upper bounds for the state $\rho(p, \phi = \pi/2)$, given by Eq. (46), as a function of the parameter p : The CC discord, D_S [solid (blue) curve], and CQ and QC discords, $D_A = D_B$ [dotted (magenta) curve], together with the adaptive upper bound, $D_S^{(\text{aub})}$ [dashed (red) curve], and unoptimized nonadaptive upper bounds, $D_{S11}^{(\text{nub})} = D_{S22}^{(\text{nub})}$ [dot-dashed (green) curve]. We note that the optimized upper bound $\tilde{D}_S^{(\text{aub})} = D_S$ and $D_S^{(\text{aub})} = \tilde{D}_{S12}^{(\text{aub})} = \tilde{D}_{S21}^{(\text{aub})}$ for any p . All the upper bounds, except $\tilde{D}_S^{(\text{aub})}$, are discontinuous at $p = 1/2$, while the corresponding vertical lines are added for clarity only.

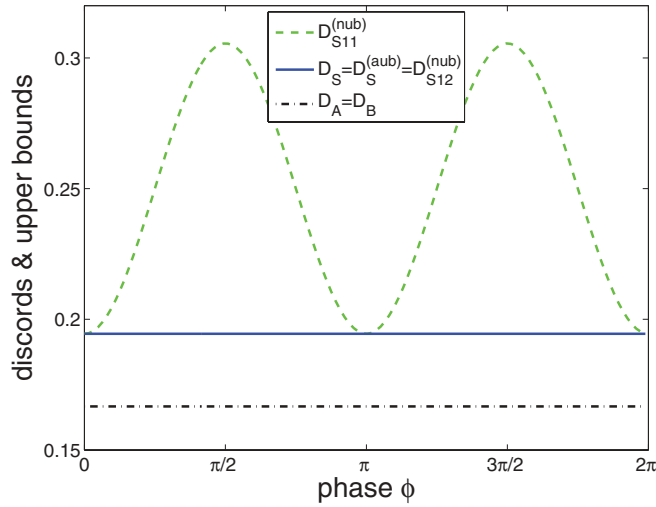


FIG. 3. (Color online) Same as Fig. 2, but for the state $\rho(p, \phi)$ as a function of phase ϕ for fixed $p = 2/3$.

for $0 \leq p \leq 1$. We find that the CC discord for these states is given by

$$D_S = \frac{1}{4} \min[2p^2, 7p^2 - 8p + 3] = \begin{cases} \frac{1}{2}p^2 & \text{if } p \leq \frac{3}{5}, \\ \frac{1}{4}(7p^2 - 8p + 3) & \text{otherwise.} \end{cases} \quad (47)$$

By contrast, the CQ and QC discords are given by

$$D_A = D_B = \frac{1}{2} \min(p^2, 3p^2 - 3p + 1) = \begin{cases} \frac{1}{2}p^2 & \text{if } p \leq \frac{1}{2}, \\ \frac{1}{2}(3p^2 - 3p + 1) & \text{otherwise.} \end{cases} \quad (48)$$

Some details of the calculation of the discords are given in Appendix C. Moreover, we find the adaptive upper bound for state $\rho(p, \phi)$ to be

$$D_S^{(\text{aub})} = D_{S'} = D_{S''} = \begin{cases} \frac{1}{2}p^2 & \text{if } p \leq \frac{1}{2}, \\ \frac{1}{4}(7p^2 - 8p + 3) & \text{otherwise.} \end{cases} \quad (49)$$

It is seen that $D_S^{(\text{aub})} = D_S$ for $0 \leq p \leq 1/2$ and $3/5 \leq p \leq 1$.

The nonadaptive and adaptive upper bounds for this state can be optimized as described in the next section. All these discords and upper bounds are shown in Fig. 2. In particular, we observe discontinuity of the upper bounds at $p = 1/2$. We find that the upper bound $D_S^{(\text{aub})}$ (and $D_S^{(\text{nub})}$) has two different limits:

$$\lim_{p \rightarrow 1/2^-} D_S^{(\text{aub})} = \frac{1}{8}, \quad \lim_{p \rightarrow 1/2^+} D_S^{(\text{aub})} = \frac{3}{16}. \quad (50)$$

By contrast, the asymmetric discords $D_A = D_B$, symmetric discord D_S , and optimized upper bounds $\tilde{D}_S^{(\text{aub})}$ (as discussed in the next subsection) are continuous functions of any p . Anyway, none of the discords has continuous first derivative in p .

VI. IMPROVED UPPER BOUNDS

A. Optimization over degenerate measurement outcomes

If the maximal eigenvalues of operators $K_{x,y}$ and/or $L_{x,y}$ are degenerate, then the adaptive and nonadaptive upper bounds can be optimized by taking the minimum for the eigenvectors corresponding to these maximum eigenvalues. Here, we describe this method in brief and give an example explaining Figs. 2 and 3.

First, it is worth recalling now a classic linear-algebraic theorem stating that eigenvectors of degenerate matrices are not necessarily orthogonal, but they can be made orthogonal and complete, as in the nondegenerate case, by applying Gram-Schmidt's orthogonalization procedure. This is possible by having the additional freedom of replacing the eigenvectors corresponding to a degenerate eigenvalue with their linear combinations.

Let us denote eigenvectors $|\hat{k}_x^{(i)}\rangle$ ($|\hat{k}_y^{(i)}\rangle$) corresponding to the same maximum degenerate eigenvalue of operator K_x (K_y), given by Eq. (27) [Eq. (28)]. Analogously, we denote eigenvectors $|\hat{l}_x^{(ij)}\rangle$ and $|\hat{l}_y^{(ij)}\rangle$ corresponding to the maximum degenerate eigenvalues of operators:

$$L_x^{(i)} = |x\rangle\langle x| + T |\hat{k}_y^{(i)}\rangle\langle \hat{k}_y^{(i)}| T^T, \quad (51)$$

$$L_y^{(i)} = |y\rangle\langle y| + T^T |\hat{k}_x^{(i)}\rangle\langle \hat{k}_x^{(i)}| T, \quad (52)$$

respectively. Thus, by applying these eigenvectors to Eqs. (31), (32), and (38), one can obtain norms $\|\sigma_{S_0}^{(ij)}\|^2$, $\|\sigma_{S'}^{(ij)}\|^2$, and $\|\sigma_{S''}^{(ij)}\|^2$, resulting in

$$D_{Sij}^{(\text{aub})} = \min_{r=S', S''} (\|\rho\|^2 - \|\sigma_r^{(ij)}\|^2), \quad (53)$$

$$D_{Sij}^{(\text{nub})} = \|\rho\|^2 - \|\sigma_{S_0}^{(ij)}\|^2. \quad (54)$$

Then the optimized adaptive and nonadaptive upper bounds are simply given by

$$D_S^{(\text{aub})} = \min_{i,j} D_{Sij}^{(\text{aub})}, \quad D_S^{(\text{nub})} = \min_{i,j} D_{Sij}^{(\text{nub})}, \quad (55)$$

respectively.

Example. Let us analyze again the state $\rho(p, \phi)$, given by Eq. (46). Operator K_x is degenerate, as given by Eq. (C2), so we can choose $|\hat{k}_x^{(i)}\rangle = |i\rangle$. Simple calculation shows that one can also choose $|\hat{l}_x^{(ij)}\rangle = |j\rangle$ for $i, j = 1, 2$. We find that the nonadaptive upper bound for $i = 1, 2$ is equal to

$$D_{Sii}^{(\text{nub})} = \begin{cases} \frac{1}{2}p^2 & \text{if } p \leq \frac{1}{2}, \\ \frac{1}{4}[p^2(\cos^2 \phi) - 8p + 3] & \text{otherwise,} \end{cases} \quad (56)$$

as shown by the dot-dashed (green) curves in Figs. 2 and 3. By contrast, $D_{S12}^{(\text{nub})} = D_{S21}^{(\text{nub})} = D_S^{(\text{aub})}$ as given by Eq. (49). So, finally,

$$D_S^{(\text{nub})} = \min(D_{S11}^{(\text{nub})}, D_{S12}^{(\text{nub})}) = D_{S12}^{(\text{nub})} = D_S^{(\text{aub})}, \quad (57)$$

as shown by the dashed (red) curve in Fig. 2. Note that such degenerate-value optimization for $D_S^{(\text{aub})}$ is unnecessary for this state.

By analyzing our formulas and Fig. 2, we can observe that (i) $D_A = D_B \neq D_S$ for $p \in (\frac{1}{2}, 1)$, (ii) $D_S^{(11)} \neq D_S$ for $p \in (\frac{1}{2}, 1)$ if $\phi \neq 0$, and (iii) $D_S^{(\text{aub})} = D_S^{(\text{nub})} = D_{S11}^{(\text{nub})}(\phi =$

$0) \neq D_S$ for $p \in (\frac{1}{2}, \frac{3}{5})$. We observe that the unoptimized nonadaptive bound can be much greater than the adaptive bound if $\phi \neq 0$ and $\frac{1}{2} < p \leq 1$, thus including the case for Bell's states ($p = 1$). In Fig. 3, we analyze the state $\rho(p, \phi)$ for $p = 2/3$. We observe here that (i) the symmetric discord [solid (blue) line] is equal to the adaptive upper bound, $D_S = D_S^{(aub)} = 7/36$; (ii) the asymmetric discords [dot-dashed (black) line] are $D_A = D_B = 1/6$; and (iii) the nonadaptive upper bound [dotted (red) curve] depends on ϕ as $D_{S11}^{(nub)} = D_S + \sin^2(\phi)/9$. Finally, we conclude that $D_S = D_S^{(aub)} = D_S^{(nub)} = D_{S12}^{(nub)} \leq D_{S11}^{(nub)}$ for $0 \leq p \leq 1/2$ and $3/5 \leq p \leq 1$. We see that the nonadaptive bounds without optimization, on the other hand, can fare rather badly as an estimator of the CC discord.

B. Optimization by locally nonoptimal measurements

Here, we suggest optimizing the adaptive upper bound by locally nonoptimal measurements, i.e., optimizing over all measurement outcomes corresponding to all (for $i, j = 1, 2, 3$) measurements of party A (B) on ρ producing (usually not the closest) state $\sigma_A^{(i)}$ ($\sigma_B^{(i)}$) and then measurements of party B (A) on this state producing the state $\sigma_{S'}^{(ij)}$ ($\sigma_{S''}^{(ij)}$). Thus, we describe the optimization of the adaptive upper bound over all eigenvectors of K_m and L_m ($m = x, y$) corresponding to all eigenvalues instead of taking only those eigenvectors corresponding to the maximum eigenvalues of these operators. This somehow counterintuitive method can in fact be efficient for the adaptive upper bound since L_m are constructed via eigenvectors of K_m . Clearly, the method cannot improve the nonadaptive upper bound, as the operators L_m are not used there.

The optimized adaptive upper bound $\tilde{D}_S^{(aub)}$ can be defined in analogy to Eq. (55) as follows:

$$\tilde{D}_S^{(aub)} = \min_{i,j=1,2,3} D_{Sij} = \|\rho\|^2 - \max_{r=S',S''} \max_{i,j=1,2,3} \|\sigma_r^{(ij)}\|^2. \tag{58}$$

By contrast to Eq. (55), the optimization is over 2×9 parameters for any state, independent of its degeneracy. It is convenient to form 3×3 matrices with elements $\|\sigma_r^{(ij)}\|^2$ as done in the following.

Example. Again, we analyze the state, given by Eq. (46). For each of the three eigenvectors $|\hat{k}_m^{(i)}\rangle$ of K_m (for $m = x, y$), given by Eq. (C2), we find three orthogonal eigenvectors $|\hat{l}_m^{(ij)}\rangle$, according to Eqs. (51) and (52). Then we can calculate $\|\sigma_{S'}^{(ij)}\|^2 = \|\sigma_{S''}^{(ij)}\|^2$ and create, e.g., the following matrices:

$$\left[\|\sigma_{S'}^{(ij)}\|^2 \right] = \begin{bmatrix} \frac{1}{4} & A & C \\ \frac{1}{4} & A & C \\ C & C & B \end{bmatrix} \quad \text{if } p \leq \frac{1}{2}, \tag{59}$$

$$\left[\|\sigma_{S'}^{(ij)}\|^2 \right] = \begin{bmatrix} C & C & B \\ \frac{1}{4} & C & A \\ \frac{1}{4} & C & A \end{bmatrix} \quad \text{if } p > \frac{1}{2}, \tag{60}$$

where $A = (1 + T_{11}^2)/4 = (1 + p^2)/4$, $B = (1 + 2x_3^2 + T_{33}^2)/4 = [1 + 2(1 - p)^2 + (1 - 2p)^2]/4$, and $C = (1 + x_3^2)/4 = [1 +$

$(1 - p)^2]/4$. Any order of the eigenvectors (and, thus, the order of the elements in the above matrices) can be applied. For convenience, we ordered them here by the value of the corresponding eigenvalues. Then we obtain

$$\tilde{D}_S^{(aub)} = \|\rho\|^2 - \max(A, B, C) = \begin{cases} \|\rho\|^2 - B & \text{if } p \leq \frac{3}{5}, \\ \|\rho\|^2 - A & \text{otherwise,} \end{cases}$$

where $\|\rho\|^2 = 2p(p - 1) + 1$ (see Appendix C). Thus, we conclude that the optimized upper bound is equal to the CC discord for any $p \in [0, 1]$:

$$\tilde{D}_S^{(aub)} = \frac{1}{4} \min[2p^2, 7p^2 - 8p + 3] = D_S. \tag{61}$$

in agreement with Eq. (47). Note that $A = B$ for $p = 3/5$ and $A = C$ for $p = 1/2$. So, $\tilde{D}_S^{(aub)}$ is continuous at $p = 1/2$, contrary to discontinuous $D_S^{(nub)}$ and $D_S^{(aub)}$ (compare broken and solid curves in Fig. 2).

In conclusion, for $\rho(p, \phi)$ with $1/2 < p < 3/5$ and any ϕ , we have the following inequalities:

$$D_A = D_B < D_S = \tilde{D}_S^{(aub)} < D_S^{(aub)} = D_S^{(nub)}. \tag{62}$$

This example demonstrates the usefulness of the optimization procedure by calculating the upper bounds for all possible measurements rather than only for those measurements corresponding to the maximum eigenvalues of K_m and L_m ($m = x, y$).

C. Iterative procedure for the adaptive upper bound

Here, we describe in detail the iterative procedure described in Sec. III C for the adaptive upper bound $D^{(aub)}$ and give some examples. The n th iteration of the adaptive upper bound, $D_S^{(aubn)}$, can be calculated as

$$D_S^{(aubn)} = \|\rho\|^2 - \max(\|\sigma_{S'}^{(n)}\|^2, \|\sigma_{S''}^{(n)}\|^2), \tag{63}$$

where our old $D_S^{(aub)}$ is just $D_S^{(aub0)}$ and

$$\begin{aligned} \|\sigma_{S'}^{(n)}\|^2 &= \frac{1}{4} (1 + \langle \hat{k}_x^{(n)} | x \rangle^2 + \langle \hat{l}_y^{(n)} | y \rangle^2 + \langle \hat{k}_x^{(n)} | T | \hat{l}_y^{(n)} \rangle^2), \\ \|\sigma_{S''}^{(n)}\|^2 &= \frac{1}{4} (1 + \langle \hat{l}_x^{(n)} | x \rangle^2 + \langle \hat{k}_y^{(n)} | y \rangle^2 + \langle \hat{l}_x^{(n)} | T | \hat{k}_y^{(n)} \rangle^2), \end{aligned}$$

where $|\hat{k}_x^{(n)}\rangle = |\hat{l}_x^{(n-1)}\rangle$ and $|\hat{k}_y^{(n)}\rangle = |\hat{l}_y^{(n-1)}\rangle$, while $|\hat{l}_x^{(n)}\rangle, |\hat{l}_y^{(n)}\rangle, |\hat{k}_x^{(0)}\rangle$, and $|\hat{k}_y^{(0)}\rangle$ are the eigenvectors corresponding to the maximum eigenvalues of

$$L_x^{(n)} = |x\rangle\langle x| + T |\hat{k}_y^{(n)}\rangle\langle \hat{k}_y^{(n)}| T^T, \tag{64}$$

$$L_y^{(n)} = |y\rangle\langle y| + T^T |\hat{k}_x^{(n)}\rangle\langle \hat{k}_x^{(n)}| T, \tag{65}$$

$$K_x^{(0)} \equiv K_x = |x\rangle\langle x| + T T^T, \tag{66}$$

$$K_y^{(0)} \equiv K_y = |y\rangle\langle y| + T^T T, \tag{67}$$

respectively. For randomly generated rank 4 states (thus, usually, with nondegenerate eigenvalues of $K_{x,y}^{(0)}$ and $L_{x,y}^{(0)}$), the procedure is usually effective, as can be shown by calculating the difference

$$\Delta_n \equiv D_S^{(aubn)} - D_S$$

between the adaptive upper bound after the n th iteration and the exact value of the CC discord.

TABLE I. Examples of application of the iteration procedure for the adaptive upper bound $D_S^{(\text{aub})}$ for the states given by Eqs. (68), (71), and (72) as described in Sec. VIC. The accuracy of the procedure is shown by the difference Δ_n between the adaptive upper bound after the n th iteration, $D_S^{(\text{aub } n)}$, and the exact value of the CC discord, D_S .

Iteration no.	$\Delta_n = D_S^{(\text{aub } n)} - D_S$		
	State (68)	State (71)	State (72)
0	8.85×10^{-4}	4.28×10^{-5}	1.71×10^{-4}
1	0	4.77×10^{-7}	8.00×10^{-6}
2	–	5.53×10^{-9}	3.90×10^{-7}
3	–	6.44×10^{-11}	1.92×10^{-8}
4	–	10^{-13}	9.50×10^{-10}
5	–	10^{-15}	4.69×10^{-11}

Let us discuss just a few examples.

Example 1. Let us analyze state $\rho = f(|x\rangle, |y\rangle, T)$, described by

$$|x\rangle = |y\rangle = \frac{1}{4}[1, 1, 1]^T, \quad T = \frac{1}{4}\text{diag}([1, -1, 0]), \quad (68)$$

First, we calculate the closest CQ state to be given in Bloch's representation as $\sigma_A^* = f(|x_A\rangle, |x\rangle, T_A)$, where

$$|x_A\rangle = t \begin{bmatrix} 1 + \sqrt{3} \\ 1 + \sqrt{3} \\ 2 \end{bmatrix}, \quad T_A = \begin{bmatrix} t & -t & 0 \\ t & -t & 0 \\ \frac{1}{8\sqrt{3}} & -\frac{1}{8\sqrt{3}} & 0 \end{bmatrix}, \quad (69)$$

with $t = (3 + \sqrt{3})/48$. Analogously, the closest QC state is $\sigma_B^* = f(|x\rangle, |x_A\rangle, T_A^T)$. Thus, the CQ and QC discords are given by $D_A = D_B = (3 - \sqrt{3})/64 = 0.0198\dots$. By contrast, the closest CC state is much simpler as given by $\sigma_S^* = f(|x\rangle, |x\rangle, Z)$, where Z is the 0 matrix. Thus, the CC discord is simply equal to $D_S = 1/32 = 0.031\dots$. The nonadaptive upper bound is $D_S^{(\text{nub})} = 5(3 - \sqrt{3})/192 = 0.033\dots$, which is obtained as the Hilbert-Schmidt distance from ρ to the CC state $\sigma_{S_0} = f(|x_A\rangle, |x_A\rangle, Z)$, where $|x_A\rangle$ is given in Eq. (69). The CC states, defined by Eqs. (25) and (26), are equal to $\sigma_{S'} = f(|x_A\rangle, |x\rangle, Z)$ and $\sigma_{S''} = f(|x\rangle, |x_A\rangle, Z)$, respectively. Thus, the (initial) adaptive upper bound is $D_S^{(\text{aub})} \equiv D_S^{(\text{aub } 0)} = (21 - 5\sqrt{3})/384 = 0.032\dots$. Our iteration procedure of the adaptive upper bounds converges to D_S already in the first iteration as $D_S^{(\text{aub } 1)} = 1/32$ (see Table I) since the CC state $\sigma_{S'}^{(1)} = \sigma_{S''}^{(1)} = f(|x\rangle, |x\rangle, Z) = \sigma_S$. Thus, for the analyzed state, we have the following inequalities:

$$D_A = D_B < D_S = D_S^{(\text{aub } 1)} < D_S^{(\text{aub})} < D_S^{(\text{nub})}. \quad (70)$$

Example 2. Another state is given by the same $|x\rangle = |y\rangle$ as in Eq. (68), but for

$$T = \frac{1}{4}\text{diag}([1, 1, 0]). \quad (71)$$

We find that the CQ and QC discords are $D_A = D_B = (3 - \sqrt{3})/64$ as in the former example, the CC discord is given by $D_S = 0.02322\dots$, the nonadaptive upper bound is $D_S^{(\text{nub})} = (28 - 11\sqrt{3})/384 = 0.02330\dots$, and the adaptive upper bound is $D_S^{(\text{aub})} = [57 - 11\sqrt{3} - \sqrt{6(62 + 3\sqrt{3})}]/768 = 0.02326\dots$. The iteration procedure converges to D_S but not as rapidly as in the former example (see Table I for details).

Example 3. Now, let us analyze a state with $|x\rangle \neq |y\rangle$ as defined by

$$|x\rangle = \frac{1}{6}[1, 2, 3]^T, \quad |y\rangle = \frac{6}{7}|x\rangle, \quad T = \frac{1}{8}\text{diag}([1, 2, 3]). \quad (72)$$

Analytical formulas for the discords and their upper bounds are quite lengthy for this state, so we give only their approximate numerical values. The QC discord is $D_B \approx 0.0259$, the CQ discord is $D_A \approx 0.0262$, the CC discord is $D_S \approx 0.0280$, the nonadaptive upper bound is $D_S^{(\text{nub})} \approx 0.0284$, and the adaptive upper bound is $D_S^{(\text{aub})} \approx 0.0281$. The adaptive upper bounds $D_S^{(\text{aub } n)}$ after the n th iteration are listed in Table I. In conclusion, we have the following inequalities:

$$D_B < D_A < D_S = D_S^{(\text{aub } 4)} - O(10^{-10}) < D_S^{(\text{aub})} < D_S^{(\text{nub})}. \quad (73)$$

All the above examples show how rapidly the iterations approach the correct values of the CC discord. Now, we give a counterexample.

Example 4. The iteration procedure fails, e.g., for the state, given by Eq. (46) for $1/2 < p < 3/5$ (see Fig. 2), as $\Delta_n = \Delta_0 > 0$ for $n = 1, 2, \dots$. In general, this can be explained as follows:

Criterion. If, for a given two-qubit state, the n th iteration of the adaptive upper bound $D_S^{(\text{aub } n)}$ (in particular, for $n = 0$) differs from the CC discord D_S , and $|\hat{k}_x^{(n)}\rangle = |\hat{l}_y^{(n)}\rangle$ and $|\hat{k}_y^{(n)}\rangle = |\hat{l}_x^{(n)}\rangle$, then the iteration procedure does not converge to D_S as $D_S^{(\text{aub } n+k)} = D_S^{(\text{aub } n)} \neq D_S$ for $k = 1, 2, \dots$.

Finally, we note that this iteration procedure can be improved by replacing $D_S^{(\text{aub } n)}$ with the optimized $\tilde{D}_S^{(\text{aub } n)}$ as described in the Sec. VIB.

VII. CONCLUSIONS

We have shown that the geometric measures of quantum correlations, i.e., the CC, CQ and QC discords, are equal to the minimal purity deficit under specific von Neumann's measurements compatible with the CC, CQ and QC classes of states, respectively. This allowed us to quickly reproduce known results in the case of qubits and also to give some strong arguments that the CC discord may not, in general, be described analytically even for a two-qubit state. The best general two-qubit formula, given by Eqs. (B1)–(B6), still requires minimalization over two variables. This is in contrast to the CQ and QC discords for which analytical two-qubit formulas are available. Therefore, we focused on analytical approximations of the CC discord. We proposed nonadaptive (i.e., simple product) and adaptive upper bounds for the CC discord and applied them for two-qubit states. We showed that they are tight and faithful, so they can be used as independent tests of nonclassical quantum correlations. The adaptive upper bound corresponds to an optimal measurement on one of the parties conditioned an optimal measurement on the other party. We also described a method of improving the adaptive upper bound by nonoptimal single-party measurements. This refined bound gives exact values of the CC discord for (probably) all classes of states for which there are known analytical expressions. For randomly generated states, the bound usually

differs from the CC discord by the order 10^{-4} or 10^{-5} . Moreover, we described an iterative procedure for the adaptive upper bound, which usually quickly converges to the CC discord. We believe that this estimation of the symmetric discord will play a role in analyzing the cases where all the subsystems of a given quantum system interact with the environment *on equal footing*. For those cases it will probably be more adequate than asymmetric discord, which is based on the system-apparatus picture.

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APPENDIX A: PROOFS OF OBSERVATIONS AND LEMMAS IN SECTION II

Proof of Observation 1. Since $\mathcal{M}_X(\rho) \subset \Omega_X$, by definition, the right-hand side of Eq. (2) is not greater than that of Eq. (3). However, one can show that the opposite ordering of these expressions can occur, hence proving Observation 1. Indeed, choose any measurement $\tilde{\mathcal{M}}_X$ commuting with σ_X^* . Then the difference of Eqs. (2) and (3) is equal to $S(\rho \parallel \sigma_X^*) - S(\rho \parallel \tilde{\mathcal{M}}_X(\rho)) = S(\tilde{\mathcal{M}}_X(\rho) \parallel \sigma_X^*) \geq 0$, where the first equality is due to Lemma 1 below. Therefore $S(\tilde{\mathcal{M}}_X(\rho) \parallel \sigma_X^*) = 0$, i.e., $\sigma_X^* = \tilde{\mathcal{M}}_X(\rho)$, where the measurement is the optimal one. Lemma 1 further furnishes the equivalence between the deficit $\Delta_X(\rho)$ and $D_X^R(\rho)$ of Eq. (3).

Proof of Lemma 1. Consider any von Neumann's measurement $\mathcal{M}(\cdot) = \sum_i P_i(\cdot)P_i$ for orthogonal projectors $\{P_i\}$, $\sum_i P_i = I$. Since any function of a Hermitian operator commutes with the operator itself, one obtains $f(\mathcal{M}(G)) = \mathcal{M}f(\mathcal{M}(G))$, and consequently, $\text{tr}[Ff(\mathcal{M}(G))] = \text{tr}[F\mathcal{M}(f(\mathcal{M}(G)))] = \text{tr}[F\sum_i P_i f(\mathcal{M}(G))P_i] = \text{tr}[\sum_i P_i F P_i f(\mathcal{M}(G))] = \text{tr}[\mathcal{M}(F)f(\mathcal{M}(G))]$ for any Hermitian F and G .

Proof of Observation 2. To prove this Observation for the symmetric discord D_S , we consider

$$D_S(\rho) = \text{tr}(\rho^2) + \min_{\sigma \in \Omega_S} [\text{tr}(\sigma^2) - 2\text{tr}(\rho\sigma)] \quad (\text{A1})$$

optimized over all the CC states σ with eigenvectors formed by two orthonormal bases $\mathcal{B}_A \otimes \mathcal{B}_B := \{|e_i\rangle|f_j\rangle\}$ and some eigenvalues $\{p_{ij}\} \equiv \vec{p}_S$. We may rewrite Eq. (A1) explicitly as

$$D_S(\rho) = \text{tr}(\rho^2) - \min_{\vec{p}_S, \mathcal{B}_A \otimes \mathcal{B}_B} [2\text{tr}(\rho\sigma) - \text{tr}(\sigma^2)]. \quad (\text{A2})$$

Let $\mathcal{B}_A^* \otimes \mathcal{B}_B^*$ be an optimal basis defining naturally the von Neumann measurement $\mathcal{M}_A^* \otimes \mathcal{M}_B^* \equiv \mathcal{M}_S^*$. The variational state defined in this basis of course satisfies $\tilde{\mathcal{M}}_S^*(\sigma) = \sigma$ and so (by Lemma 1) $\text{tr}(\rho\sigma) = \text{tr}[\tilde{\mathcal{M}}_S^*(\rho)\sigma]$. Denoting by \vec{q}_S the diagonal of the state $\tilde{\mathcal{M}}_S^*(\rho)$ (which is already of the CC type), we obtain $D_S(\rho) = \text{tr}(\rho^2) - \max_{\vec{p}_S} (2\vec{q}_S \vec{p}_S - \vec{p}_S^2)$, which yields the optimal spectrum $\vec{p}_S^* = \vec{q}_S$. This concludes the proof that the optimal state σ^* in Eq. (A1) satisfies $\sigma^* = \tilde{\mathcal{M}}_S^*(\rho)$. This, combined with Lemma 1, implies both Eqs. (5) and (6).

Consider now the asymmetric discord D_A , which is given by

$$D_A(\rho) = \min_{\{p_i, \sigma_i\}} \min_{\mathcal{B}_A = \{|e_i\rangle\}} [\text{tr}(\rho^2) - 2\text{tr}(\rho\sigma) + \text{tr}(\sigma^2)], \quad (\text{A3})$$

where $\sigma = \sum_i p_i |e_i\rangle\langle e_i| \otimes \sigma_i$. Let $\mathcal{B}_A^* = \{|e_i^*\rangle\}$ be an optimal basis in Eq. (A3) now defining the von Neumann measurement \mathcal{M}_A^* and the partially optimized class of states $\sigma' = \sum_i p_i |e_i^*\rangle\langle e_i^*| \otimes \sigma'_i$ which clearly satisfies $[\mathcal{M}_A^* \otimes I_B](\sigma') = \sigma'$. By Lemma 1,

$$D_A(\rho) = \text{tr}(\rho^2) + \min_{\{p_i, \sigma'_i\}} \sum_i [p_i^2 \text{tr}((\sigma'_i)^2) - 2p_i q_i \text{tr}(\sigma'_i \rho'_i)], \quad (\text{A4})$$

where the parameters come from a new state,

$$\rho' \equiv [\mathcal{M}_A^* \otimes I_B](\rho) = \sum_i q_i |e_i^*\rangle\langle e_i^*| \otimes \rho'_i. \quad (\text{A5})$$

For all measurements \mathcal{M}_i leaving ρ'_i values invariant we have $\text{tr}[(\sigma'_i)^2] = \text{tr}[\mathcal{M}_i(\sigma'_i)^2] + \delta_i$ (with $\delta_i \geq 0$), since von Neumann's measurements do not increase purity. Using Lemma 1 again, we therefore have

$$\begin{aligned} & \min_{\{p_i, \sigma'_i\}} \sum_i [p_i^2 \text{tr}((\sigma'_i)^2) - 2p_i q_i \text{tr}(\sigma'_i \rho'_i)] \\ &= \min_{\{p_i, \sigma'_i\}} \sum_i [p_i^2 \text{tr}(\mathcal{M}_i(\sigma'_i)^2) + \delta_i - 2p_i q_i \text{tr}(\mathcal{M}_i(\sigma'_i) \rho'_i)] \\ &\geq \min_{\{p_i, \sigma'_i\}} \sum_i [p_i^2 \text{tr}(\mathcal{M}_i(\sigma'_i)^2) - 2p_i q_i \text{tr}(\mathcal{M}_i(\sigma'_i) \rho'_i)] \\ &= \min_{\{p_i, \tilde{\sigma}'_i = \mathcal{M}_i(\sigma'_i)\}} \sum_i [p_i^2 \text{tr}((\tilde{\sigma}'_i)^2) - 2p_i q_i \text{tr}(\tilde{\sigma}'_i \rho'_i)] \\ &= \min_{\tilde{\sigma}'} [\text{tr}((\tilde{\sigma}')^2) - 2\text{tr}(\tilde{\sigma}' \rho')], \end{aligned} \quad (\text{A6})$$

where

$$\tilde{\sigma}' = \sum_i p_i |e_i^*\rangle\langle e_i^*| \otimes \mathcal{M}_i(\sigma'_i). \quad (\text{A7})$$

Since $\tilde{\sigma}'$ and ρ' commute having product eigenvectors (which, however, *do not form* a product of the two eigenbases in general), we are left only with the final problem of finding optimal eigenvalues of $\tilde{\sigma}'$. In analogy to the solution of Eq. (A2), one concludes immediately that the optimal spectrum is the same as that of ρ' . Thus, the optimal CQ state must be equal to ρ' , which is just the original ρ subjected to some specific measurement $\mathcal{M}_A^* \otimes I_B$. This concludes the proof for the CQ-type discord and thus, finally, the proof of Observation 2.

Proof of Lemma 2. Property i is immediate since the set Ω_S of all the CC correlated states is a subset of the sets Ω_A and Ω_B of the CQ and QC correlated states as shown intuitively in Fig. 1. Property ii follows from the fact that for $D_A(\rho) = 0$ the optimal measurement \mathcal{M}_B^* providing D_B already reduces the state ρ to a CC state. This means that combining it with the measurement \mathcal{M}_A commuting with the left reduction of the state yields the same value D_B . This value, based on product measurement, corresponds by definition (4) to some upper bound of the CC discord D_S . On the other hand, D_B is, by property i, a lower bound on the CC discord. Thus $D_S = D_B$ and property iii is implied by property ii.

APPENDIX B: NUMERICAL CALCULATION OF THE CC DISCORD

For completeness, we give an explicit formula for numerical calculation of the CC discord for an arbitrary two-qubit state ρ as

$$D_S(\rho) = \|\rho\|^2 - \max_{\theta, \phi} \|\sigma_S(\theta, \phi)\|^2 = \|\rho\|^2 - \|\sigma_S^*\|^2, \quad (\text{B1})$$

where σ_S [and thus $\sigma_S^* = f(|x_S^*\rangle, |y_S^*\rangle, T_S^*)$] can be expressed solely in terms of the versor

$$|\hat{x}_S\rangle = \frac{|x_S\rangle}{\sqrt{\langle x_S|x_S\rangle}} = [\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta]^T,$$

as follows:

$$\begin{aligned} 4\|\sigma_S^*\|^2 &= 1 + \langle x_S^*|x_S^*\rangle + \langle y_S^*|y_S^*\rangle + \langle x_S^*|T_S^*|y_S^*\rangle \\ &= 1 + \langle x_S^*|x\rangle + \langle y_S^*|y\rangle + \langle x_S^*|T|y_S^*\rangle \\ &= 1 + \max_{\hat{x}_S, \hat{y}_S} (\langle \hat{x}_S|x\rangle^2 + \langle \hat{y}_S|y\rangle^2 + \langle \hat{x}_S|T|\hat{y}_S\rangle^2) \\ &= 1 + \max_{\hat{x}_S} [\lambda_y(\hat{x}_S) + \langle \hat{x}_S|x\rangle^2] \\ &= 1 + \max_{\hat{y}_S} [\lambda_x(\hat{y}_S) + \langle \hat{y}_S|y\rangle^2], \end{aligned} \quad (\text{B2})$$

where the quantity $\lambda_y(\hat{x}_S)$ [$\lambda_x(\hat{y}_S)$] is the maximal eigenvalue of the rank 2 matrix $T|\hat{y}_S\rangle\langle\hat{y}_S|T^T + |x\rangle\langle x|$ ($T^T|\hat{x}_S\rangle\langle\hat{x}_S|T + |y\rangle\langle y|$). So, explicitly,

$$\lambda_y(\hat{x}_S) = h_+ + \sqrt{\langle \hat{x}_S|T|y\rangle^2 + h_-^2}, \quad (\text{B3})$$

and

$$\lambda_x(\hat{y}_S) = g_+ + \sqrt{\langle x|T|\hat{y}_S\rangle^2 + g_-^2}, \quad (\text{B4})$$

where

$$h_{\pm} = \frac{1}{2}(\langle y|y\rangle \pm \langle \hat{x}_S|T T^T|\hat{x}_S\rangle), \quad (\text{B5})$$

$$g_{\pm} = \frac{1}{2}(\langle x|x\rangle \pm \langle \hat{y}_S|T^T T|\hat{y}_S\rangle), \quad (\text{B6})$$

in agreement with Ref. [9].

APPENDIX C: CALCULATION OF DISCORDS FOR MIXTURES OF $|00\rangle$ AND BELL'S STATES

Here, we give more details of our calculation of the CC and the CQ and QC discords for the states $\rho(p, \phi)$ defined by Eq. (46).

The correlation matrix T of Bloch's representation for state $\rho(p, \phi)$ reads as

$$T = \begin{bmatrix} p \cos\phi & -p \sin\phi & 0 \\ p \sin\phi & p \cos\phi & 0 \\ 0 & 0 & 1 - 2p \end{bmatrix}, \quad (\text{C1})$$

and the local Bloch's vectors are $|x\rangle = |y\rangle = [0, 0, 1 - p]^T$. First, we note that

$$K_x = K_y = |x\rangle\langle x| + T T^T = \begin{bmatrix} p^2 & 0 & 0 \\ 0 & p^2 & 0 \\ 0 & 0 & q \end{bmatrix}, \quad (\text{C2})$$

where $q = (1 - 2p)^2 + (1 - p)^2$. Since $p^2 \leq q$ is fulfilled if $p \in [0, \frac{1}{2}]$, so we have to analyze two solutions for $p \leq \frac{1}{2}$ and $p > \frac{1}{2}$. Thus, the CQ and QC discords are

$$\begin{aligned} D_A = D_B &= \frac{1}{4}[\text{tr}(K_x) - \max \text{eig}(K_x)] \\ &= \frac{1}{4}[7p^2 - 6p + 2 - \max(q, p^2)] \\ &= \frac{1}{2} \min(p^2, 3p^2 - 3p + 1). \end{aligned} \quad (\text{C3})$$

We can also calculate the CC discord as follows. The norm $\|\sigma_S\|^2$ is given by

$$\begin{aligned} 4\|\sigma_S\|^2 - 1 &= \max_{\hat{x}_S, \hat{y}_S} (\langle \hat{x}_S|x\rangle^2 + \langle \hat{y}_S|y\rangle^2 + \langle \hat{x}_S|T|\hat{y}_S\rangle^2) \\ &= \max(\langle 1|x\rangle^2 + \langle 1|y\rangle^2 + \langle 1|T|1\rangle^2, \langle 3|x\rangle^2 \\ &\quad + \langle 3|y\rangle^2 + \langle 3|T|3\rangle^2) \\ &= \max[p^2, 2(1 - p)^2 + (1 - 2p)^2]. \end{aligned} \quad (\text{C4})$$

Moreover, $\|\rho\|^2 = 2p(p - 1) + 1$, since $\langle x|x\rangle = \langle y|y\rangle = (1 - p)^2$ and $\|T\|^2 = (1 - 2p)^2 + 2p^2$. Thus, finally, we obtain $D_S = \|\rho\|^2 - \|\sigma_S\|^2$ given by Eq. (47). The geometric discords $D_A = D_B$ and D_S for this state are plotted in Figs. 2 and 3.

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