# Quantum Correlation with Sandwiched Relative Entropies: Advantageous as Order Parameter in Quantum Phase Transitions

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Quantum discord is a measure of quantum correlations beyond the entanglement-separability paradigm. It is conceptualized by using the von Neumann entropy as a measure of disorder. We introduce a class of quantum correlation measures as differences between total and classical correlations, in a shared quantum state, in terms of the sandwiched relative Rényi and Tsallis entropies. We compare our results with those obtained by using the traditional relative entropies. We find that the measures satisfy all the plausible axioms for quantum correlations. We evaluate the measures for shared pure as well as paradigmatic classes of mixed states. We show that the measures can faithfully detect the quantum critical point in the transverse quantum Ising model and find that they can be used to remove an unquieting feature of nearest-neighbor quantum discord in this respect. Furthermore, the measures provide better finite-size scaling exponents of the quantum critical point than the ones for other known order parameters, including entanglement and information-theoretic measures of quantum correlations.

## I. INTRODUCTION

Characterization and quantification of quantum correlation [1, 2] play a central role in quantum information. Entanglement, in particular, has been successfully identified as a useful resource for different quantum communication protocols [3] and computational tasks [4]. Moreover, it has also been employed to study cooperative quantum phenomena like quantum phase transitions in many-body systems [5, 6]. However, in the recent past, several quantum phenomena of shared systems have been discovered in which entanglement is either absent or does not play any significant role. Locally indistinguishable orthogonal product states [7] (c.f. [8]) is a prominent example where entanglement does not play an important role. The role of entanglement is also unclear in the model of deterministic quantum computation with one quantum bit [9–11]. Such phenomena motivated the search for concepts and measures of quantum correlation independent of the entanglement-separability paradigm. Introduction of quantum discord [12, 13] is one of the most important advancements in this direction and has inspired a lot of research activity [2]. It has thereby emerged that quantum correlations, independent of entanglement, can also be a useful ingredient in several quantum information processing tasks [2]. Other measures in the same direction include quantum work deficit [14], measurement-induced nonlocality [15], and quantum deficit [16] (see also [17]). These measures can be generally considered to be quantum correlation measures within an "information-theoretic paradigm".

In classical as well as quantum information theory, one of the most important pillars is the framework of entropy [18], which quantifies the ignorance or lack of information in the relevant physical system. Moreover, it helps to understand information theory from a thermodynamic perspective. Almost all the quantum correlation measures incorporate entropic functions in various forms. And, most of the quantum correlation measures are defined by using the von Neumann entropy [19]. The operational significance of von Neumann entropy has been widely recognized in numerous scenarios in quantum information theory. Nonetheless, there are classes of generalized entropies like the Rényi [20] and Tsallis [21] entropies, which are also operationally significant in important physical scenarios. Both the Rényi and Tsallis entropies reduce to the von Neumann entropy when the entropic parameter $\alpha \to 1$. For $\alpha \in (0, 1)$, the relative Rényi entropy appears in the quantum Chernoff bound which determines the minimal probability of error in discriminating two different quantum states in the setting of asymptotically many copies [22]. In Ref. [23], it was shown that the relative Rényi entropy is relevant in binary quantum state discrimination, for the same range of $\alpha$. The concept of Rényi entropy has also been found to be useful in the context of holographic theory [24]. It has also been found useful in dealing with several condensed matter systems [25]. The significance of the Tsallis entropy in quantum information theory has been established in the context of quantifying entanglement [26], local realism [27], and entropic uncertainty relations [28] (see also [29]). Both the Rényi and Tsallis entropies have important applications in classical as well as quantum statistical mechanics and thermodynamics [30].

While there are important interpretational and operational breakthroughs that have been obtained by using the concept of quantum discord, there are also several intriguing unanswered questions and thriving controversies [2, 31]. It is therefore interesting and important to look back upon the conceptual foundations of quantum discord and inquire whether certain changes, subtle or substantial, in those concepts lead us to a better understanding of the controversies and the unanswered questions. Towards this aim, we introduce measures of the total, classical, and quantum correlations of a bipartite quantum state in terms of the entire class of relative Rényi and Tsallis entropy distances. We show that the measures satisfy all the required properties of bipartite

correlations. We then evaluate the quantum correlation measure for several paradigmatic classes of states. As an application, we find that the quantum correlation measures, via relative Rényi and Tsallis entropies, can indicate quantum phase transitions and give better finite-size scaling exponents than the other known order parameters. Importantly, we show that the conceptualization of the measures in terms of Rényi and Tsallis entropies solves an incommodious feature regarding the behavior of nearest-neighbor quantum discord in a second order phase transition.

There are at least two distinct ways in which the relative Rényi and Tsallis entropies are defined, and are usually referred to as the "traditional" [32] and "sandwiched" [33, 34] varieties. The sandwiched varieties incorporate the noncommutative nature of density matrices in an elegant way, and it is therefore natural to expect that it will play an important role in fundamentals and applications. Indeed, the sandwiched relative Rényi entropy has been used to show that the strong converse theorem for the classical capacity of a quantum channel holds for some specific channels [33]. Moreover, an operational interpretation of the sandwiched relative Rényi entropy in the strong converse problem of quantum hypothesis testing is noted for $\alpha > 1$ [35]. On the other hand, the sandwiched relative Tsallis entropy has recently been shown to be a better witness of entanglement [36] than the traditional one [26]. The relative min- and max-entropies [37–39], which can be obtained from the sandwiched relative Rényi entropy for specific choices of $\alpha$, play significant roles in providing bounds on errors of one-shot entanglement cost [40], on the one-shot classical capacity of certain quantum channels [41], and in several scenarios in non-asymptotic quantum information theory [42]. In Ref. [43], connection of max- relative entopy with frustration in quantum many body systems has been established.

The paper is organized as follows. In Sec. II, we discuss the relative Rényi and Tsallis entropies. In Sec. III, we talk about the usual quantum discord. The Rényi and Tsallis quantum correlations are defined in Sec. IV, where we also derive their properties and evaluate them for paradigmatic classes of bipartite quantum states. Some special cases like the "linear", "min-", and "max-" quantum discord are also formulated and discussed there. The quantum correlation measure is then applied for detecting quantum phase transition in a quantum many-body system in Sec. V. We present a conclusion in Sec. VI.

## II. RELATIVE RÉNYI AND TSALLIS ENTROPIES

The Rényi [20, 44] and Tsallis [21, 45] entropies of a density operator $\rho$ are given respectively by,

$$S_\alpha^R(\rho) = \frac{1}{1-\alpha} \log \mathrm{tr}[\rho^\alpha], \tag{1}$$

$$S_\alpha^T(\rho) = \frac{\mathrm{tr}[\rho^\alpha] - 1}{1-\alpha}. \tag{2}$$

$$\tag{3}$$

Here, the parameter $\alpha \in (0,1) \cup (1,\infty)$, unless mentioned otherwise. All logarithms in this paper are with base 2. Both the entropies reduce to the von Neumann entropy [19], $S(\rho) = -\mathrm{tr}(\rho \log \rho)$, when $\alpha \to 1$. In Ref. [46], both the Rényi and Tsallis entropies are derived from a generalized form of entropy and several interesting properties of them are discussed. The Tsallis entropy for $\alpha = 2$ is called the linear entropy, $S_L(\rho)$, given by

$$S_L(\rho) = 1 - \mathrm{tr}[\rho^2]. \tag{4}$$

The traditional quantum relative Rényi entropy between two density operators $\rho$ and $\sigma$ is defined as

$$S_\alpha^R(\rho||\sigma) = \frac{\log[\mathrm{tr}\left(\rho^\alpha \sigma^{1-\alpha}\right)]}{\alpha - 1}. \tag{5}$$

Note that all the quantum relative entropies, traditional or sandwiched, discussed in this paper, are defined to be $+\infty$ if the kernel of $\sigma$ has non-trivial intersection with the support of $\rho$, and is finite otherwise. $S_\alpha^R(\rho||\sigma)$ reduces to the usual quantum relative entropy [47], $S(\rho||\sigma)$, when $\alpha \to 1$, where

$$S(\rho||\sigma) = -S(\rho) - \mathrm{tr}(\rho \log \sigma). \tag{6}$$

Recently, a generalized version of the quantum relative Rényi entropy (called "sandwiched" relative Rényi entropy) has been introduced, by considering the non commutative nature of density operators [33, 34]. It is defined as

$$\tilde{S}_\alpha^R(\rho||\sigma) = \frac{1}{\alpha - 1} \log \left[ \mathrm{tr}\left( \sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right]. \tag{7}$$

Note that $\tilde{S}_\alpha^R(\rho||\sigma)$ also reduces to $S(\rho||\sigma)$ when $\alpha \to 1$. In Ref. [33, 34, 48–50] several interesting properties of the sandwiched Rényi entropy have been established. Here, we mention some of them (for two density operators $\rho$ and $\sigma$) which we will use later in this paper.

1. $\tilde{S}_\alpha^R(\rho||\sigma) \geq 0$.

2. $\tilde{S}_\alpha^R(\rho||\sigma) = 0$ if and only if $\rho = \sigma$.

3. For $\alpha \in [\frac{1}{2}, 1) \cup (1, \infty)$ and for any completely positive trace-preserving map (CPTPM) $\mathcal{E}$, we have the data processing inequality, $\tilde{S}_\alpha^R(\rho||\sigma) \geq \tilde{S}_\alpha^R(\mathcal{E}(\rho)||\mathcal{E}(\sigma))$ [48].

4. $\tilde{S}_\alpha^R(\rho||\sigma)$ is invariant under all unitaries $U$, i.e., $\tilde{S}_\alpha^R(U\rho U^\dagger||U\sigma U^\dagger) = \tilde{S}_\alpha^R(\rho||\sigma)$ .

The traditional quantum relative Tsallis entropy between two density operators $\rho$ and $\sigma$ is defined as

$$S_\alpha^T(\rho||\sigma) = \frac{\text{tr}\left(\rho^\alpha \sigma^{1-\alpha}\right) - 1}{\alpha - 1}. \qquad (8)$$

The sandwiched relative Tsallis entropy between two density operators $\rho$ and $\sigma$ is given by [36]

$$\tilde{S}_\alpha^T(\rho||\sigma) = \frac{\text{tr}\left[\left(\sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}}\right)^\alpha\right] - 1}{\alpha - 1}. \qquad (9)$$

Both $S_\alpha^T(\rho||\sigma)$ and $\tilde{S}_\alpha^T(\rho||\sigma)$ also reduce to $S(\rho||\sigma)$ when $\alpha \to 1$. It can be easily verified that the properties (1-4), satisfied by $\tilde{S}_\alpha^R(\rho||\sigma)$ are also satisfied by $\tilde{S}_\alpha^T(\rho||\sigma)$. In this paper, we will predominantly use the sandwiched version of both the relative entropies. Hereafter, by relative entropy, we will mean the sandwiched form of the relative entropies, unless mentioned otherwise. Some of the important special cases of the Rényi and Tsallis relative entropies are given below.

**a.** *Relative Linear Entropy*: At $\alpha = 2$, $\tilde{S}_\alpha^T(\rho||\sigma)$ gives the relative linear entropy,

$$S_L(\rho||\sigma) = \tilde{S}_2^T(\rho||\sigma). \qquad (10)$$

The relative linear entropy has also been defined in the literature by using the traditional version of the relative entropy at $\alpha = 2$. However, in this paper, we will use the relative linear entropy defined only through the sandwiched relative entropy (at $\alpha = 2$).

**b.** *Relative Collision Entropy*: At $\alpha = 2$, $\tilde{S}_\alpha^R(\rho||\sigma)$ has been called the relative collision entropy [37],

$$S_C(\rho||\sigma) = \tilde{S}_2^R(\rho||\sigma). \qquad (11)$$

**c.** *Relative Min- and Max-Entropies*: In [51], it is pointed out that at $\alpha = \frac{1}{2}$, $\tilde{S}_\alpha^R(\rho||\sigma)$ gives relative min-entropy [39],

$$S_{min}(\rho||\sigma) = \tilde{S}_{\frac{1}{2}}^R(\rho||\sigma). \qquad (12)$$

Note that

$$S_{min}(\rho||\sigma) = -2\log F(\rho, \sigma), \qquad (13)$$

where $F(\rho, \sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_1 = \text{tr}|\sqrt{\rho}\sqrt{\sigma}|$ is the fidelity between the states $\rho$ and $\sigma$. It is shown in [34], that the relative max-entropy [38] is nothing but relative Rényi entropy, when $\alpha \to \infty$ i.e.

$$S_{max}(\rho||\sigma) = \tilde{S}_{\alpha \to \infty}^R(\rho||\sigma), \qquad (14)$$

where

$$S_{max}(\rho||\sigma) = \inf(\lambda : \rho \le 2^\lambda \sigma). \qquad (15)$$

## III. QUANTUM DISCORD

Quantum discord is a measure of quantum correlations of bipartite quantum states that is independent of the entanglement-separability paradigm [12, 13]. It can be conceptualized from several perspectives. An approach that is intuitively satisfying, is to define it as the difference between the total correlation and the classical correlation for a bipartite quantum state $\rho_{AB}$. The total correlation is defined as the quantum mutual information of $\rho_{AB}$, which is given by

$$\mathcal{I}(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \qquad (16)$$

where $\rho_A$ and $\rho_B$ are the local density matrices of $\rho_{AB}$. The mutual information $\mathcal{I}(\rho_{AB})$ can also be expressed in terms of the usual quantum relative entropy as

$$\mathcal{I}(\rho_{AB}) = \min_{\{\sigma_A, \sigma_B\}} S(\rho_{AB}||\sigma_A \otimes \sigma_B). \qquad (17)$$

This follows from the fact that

$$\begin{aligned}
&\min_{\{\sigma_A, \sigma_B\}} S(\rho_{AB}||\sigma_A \otimes \sigma_B) \\
&= \min_{\{\sigma_A, \sigma_B\}} \{-S(\rho_{AB}) - \text{tr}(\rho_A \log \sigma_A) \\
&\quad - \text{tr}(\rho_B \log \sigma_B)\},
\end{aligned}$$

and the non-negativity of relative von Neumann entropy between two density matrices. Therefore, the quantum mutual information is the minimum usual relative entropy distance of the state $\rho_{AB}$ from the set of all completely uncorrelated states, $\sigma_A \otimes \sigma_B$, whence we obtain a ground for interpreting the quantum mutual information as the total correlation in the state. Further evidence in this direction is provided in [52–55]. The classical correlation is given in terms of the measured conditional entropy, and is defined as [12, 13]

$$\mathcal{J}(\rho_{AB}) = S(\rho_A) - S(\rho_{A|B}), \qquad (18)$$

where

$$S(\rho_{A|B}) = \min_{\{P_i\}} \sum_i p_i S(\rho_{A|i}) \qquad (19)$$

is the conditional entropy of $\rho_{AB}$, conditioned on measurements at $B$ with rank-one projection-valued measurements $\{P_i\}$. Here, $\rho_{A|i} = \frac{1}{p_i}\text{tr}_B[(\mathbb{I}_A \otimes P_i)\rho(\mathbb{I}_A \otimes P_i)]$ is the conditional state which we get with probability $p_i = \text{tr}_{AB}[(\mathbb{I}_A \otimes P_i)\rho(\mathbb{I}_A \otimes P_i)]$, where $\mathbb{I}_A$ is the identity operator on the Hilbert space of $A$. $\mathcal{J}(\rho_{AB})$ can also be defined in terms of the mutual information as

$$\mathcal{J}(\rho_{AB}) = \max_{\{P_i\}} \mathcal{I}(\rho'_{AB}), \qquad (20)$$

where

$$\rho'_{AB} = \sum_i (\mathbb{I}_A \otimes P_i)\rho_{AB}(\mathbb{I}_A \otimes P_i). \qquad (21)$$

The classical correlation can therefore be seen as the minimum relative entropy distance of the state $\rho'_{AB}$ from all uncorrelated states, maximized over all rank-one projective measurements on $B$, and is given by

$$\mathcal{J}(\rho_{AB}) = \max_{\{P_i\}} \min_{\{\sigma_A, \sigma_B\}} S(\rho'_{AB} || \sigma_A \otimes \sigma_B). \qquad (22)$$

The maximization in Eq. (22) or in Eq. (18) ensure that $\mathcal{J}(\rho_{AB})$ quantifies the maximal content of classical correlation present in the bipartite state $\rho_{AB}$. Hence, if we subtract $\mathcal{J}(\rho_{AB})$ from the total correlation, the remaining correlation is "purely" quantum, and is defined as [12, 13]

$$\mathcal{D}(\rho_{AB}) = \mathcal{I}(\rho_{AB}) - \mathcal{J}(\rho_{AB}). \qquad (23)$$

## IV. TOTAL, CLASSICAL, AND QUANTUM CORRELATIONS AS RELATIVE ENTROPIES

In this section, we define the total, classical, and quantum correlation in terms of the sandwiched relative Rényi and Tsallis entropies. We discuss the properties of these measures and evaluate them for several important families of bipartite quantum states. In the final subsection, we also compare the results with those obtained with traditional relative entropies.

### A. Generalized Mutual Information as Total Correlation

We define the generalized mutual information of $\rho_{AB}$ as

$$\mathcal{I}_\alpha^\Gamma(\rho_{AB}) = \min_{\{\sigma_A, \sigma_B\}} \tilde{S}_\alpha^\Gamma(\rho_{AB} || \sigma_A \otimes \sigma_B). \qquad (24)$$

Here, the minimum is taken over all density matrices, $\sigma_A$ and $\sigma_B$. The relative entropy, although not a metric on the operator space, is a measure of the distance between two quantum states. $\tilde{S}_\alpha^\Gamma(\rho_{AB} || \sigma_A \otimes \sigma_B)$ is a distance between the quantum state $\rho_{AB}$ and a completely uncorrelated state $\sigma_A \otimes \sigma_B$. Here, and hereafter, the superscript $\Gamma$ is either $R$ or $T$, depending on whether it is the Rényi or Tsallis variety that is considered. The corresponding minimum distance can be interpreted as the total correlation present in the system. The generalized mutual information $\mathcal{I}_\alpha^\Gamma(\rho_{AB})$ becomes equal to the usual quantum mutual information $\mathcal{I}(\rho_{AB})$ when $\alpha \to 1$:

$$\begin{aligned} \lim_{\alpha \to 1} \mathcal{I}_\alpha^\Gamma(\rho_{AB}) &= \lim_{\alpha \to 1} \min_{\{\sigma_A, \sigma_B\}} \tilde{S}_\alpha^\Gamma(\rho_{AB} || \sigma_A \otimes \sigma_B). \\ &= \min_{\{\sigma_A, \sigma_B\}} S(\rho_{AB} || \sigma_A \otimes \sigma_B) \\ &\equiv \mathcal{I}(\rho_{AB}). \end{aligned} \qquad (25)$$

### B. Classical and Quantum Correlation

The Rényi or Tsallis version of the classical correlation, denoted by $\mathcal{J}_\alpha^\Gamma(\rho_{AB})$, is defined as

$$\mathcal{J}_\alpha^\Gamma(\rho_{AB}) = \max_{\{P_i\}} \min_{\{\sigma_A, \sigma_B\}} \tilde{S}_\alpha^\Gamma(\rho'_{AB} || \sigma_A \otimes \sigma_B), \quad (26)$$

where $\rho'_{AB}$ is obtained by performing rank-1 projective measurements as in the definition of original classical correlation (in Eq. (21)).

Therefore, quantum correlation using generalized entropies is defined as

$$\mathcal{D}_\alpha^\Gamma(\rho_{AB}) = \mathcal{I}_\alpha^\Gamma(\rho_{AB}) - \mathcal{J}_\alpha^\Gamma(\rho_{AB}), \qquad (27)$$

with $\alpha \in [\frac{1}{2}, 1) \cup (1, \infty)$. By using the data processing inequality, which holds in this range of $\alpha$, one can prove the non-negativity of the quantum correlation [48]. We now look into the properties of $\mathcal{D}_\alpha^\Gamma(\rho_{AB})$, which provide independent support for identifying the quantities as correlation measures.

**Property 1**. $\mathcal{I}_\alpha^\Gamma, \mathcal{J}_\alpha^\Gamma \geq 0$ since $\tilde{S}_\alpha^\Gamma(\rho || \sigma) \geq 0$.

**Property 2**. $\mathcal{I}_\alpha^\Gamma, \mathcal{J}_\alpha^\Gamma$ are vanishing, and therefore, $\mathcal{D}_\alpha^\Gamma = 0$, for any product state, $\rho_{AB} = \rho_A \otimes \rho_B$, as $\tilde{S}_\alpha^R(\rho || \rho) = 0$. The proof for the vanishing of total correlations follows by noting that the product state in the argument itself is the state which gives the optimal relative entropy distance. A similar argument, but for the measured state, holds for the classical correlation.

Moreover, $\mathcal{D}_\alpha^\Gamma = 0$ for any quantum-classical state, i.e. any state of the form $\sum_i p_i \rho_i^A \otimes (|i\rangle\langle i|)^B$, where $\{p_i\}$ forms a probability distribution, $\{|i\rangle\}$ forms an orthonormal basis, and $\rho_i$ are density matrices, when the measurement is performed on the $B$ part.

**Property 3**. $\mathcal{I}_\alpha^\Gamma, \mathcal{J}_\alpha^\Gamma$ remain invariant under local unitaries, which follow from the fact that $\tilde{S}_\alpha^R(\rho || \sigma)$ is invariant under all unitaries $U$. Hence, $\mathcal{D}_\alpha^\Gamma$ is also invariant under local unitaries.

**Property 4**. $\mathcal{I}_\alpha^\Gamma, \mathcal{J}_\alpha^\Gamma$ are non increasing under local operations, which follow from the data processing inequality, $\tilde{S}_\alpha^R(\rho || \sigma) \geq \tilde{S}_\alpha^R(\mathcal{E}(\rho) || \mathcal{E}(\sigma))$, for any CPTPM $\mathcal{E}$.

**Property 5**. $\mathcal{D}_\alpha^\Gamma$ is non-negative, as $\mathcal{J}_\alpha^\Gamma$ is upper bounded by $\mathcal{I}_\alpha^\Gamma$. The latter statement is due to the fact that $\mathcal{J}_\alpha^\Gamma$ is obtained by performing a local measurement on $\rho_{AB}$, and we know from the data processing inequality that $\tilde{S}_\alpha^\Gamma$ is monotone under CPTPM.

The classical correlation measure that we have defined here, satisfies all the plausible properties for classical correlation proposed in Ref. [12], except the one which states that for pure states, the classical correlation reduces to the von Neumann entropy of the subsystems. We wish to mention that this property is natural for the measure which involves the von Neumann entropy, and is not expected to be followed by the measures with generalized entropies. This is because the definition of classical correlation in terms of the relative entropy reduces naturally to the one in terms of the conditional entropy in the case of the von Neumann entropy.

We use the convention that each of the definitions of $\mathcal{I}_\alpha^\Gamma$, $\mathcal{J}_\alpha^\Gamma$ and $\mathcal{D}_\alpha^\Gamma$ also incorporates a division by log 2 bits, whence all the definitions can be considered to be dimensionless.

We note here that there has been previous attempts to define quantum discord by using Tsallis entropies [56–58]. These definitions however do not always guarantee positivity of the quantum discord, so defined. Also, the corresponding total and classical correlations are not necessarily monotonic under local operations. Ref. [59] defines a quantum correlation by considering the difference between the Tsallis entropies of the post-measured and pre-measured states. In Ref. [60], a Gaussian quantum correlation is defined by using the Rényi entropy for $\alpha = 2$. After completion of the current paper, we came to know about the work in Ref. [61], which states that quantum discord can be defined using sandwiched relative entropy, with a definition of quantum mutual information of a bipartitite quantum state $\rho_{AB}$, given by $\mathcal{I}'^R_\alpha(\rho_{AB}) = \min_{\{\sigma_B\}} \tilde{S}^R_\alpha(\rho_{AB}||\rho_A \otimes \sigma_B)$ (cf. Eq. (24)). The definition of mutual information used here and in Ref. [62] (published version of this paper) use $\sigma_A$ in place of $\rho_A$, which makes $\mathcal{I}'^R_\alpha$, a special case of it. By "special case", it is meant that the optimization performed in this work is over a class of states that contains the class of states used in [61]. The Rényi quantum discord was later defined by the authors of [61] in terms of generalized conditional mutual information [63], an approach that is very different from the one followed in this work.

### C. Special Cases

#### 1. Linear Quantum Discord

The relative linear entropy can be used to define the "linear quantum discord", given by

$$\mathcal{D}_L(\rho_{AB}) = \mathcal{I}_2^T(\rho_{AB}) - \mathcal{J}_2^T(\rho_{AB}), \qquad (28)$$

where $\mathcal{I}_2^T(\rho_{AB})$ and $\mathcal{J}_2^T(\rho_{AB})$ are defined by using the relative linear entropy, given in Eq. (10).

#### 2. Min- and Max-Quantum Discords

We also define the "min- and max-quantum discords" by considering relative min- and max-entropies as

$$\mathcal{D}_{min}(\rho_{AB}) = \mathcal{I}_{\frac{1}{2}}^R(\rho_{AB}) - \mathcal{J}_{\frac{1}{2}}^R(\rho_{AB}), \qquad (29)$$

and

$$\mathcal{D}_{max}(\rho_{AB}) = \mathcal{I}_{\alpha \to \infty}^R(\rho_{AB}) - \mathcal{J}_{\alpha \to \infty}^R(\rho_{AB}). \qquad (30)$$

### D. Pure States

Any bipartite pure state of two qubits can be written, using Schmidt decomposition, as

$$|\psi_{AB}\rangle = \sum_{i=0}^{1} \sqrt{\lambda_i}|i_A i_B\rangle, \qquad (31)$$

where $\lambda_i$ are non-negative real numbers satisfying $\sum_i \lambda_i = 1$. Since a bipartite pure state is symmetric, it is expected that the state $\sigma_A \otimes \sigma_B$, which minimizes the relative entropy of $|\psi_{AB}\rangle$ with uncorrelated states, is also symmetric. Numerical studies support this view. This fact is not only true for pure bipartite states, but it holds for all symmetric bipartitite states that are considered in this paper. Moreover, numerical results indicate that for arbitrary $|\psi_{AB}\rangle$, the state $\sigma^A \otimes \sigma^B$ which gives the minimum, is diagonal in the Schmidt basis of $|\psi_{AB}\rangle$. To numerically evaluate the minimum relative entropy distance of a bipartite quantum state $\rho_{AB}$ from product states, we begin by randomly generating bipartite product states $\sigma_A \otimes \sigma_B$. Then we calculate the relative entropies between $\rho_{AB}$ and all such $\sigma_A \otimes \sigma_B$. The minimum of these relative entropies is considered to be the minimum relative entropy distance. We repeat the procedure for a larger set of randomly chosen product states. We terminate the process when the minimum does not change within the required precision. Note that the numerical study is performed without the assumptions that the product state at which the minimum is attained is symmetric and that it is diagonal in the Schmidt basis. We have followed the same procedure throughout the paper to numerically evaluate the different correlations. Therefore, the minimum $\sigma_A$ or $\sigma_B$ is given by

$$\sigma_A = \sigma_B = \sigma \equiv \sum_{i=0}^{1} a_i|i\rangle\langle i|, \qquad (32)$$

where $a_i$ are non-negative real numbers satisfying $\sum_i a_i = 1$. With these assumptions, the total correlation of $|\psi_{AB}\rangle$ is given by

$$\mathcal{I}_\alpha^R(|\psi_{AB}\rangle) = \min_{\{a\}} \frac{1}{\alpha - 1} \log \left[ \lambda a^{\frac{2(1-\alpha)}{\alpha}} \right.$$
$$\left. + (1-\lambda)(1-a)^{\frac{2(1-\alpha)}{\alpha}} \right]^\alpha, \qquad (33)$$

where $a_0 = a$, $a_1 = 1-a$, $\lambda_0 = \lambda$, $\lambda_1 = 1-\lambda$. The value of $a$ is obtained from the condition

$$\frac{1}{a} = \left( \frac{\lambda}{1-\lambda} \right)^{\frac{\alpha}{2-3\alpha}} + 1, \qquad (34)$$

for $\alpha \in (2/3, 1) \cup (1, \infty)$. For $\frac{1}{2} \leq \alpha \leq \frac{2}{3}$, the minimization in Eq. (33) yields

$$\mathcal{I}_\alpha^R(|\psi_{AB}\rangle) = \frac{\alpha}{\alpha - 1} \log \left[ \max\{\lambda, 1-\lambda\} \right]. \qquad (35)$$

For pure states, numerical searches indicate that the classical correlation is independent of the measurement basis. We consider measurement performed in the Schmidt basis for calculating the classical correlation of the original state. Just like the total correlation in the original state, the $\sigma_A \otimes \sigma_B$, which minimizes the relative entropy of the post-measurement state with uncorrelated states, is symmetric, since we perform the projective measurement in the Schmidt basis. Moreover, from numerical results, we find that $\sigma_A \otimes \sigma_B$ is again diagonal in the Schmidt basis of $|\psi_{AB}\rangle$. The Rényi classical correlation of $|\psi_{AB}\rangle$ is therefore given by

$$\mathcal{J}_\alpha^R(|\psi_{AB}\rangle) = \min_{\{a\}} \frac{1}{\alpha-1} \log\left[\lambda^\alpha a^{2(1-\alpha)}\right.$$
$$\left. + (1-\lambda)^\alpha (1-a)^{2(1-\alpha)}\right]. \quad (36)$$

The value of $a$ is obtained from the condition

$$\frac{1}{a} = \left(\frac{\lambda}{1-\lambda}\right)^{\frac{\alpha}{1-2\alpha}} + 1, \quad (37)$$

for $\alpha \in (1/2, 1) \cup (1, \infty)$.

The linear quantum discord for $|\psi_{AB}\rangle$ is given by

$$\mathcal{D}_L(|\psi_{AB}\rangle) = \left(\sqrt{\lambda} + \sqrt{1-\lambda}\right)^4 - \left(\sqrt{\lambda} + \sqrt{1-\lambda}\right)^2. \quad (38)$$

We find that the min-quantum discord is vanishing for every two-qubit pure state. We believe that this is a peculiarity of some elements of the class of information-theoretic quantum correlation measures that are defined according to the premise that subtracting classical correlations from total correlations will produce quantum correlations. This may perhaps be paralleled with the fact that although it was perhaps considered desirable that all entanglement measures should possess the property that they should vanish for separable states and only for separable states, the discovery of bound entangled states [64] led us to the fact that distillable entanglement [65] can vanish for certain entangled states as well. It should be noted that in contradistinction to distillable entanglement, the min-quantum discord can be non-zero for certain separable states, indicating that at least in this sense, the space of information-theoretic quantum correlations is richer than the space of entanglement measures.

The max-quantum discord for $|\psi_{AB}\rangle$ is given by

$$\mathcal{D}_{max}(|\psi_{AB}\rangle) = \log\left[\frac{(\sqrt[3]{\lambda} + \sqrt[3]{1-\lambda})^3}{(\sqrt{\lambda} + \sqrt{1-\lambda})^2}\right]. \quad (39)$$

In Fig. 1, we plot the Rényi quantum correlation of $|\psi_{AB}\rangle$ for various values of $\alpha$. We have also performed the entire calculations for the Tsallis discord and find that its behavior is qualitatively similar to the Rényi discord. In Fig. 2, we have exhibited the Tsallis discord for bipartite pure states, which clearly indicate the similarity between the two discords. In the rest of the paper, we will only plot the Rényi discord.
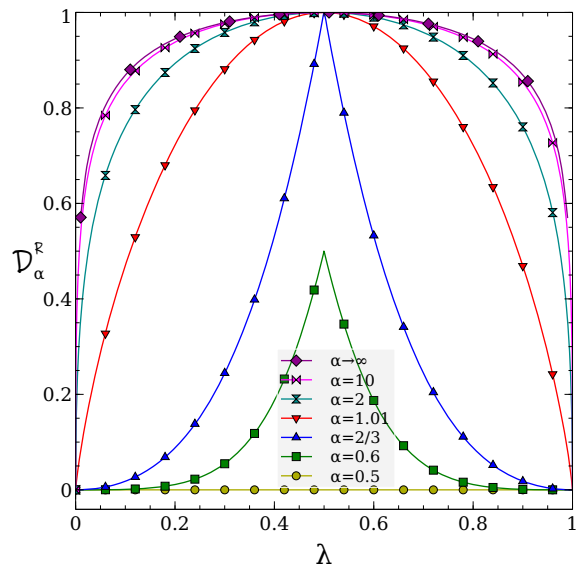


FIG. 1. (Color online.) Rényi quantum correlation, $\mathcal{D}_\alpha^R$, with respect to $\lambda$, of $|\psi_{AB}\rangle = \sqrt{\lambda}|00\rangle + \sqrt{(1-\lambda)}|11\rangle$, for different $\alpha$. Both axes are dimensionless.
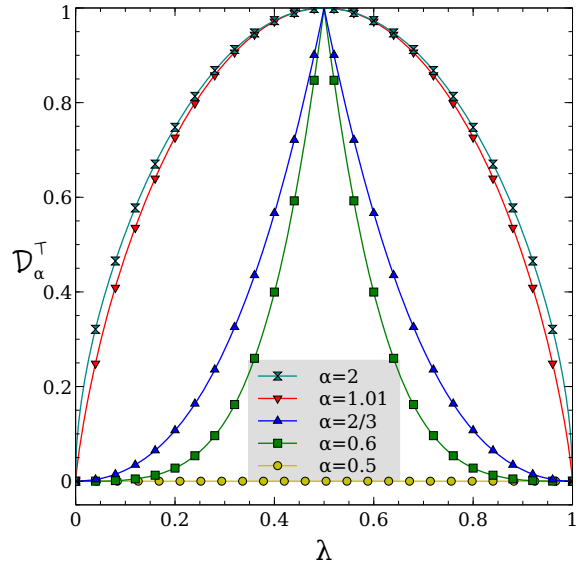


FIG. 2. (Color online.) Tsallis quantum correlation, $\mathcal{D}_\alpha^T$, with respect to $\lambda$, of $|\psi_{AB}\rangle = \sqrt{\lambda}|00\rangle + \sqrt{(1-\lambda)}|11\rangle$, for different $\alpha$. Both axes are dimensionless. The values of the Tsallis quantum correlation are normalized, whenever possible, so that the maximal quantum correlations are of unit value.

### E. Mixed States: Some Examples

**(i) Werner States:** Consider the Werner state, given by

$$\rho_W = p|\psi^-\rangle\langle\psi^-| + (1-p)\frac{I}{4},$$

where $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$, $I$ denotes the identity operator on the two-qubit Hilbert space, and $0 \leq p \leq 1$. Suppose the $\sigma_A^{min}$ and $\sigma_B^{min}$ are the optimal $\sigma_A$ and $\sigma_B$ which minimizes the relative Rényi entropy of $\rho_W$ with uncorrelated states. Using the fact that the Werner state is symmetric and local unitarily invariant, we choose

$$\sigma_A^{min} = \sigma_B^{min} = \sigma \equiv a_0|0\rangle\langle 0| + a_1|1\rangle\langle 1|, \quad (40)$$

where $a_i$ are non-negative real numbers satisfying $\sum_i a_i = 1$. Here we have assumed that $\sigma_A \otimes \sigma_B$, which minimizes the relative entropy of $\rho_W$ with uncorrelated states, is symmetric. Detail numerical study support our assumption, as mentioned in Sec. IV D. It is now possible to perform the minimization for $\alpha \in [\frac{2}{3}, 1) \cup (1, \infty)$. In this range, the relative Rényi entropy distance corresponding to the total correlations is minimum for $a_0 = a_1 = \frac{1}{2}$. Therefore, the Rényi total correlation of the Werner state for $\alpha \geq \frac{2}{3}$ ($\alpha \neq 1$) is given by

$$\mathcal{I}_\alpha^R(\rho_W) = 2 + \frac{1}{\alpha - 1} \log \frac{1}{4^\alpha} \left[ (1+3p)^\alpha + 3(1-p)^\alpha \right]. \quad (41)$$

Just like for the case of pure bipartite states, the Rényi classical correlation is again independent of measurement basis, as is expected from the property of rotational invariance of the Werner state.

Numerical observations also suggest that for $\alpha \geq \frac{1}{2}$ ($\alpha \neq 1$) and for any $p$, the relative Rényi entropy is minimum at $\sigma_A \otimes \sigma_B = \frac{I}{4}$ for the post-measurement state corresponding to the Werner state. So the Rényi classical correlation, in this range of $\alpha$, is given by

$$\mathcal{J}_\alpha^R(\rho_W) = 2 + \frac{1}{\alpha - 1} \log \frac{1}{4^\alpha} \left[ 2(1+p)^\alpha + 2(1-p)^\alpha \right]. \quad (42)$$

Hence, the Rényi quantum correlation of the Werner state for $\alpha \geq \frac{2}{3}$ ($\alpha \neq 1$) is given by

$$\mathcal{D}_\alpha^R(\rho_W) = \frac{1}{\alpha - 1} \log \left[ \frac{(1+3p)^\alpha + 3(1-p)^\alpha}{2(1+p)^\alpha + 2(1-p)^\alpha} \right]. \quad (43)$$

For $\frac{1}{2} \leq \alpha < \frac{2}{3}$, we find the Rényi quantum correlation for the Werner states by numerical evaluation. In Fig. 3, we exhibit the Rényi quantum correlation for the Werner states for different values of $\alpha$.

The Rényi quantum correlation is maximum for the Werner state at $p = 1$ for $\alpha \geq \frac{2}{3}$. The singlet state, and states that are local unitarily connected with it, is therefore maximally Rényi quantum correlated in that range of $\alpha$, among the Werner states. However, for $\frac{1}{2} \leq \alpha < \frac{2}{3}$, the Bell states are not the maximally Rényi quantum correlated states. In this range of $\alpha$, we get maximal quantum correlation among the Werner states, for a value of $p$ that is different from unity. For example, for $\alpha = 0.6$, we find that the state, $\rho_W$, with mixing parameter $p \approx 0.96$ has the maximal quantum correlation among all Werner states. For $\alpha = 1/2$, the same is at $p \approx 0.88$. For $\alpha = \frac{1}{2}$, i.e., for min-entropy, the singlet has zero quantum correlation. Indeed, all pure states have vanishing
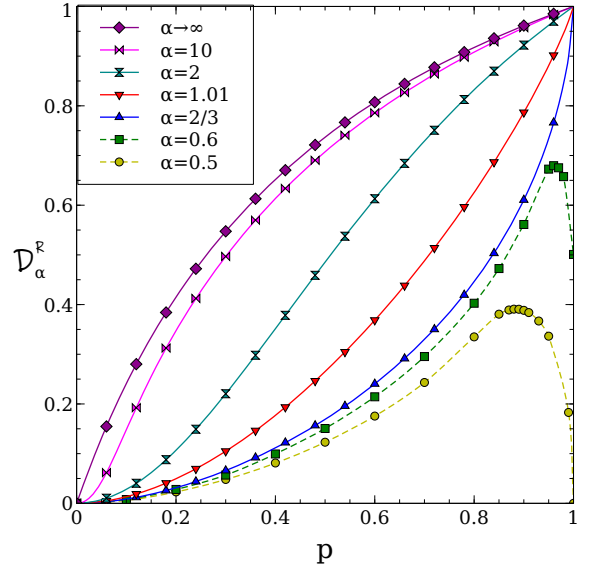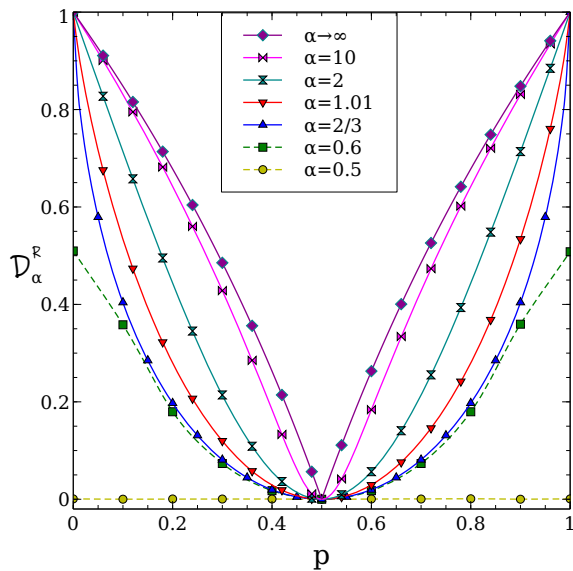


FIG. 3. (Color online.) Rényi quantum correlation, $\mathcal{D}_\alpha^R$, with respect to $p$, of the Werner state, $\rho_W = p|\psi^-\rangle\langle\psi^-| + (1-p)\frac{1}{4}I$, for different $\alpha$. Both axes are dimensionless.

min-quantum discord. We will visit this issue again in Sec. IV F.

The linear quantum discord for the Werner state is

$$\mathcal{D}_L(\rho_W) = \frac{1}{4} \left[ (1+3p)^2 + (1-p)^2 - 2(1+p)^2 \right]. \quad (44)$$

The max-quantum discord can also be calculated similarly for the Werner state and is given by

$$\mathcal{D}_{max}(\rho_W) = \log \left[ \frac{(1+3p)}{(1+p)} \right]. \quad (45)$$

We have numerically evaluated the min-quantum discord for the Werner state (see Fig. 3).

**(ii) Bell Mixture:** We consider a mixture of two Bell states, given by

$$\rho_{BM} = p|\phi^+\rangle\langle\phi^+| + (1-p)|\phi^-\rangle\langle\phi^-|,$$

where $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, $|\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$ and $0 \leq p \leq 1$. Numerical observations suggests that

$$\mathcal{I}_\alpha^\Gamma(\rho_{BM}) = \tilde{S}_\alpha^\Gamma \left( \rho_{BM} || \frac{I}{4} \right),$$

for $\alpha \geq \frac{2}{3}$ ($\alpha \neq 1$). Hence, in this range of $\alpha$,

$$\mathcal{I}_\alpha^R(\rho_{BM}) = 2 + \frac{1}{\alpha - 1} \log \left[ p^\alpha + (1-p)^\alpha \right]. \quad (46)$$

We have found numerically that if one performs measurement in the $\{|0\rangle, |1\rangle\}$ basis, the relative entropy of the post-measurement state with $\frac{I}{4}$ gives the Rényi classical correlation for the entire range of $\alpha$, i.e., for

$\alpha \in (\frac{1}{2}, 1) \cup (1, \infty)$, and it is equal to unity for any $p$ and $\alpha$. Hence for $\alpha \geq \frac{2}{3}$ ($\alpha \neq 1$),

$$\mathcal{D}_\alpha^R(\rho_{BM}) = 1 + \frac{1}{\alpha - 1} \log\left[p^\alpha + (1-p)^\alpha\right]. \qquad (47)$$

The linear quantum discord for this state is given by

$$\mathcal{D}_L(\rho_{BM}) = 8(p^2 - p) + 2. \qquad (48)$$

Similarly,

$$\mathcal{D}_{max}(\rho_{BM}) = 1 + \log\left[\max\{p, 1-p\}\right]. \qquad (49)$$

In Fig. 4, the Rényi quantum correlations for $\rho_{BM}$ is depicted for different values of $\alpha$.



FIG. 4. (Color online.) Rényi quantum correlation, $\mathcal{D}_\alpha^R$, with respect to $p$, of the Bell mixture, $\rho_{BM} = p|\phi^+\rangle\langle\phi^+| + (1-p)|\phi^-\rangle\langle\phi^-|$, for different values of $\alpha$. Both axes are dimensionless.

**(iii) Mixture of Bell state and a Product State:** Consider the state given by

$$\rho_{BN} = p|\phi^+\rangle\langle\phi^+| + (1-p)|00\rangle\langle00|.$$

The Rényi quantum correlation is calculated numerically, and in Fig. 5, we plot it for $\rho_{BN}$, for different values of $\alpha$.

### F. Sandwiched vs Traditional Relative Entropies

Until now, in this section, we have used the sandwiched relative entropy distances to define the Rényi and Tsallis quantum correlations. We now briefly consider the traditional variety for defining quantum correlation, and discuss some of its implications. In the preceding subsections, we have observed anomalous behavior of the
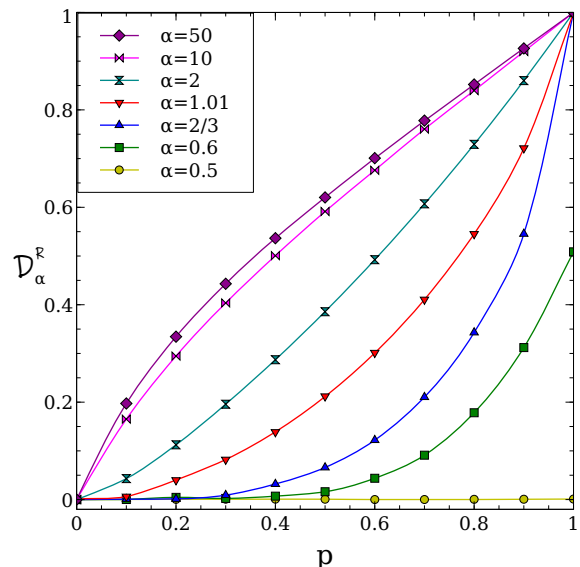


FIG. 5. (Color online.) Rényi quantum correlation, $\mathcal{D}_\alpha^R$, with respect to $p$, of $\rho_{BN} = p|\phi^+\rangle\langle\phi^+| + (1-p)|00\rangle\langle00|$, for different $\alpha$. Both axes are dimensionless.

Rényi quantum correlation in the range $\frac{1}{2} \leq \alpha < \frac{2}{3}$ for pure states, as well as in certain families of mixed states in the neighborhood of pure states. In these cases, we have, e.g., seen that the Bell states are not the maximally Rényi quantum correlated state for $\alpha < \frac{2}{3}$ and at $\alpha = \frac{1}{2}$, i.e, for the min- entropy, all pure states have vanishing quantum correlations.

We can also define quantum correlations with the traditional relative Rényi and Tsallis entropies. The properties (1-4) discussed in Sec. II, are also followed by both the traditional relative entropies [66], but the data processing inequality holds for $\alpha \in [0, 1) \cup (1, 2]$ [67]. We can therefore define quantum correlation with traditional relative entropy distances for this range of $\alpha$. If we consider the traditional relative entropies, then we do not see any anomalous behavior of the Rényi quantum correlation. But from the traditional version of the relative Rényi entropy, we do not get the min- entropy. Moreover, in [35], the authors have argued that the sandwiched relative Rényi entropy is operationally relevant in the strong converse problem of quantum hypothesis testing for $\alpha > 1$, but for $\alpha < 1$, the traditional version is more relevant from an operational point of view. The anomalous behavior of the quantum correlation with the sandwiched relative entropy distances seems to indicate that to define quantum correlation for $\alpha < 1$, the more appropriate candidates are the traditional relative entropies. Here we discuss about the traditional Rényi quantum correlation for two-qubit pure states and the Werner state.

**(i) Pure States:** Numerical observations similar to the case with the sandwiched variety, give us that the total correlation of a two-qubit pure state, $|\psi_{AB}\rangle =$

$\sum_{i=0}^{1} \sqrt{\lambda_i}|i_A i_B\rangle$, for traditional relative Rényi entropy, with $\alpha \in (\frac{1}{2}, 1)$, is given by

$$\mathcal{I}_\alpha^{TR}(|\psi_{AB}\rangle) = \min_{\{a\}} \frac{1}{\alpha-1} \log \Big[ \lambda a^{2(1-\alpha)}$$
$$+ (1-\lambda)(1-a)^{2(1-\alpha)} \Big], \qquad (50)$$

where $0 \leq a \leq 1$, and the value of $a$ is obtained from the condition

$$\frac{1}{a} = \left( \frac{\lambda}{1-\lambda} \right)^{\frac{1}{1-2\alpha}} + 1. \qquad (51)$$

The classical correlation in the traditional case in com-
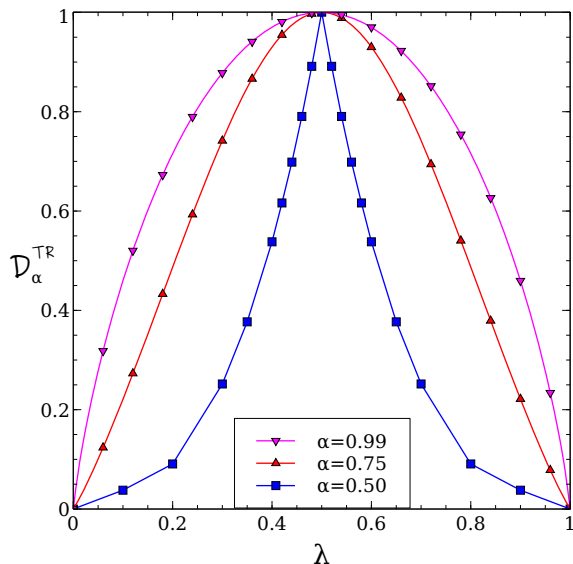


FIG. 6. (Color online.) Traditional Rényi quantum correlation, $\mathcal{D}_\alpha^{TR}$, with respect to $\lambda$, of $|\psi_{AB}\rangle = \sqrt{\lambda}|00\rangle + \sqrt{(1-\lambda)}|11\rangle$ for different $\alpha$. Both axes are dimensionless.

puted numerically. The numerical computation is performed by the same numerical recipe as mentioned in Sec. IV D.

In Fig. 6, we have plotted the $\mathcal{D}_\alpha^{TR}(|\psi_{AB}\rangle)$, for different values of $\alpha$. No anomalous behavior can be seen, and the maximally entangled states have maximal quantum correlations.

**(ii) Werner States:** Like in the sandwiched version, exploiting the rotational invariance and symmetry of the Werner state, it can be shown analytically that the total correlation of the Werner state for the traditional relative Rényi entropy, for $\alpha \in [\frac{1}{2}, 1)$, is given by

$$\mathcal{I}_\alpha^{TR}(\rho_W) = 2 + \frac{1}{\alpha-1} \log \frac{1}{4^\alpha} \big[ (1+3p)^\alpha + 3(1-p)^\alpha \big]. \qquad (52)$$

The classical correlation of the Werner state is also measurement basis independent for the traditional version,

like the sandwiched one. We get that the classical correlation, in this range, is given by

$$\mathcal{J}_\alpha^{TR}(\rho_W) = 2 + \frac{1}{\alpha-1} \log \frac{1}{4^\alpha} \big[ 2(1+p)^\alpha + 2(1-p)^\alpha \big]. \qquad (53)$$

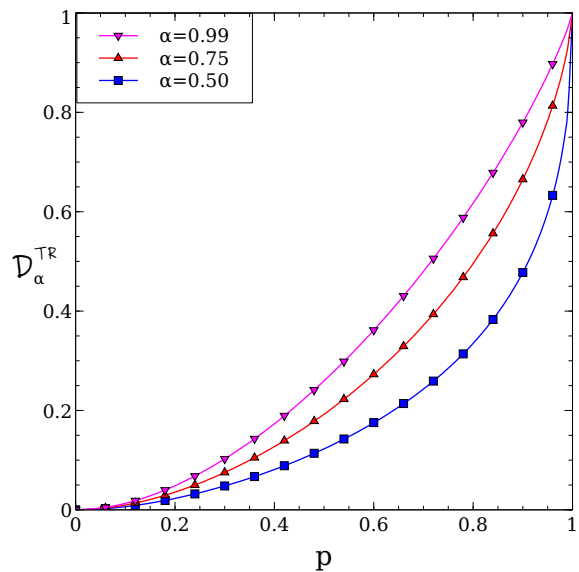The forms of the total and classical correlations, in this



FIG. 7. (Color online.) Traditional Rényi quantum correlation, $\mathcal{D}_\alpha^{TR}$, with respect to $p$ of the Werner state, $\rho_W = p|\psi^-\rangle\langle\psi^-| + (1-p)\frac{1}{4}I$, for different $\alpha$. Both axes are dimensionless.

case, are equivalent to those in the sandwiched version. But here, the range of $\alpha$ is different. Hence, for $\alpha \in [\frac{1}{2}, 1)$, the traditional Rényi quantum correlation for the Werner state is given by

$$\mathcal{D}_\alpha^{TR}(\rho_W) = \frac{1}{\alpha-1} \log \left[ \frac{(1+3p)^\alpha + 3(1-p)^\alpha}{2(1+p)^\alpha + 2(1-p)^\alpha} \right]. \qquad (54)$$

In Fig. 7, we have plotted the $\mathcal{D}_\alpha^{TR}(\rho_W)$, for different values of $\alpha$.

## V. APPLICATION: DETECTING CRITICALITY IN QUANTUM ISING MODEL

In this section, we show that the Rényi and Tsallis quantum correlations can be applied to detect cooperative phenomena in quantum many-body systems. Let us consider a system of $N$ quantum spin-1/2 particles, described by the one-dimensional quantum Ising model [68]. Such models can be simulated by using ultracold gases in a controlled way in the laboratories [5, 69], and is also known to describe Hamiltonians of materials [70]. The Hamiltonian for this system is given by

$$H = J \sum_{i=1}^{N} \sigma_i^x \sigma_{i+1}^x + h \sum_{i=1}^{N} \sigma_i^z, \qquad (55)$$

where $J$ is the coupling constant for the nearest neighbor interaction, $\sigma$'s are the Pauli spin matrices, and $h$ represents the external transverse magnetic field applied across the system. Periodic boundary condition is assumed. The Hamiltonian can be diagonalized by applying Jordan-Wigner, Fourier, and Bogoliubov transformations [68]. At zero temperature, it undergoes a quantum phase transition (QPT) driven by the transverse magnetic field at $\lambda \equiv \dfrac{h}{J} = \lambda_c \equiv 1$ [68]. Such a transition has been detected by using different order parameters [68, 71], including quantum correlation measures like concurrence [72], geometric measures [73–75], and quantum discord [76].

We now investigate the behavior of the Rényi and Tsallis quantum correlations of the nearest neighbor density matrix (reduced density matrix of two neighboring spins) at zero temperature, near the quantum critical point. Note that we have reverted back to the sandwiched version of the relative entropies in this section. The nearest neighbor bipartite density matrix, $\rho_{AB}$, of the ground state of the Hamiltonian given by Eq. (55), represented by $\rho_{AB}$, can be written [68] in terms of the diagonal two-site correlators and the average magnetization in $z$-direction. The density matrix, $\rho_{AB}$, in the thermodynamic limit of $N \to \infty$, is given by

$$\rho_{AB} = \begin{pmatrix} \alpha_+ + \dfrac{M_z}{2} & 0 & 0 & \beta_- \\ 0 & \alpha_- & \beta_+ & 0 \\ 0 & \beta_+ & \alpha_- & 0 \\ \beta_- & 0 & 0 & \alpha_+ - \dfrac{M_z}{2} \end{pmatrix}$$

where $\alpha_\pm = \dfrac{1}{4}(1 \pm T_{zz})$, $\beta_\pm = \dfrac{T_{xx} \pm T_{yy}}{4}$ with $T_{ij} = \mathrm{tr}(\sigma_i \otimes \sigma_j \rho_{AB})$ and $M_z = \mathrm{tr}(\mathbb{I}_A \otimes \sigma_z \rho_{AB})$. The correlations and transverse magnetization, for the zero-temperature state, are given by [68]

$$\begin{aligned} T^{xx}(\lambda) &= G(-1, \lambda), \\ T^{yy}(\lambda) &= G(1, \lambda), \\ T^{zz}(\lambda) &= [M^z(\lambda)]^2 - G(1, \lambda)G(-1, \lambda), \end{aligned} \tag{56}$$

where

$$G(R, \lambda) = \frac{1}{\pi} \int_0^\pi d\phi \frac{(\sin(\phi R)\sin\phi - \cos\phi(\cos\phi - \lambda))}{\Lambda(\lambda)} \tag{57}$$

and

$$M^z(\lambda) = -\frac{1}{\pi} \int_0^\pi d\phi \frac{(\cos\phi - \lambda)}{\Lambda(\lambda)}. \tag{58}$$

Here

$$\Lambda(x) = \left\{ \sin^2\phi + [x - \cos\phi]^2 \right\}^{\frac{1}{2}}, \tag{59}$$
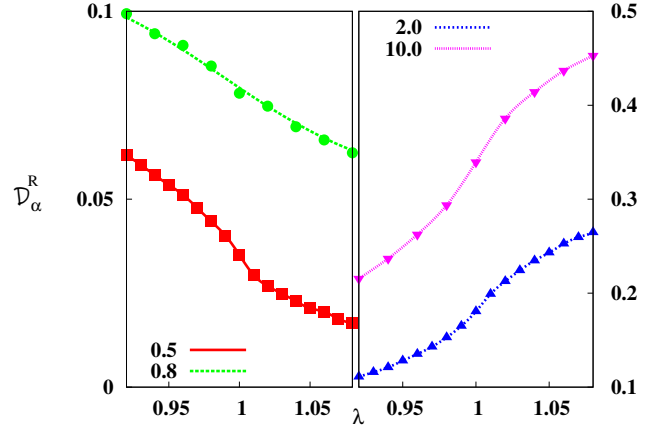
and

$$\lambda = \frac{h}{J}. \tag{60}$$



FIG. 8. (Color online.) Detecting quantum phase transitions with Rényi quantum correlations. Rényi quantum correlation, $\mathcal{D}_\alpha^R$, with respect to $\lambda$, of the nearest neighbor bipartite density matrix at zero temperature, for different values of $\alpha$. The legends indicate the values of $\alpha$. Both axes are dimensionless.

Note that $\lambda$ is a dimensionless variable. The Rényi and Tsallis quantum correlations are calculated for the state, $\rho_{AB}$, for different values of $\alpha$. In Fig. 8, we plot the Rényi quantum correlation as a function of $\lambda$ for different values of $\alpha$. QPT corresponds to a point of inflexion in the $\mathcal{D}_\alpha^\Gamma$ versus $\lambda$ curve and $\frac{d\mathcal{D}_\alpha^\Gamma}{d\lambda}$ diverges there. We claim that the derivatives of the Rényi (and the Tsallis) discords do diverge at the critical point. The seeming finiteness of the derivative at the critical point has to do with the finite spacing of the variable $\lambda$. To see this, we perform a finite-size scaling analysis of the full width at half maxima, of the peak tat is obtained around the critical point for finite size (see Fig. 9).

This feature is distinctly different from the variation of the derivative of the quantum discord with respect to $\lambda$ around the QPT point, which exhibits a point of inflexion at $\lambda = 1$ [76] (cf. [77]). It is only the second derivative of quantum discord with respect to $\lambda$, which diverges at the QPT point. This is an uncomfortable and intriguing feature of quantum discord, and is not shared by e.g. the concurrence at the same quantum critical point [72]. Therefore it is advantageous to use the Rényi and Tsallis quantum correlations to detect phase transitions and other collective phenomena in quantum many body systems, in comparison to quantum discord.

**Finite-size scaling :** The Rényi and Tsallis quantum correlations are shown in Fig. 8 to detect phase transitions in infinite systems. Ultracold gas realization of such phenomena, however, can simulate the corresponding Hamiltonian for a finite number of spins [78]. The quantum Ising model, which has been briefly described earlier in this section, can also be solved for finite-size systems [68]. We calculate the quantum correlations of nearest neighbor spins for finite spin chains using both the
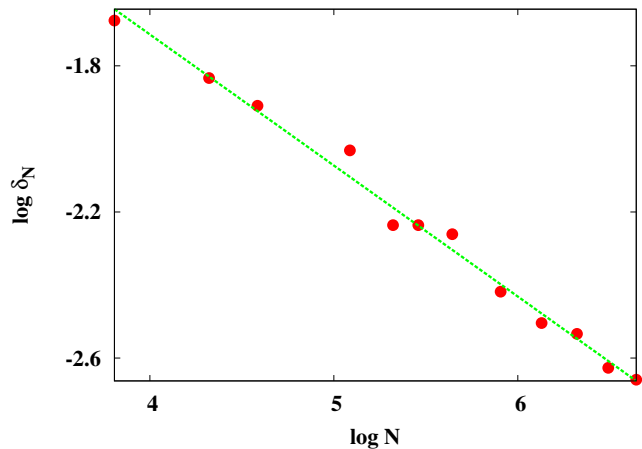
FIG. 9. (Color online.) Scaling analysis of full-width at half maxima, $\delta_N$, for $\mathcal{D}_2^R$. Both axes are dimensionless.



FIG. 10. (Color online.) Scaling analysis of Rényi quantum correlation, $\mathcal{D}_\alpha^R$, for different values of $\alpha$, in the one-dimensional quantum Ising model. The legends indicate the values of $\alpha$. Both axes are dimensionless.

Tsallis and Rényi entropies. We find that the quantum correlations detect the transition in finite-size systems too. Again, the transition point corresponds to points of inflexion in the $\mathcal{D}_\alpha^\Gamma$ versus $\lambda$ curves, and narrow bell-shaped peaks in the $\frac{d\mathcal{D}_\alpha^\Gamma}{d\lambda}$ versus $\lambda$ curves, for different values of $N$. The bell-shaped curves become more narrow and peaked with the increase of number of spins. We perform a finite-size scaling analysis of full-width at half maxima, $\delta_N$, of the $\frac{d\mathcal{D}_\alpha^\Gamma}{d\lambda}$ versus $\lambda$ curves, and the scaling exponent is e.g. -0.36 for $\mathcal{D}_2^R$ (see Fig. 9). The exponent is a measure of the rapidity with which the narrow bell-shaped peak tends to show a divergence with the increment in system size $N$. The $\log - \log$ scaling between the size, $N$, and the width, $\delta_N$, clearly indicates divergence of the derivative at infinite $N$.

We also perform finite-size scaling analyses of the $\lambda_c^N$, the value of $\lambda$ for which the derivatives of the Rényi (or Tsallis) quantum correlations with respect to $\lambda$ has a maximum for a system of $N$ spins, for several different values of $\alpha$, and obtain the corresponding scaling exponents. The exponent is a measure of the rapidity with which the QPT point, $\lambda_c^N$, in a finite size system of size $N$, approaches the QPT point, $\lambda_c$, of the infinite system, as a function of $N$.

TABLE I. The scaling exponents for both $\mathcal{D}_\alpha^R$ and $\mathcal{D}_\alpha^T$ for some values of $\alpha$.

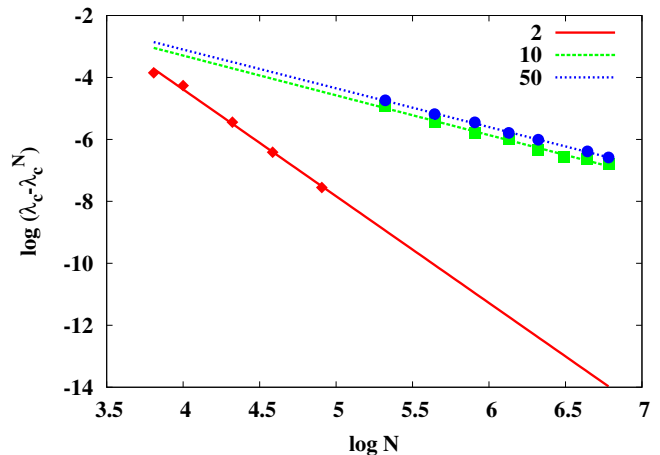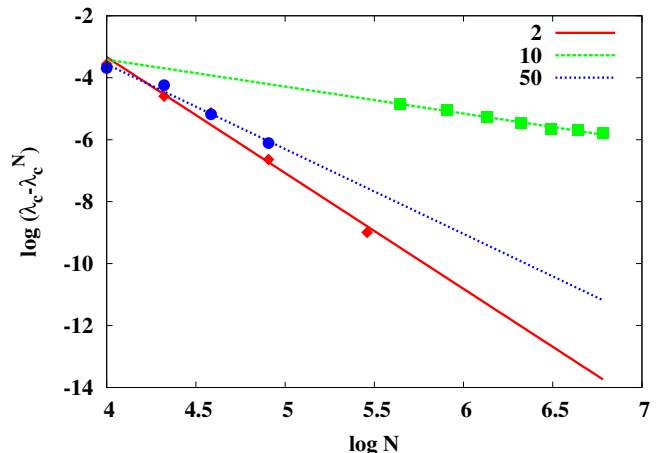| $\alpha$ | $\mathcal{D}_\alpha^R$ | $\mathcal{D}_\alpha^T$ |
|---|---|---|
| 2.0 | -3.45 | -3.74 |
| 10.0 | -1.28 | -0.87 |
| 50.0 | -1.25 | -2.74 |



FIG. 11. (Color online.) Scaling analysis of Tsallis quantum correlation, $\mathcal{D}_\alpha^T$, for different values of $\alpha$, in the one-dimensional quantum Ising model. The legends indicate the values of $\alpha$. Both axes are dimensionless.

Table I exhibits the scaling exponents for both $\mathcal{D}_\alpha^R$ and $\mathcal{D}_\alpha^T$ for some values of $\alpha$. It is found that for $\alpha = 2$, the scaling exponents are much higher for both $\mathcal{D}_\alpha^R$ and $\mathcal{D}_\alpha^T$ than any other known measures. In particular, the scaling exponents for transverse magnetization, fidelity, concurrence, quantum discord, and shared purity are respectively -1.69, -0.99, -1.87, -1.28, and -1.65 [72, 79–82].

## VI. CONCLUSIONS

Quantum discord is a quantum correlation measure, belonging to the information-theoretic paradigm, and it

has the potential to explain several quantum phenomena that cannot be explained by invoking the concept of quantum entanglement. In this paper, we have defined quantum correlations with generalized classes of entropies, viz. the Rényi and the Tsallis ones. The usual quantum discord incorporates the von Neumann entropy in its definition. We first defined the generalized mutual information in terms of sandwiched relative entropy distances. Using this definition of generalized mutual information, we introduced the generalized quantum correlations, and have shown that they fulfill the intuitively satisfactory properties of quantum correlation measures. We have evaluated the generalized quantum correlations for pure states and some paradigmatic classes of mixed states.

As an application, we find that the generalized quantum correlations can detect quantum phase transitions in the transverse quantum Ising model. Interestingly, a finite-size scaling analysis reveals that the scaling exponents obtained for the generalized quantum correla-tions can be significantly higher than the usual quantum discord as well as other order parameters, like transverse magnetization and concurrence, at the same critical point. This aspect can lead to the usefulness of these measures in quantum simulators in ultracold gas experiments, potentially realizing finite versions of quantum spin models. Moreover, while the derivative of the quantum discord provides only a point of inflexion at the quantum critical point, the derivative of the generalized quantum correlations defined here signals the same critical point via a divergence.

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