Quantum discord and its allies: a review

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We review concepts and methods associated with quantum discord and related topics. We also describe their possible connections with other aspects of quantum information and beyond, including quantum communication, quantum computation, many-body physics, and open quantum dynamics. Quantum discord in the multiparty regime and its applications are also discussed.

Contents

I. INTRODUCTION

The quantum theory of nature, formalized in the first few decades of the 20th century, contains elements that are fundamentally different from those required in the classical physics description of nature. One of the most prominent features in quantum physics is the existence of quantum correlations between different quantum systems. In a classical world, if a system in a pure state can be divided into two subsystems, then the sum of the information of the subsystems makes up the complete information of the whole system. This is no longer true in the quantum formalism. In particular, there exists quantum states consisting of two (or more) physical systems for which complete information of the whole is available, even when the subsystems are completely random. Erwin Schrödinger [1] coined the term "quantum entanglement" [2] to describe this quantum feature.

About three decades ago, with the spectacular discoveries of quantum communication and computational schemes [2–6], it has been realized that apart from its fundamental importance, entanglement can be used as a resource to efficiently achieve certain information processing tasks which cannot be performed by using unentangled states. Several of these phenomena and protocols have already been realized in the laboratories by using different physical substrates (see e.g. [7–12]).

However, a thin but steady stream of developments keep being reported which challenge the belief that entanglement is the only form of quantum correlation in shared quantum systems. For example, Knill and Laflamme [13] discovered the protocol of deterministic quantum computation with one quantum bit where the natural bipartite split of the system is unentangled, even though the phenomenon demonstrated is nonclassical, under a plausible assumption. This naturally leads to the quest for quantum correlations beyond entanglement in the same split.

Distinguishability of quantum states lies at the heart of physics [14–19]. And herein we get another whiff of evidence in the same direction, viz. quantum correlation beyond entanglement. For a single-party quantum system, a set of mutually orthogonal states can always be discriminated with certainty. For quantum systems of two (or more) parties, there is a practical and useful restriction on the set of allowed operations to consider only local quantum operations supplemented by classical communication, which has been acronymized as "LOCC" [2]. In this case, even orthogonal states may not be distinguishable. It may seem that the reason behind such indistinguishability is that entangled states cannot be created by LOCC. In sharp disagreement to such intuition, Bennett *et al.* [20] (see also [21, 22]) presented a set of pure states of two quantum spin-1 particles, that despite being product and orthogonal, cannot be locally distinguished, i.e., distinguished by LOCC-based measurement strategies. On the other hand, it was demonstrated that two pure quantum states can always be locally distinguished if they are orthogonal, irrespective of their entanglement content, and irrespective of the number of parties and their dimensions [23] (see also [24–26]). It was moreover exposed that local indistinguishability of certain ensembles of quantum states can be increased by decreasing its average entanglement [27]. These results indicate that the physical quantity or quantities responsible for the nonclassical behavior of local indistinguishability of orthogonal states is clearly of a different nature than entanglement. Indeed, the seminal paper of Bennett *et al.* [20] was titled "Quantum nonlocality without entanglement". Such a correlation quantity beyond entanglement can be the property of equal or unequal mixtures of the ensembles discussed above[1].

Peres and Wootters [32] provided a plausible reasoning that one would require to utilize non-LOCC measurement strategies to optimally distinguish between elements of a two-party quantum ensemble, where the elements are identically prepared pure qubits at the two locations (parties). Such an ensemble is therefore built of "parallel" states[2]. See also [33] in this regard. Furthermore, it was discovered by Gisin and Popescu [34] that "antiparallel" states[3] can contain more information about the spin-direction than the parallel ones. Cf. [35–37].

In another direction, a non-maximally entangled state was found to provide the best resolution for frequency measurements in presence of decoherence [38]. Furthermore, it was discovered that a non-maximally entangled state furnishes the highest violation of a certain Bell inequality [39]. It was also observed that maximally entangled states do not have a special status when considering asymptotic local transformations between two-party entangled quantum states [40].

These developments are some of the potential ones that

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[1] This review considers the question of defining quantum correlation beyond entanglement for quantum states. One may however go further and ask whether it is possible to measure this "nonlocality" in multiparty quantum ensembles. See [28, 29], and compare with [30, 31].

[2] Parallel states are product states of the form $|\uparrow_{\hat{n}}\rangle \otimes |\uparrow_{\hat{n}}\rangle$, where $|\uparrow_{\hat{n}}\rangle$ can, e.g., be the spin-up state in the $\hat{n}$-direction of a quantum spin-up system.

[3] Antiparallel states are product states of the form $|\uparrow_{\hat{n}}\rangle \otimes |\downarrow_{\hat{n}}\rangle$, where $|\uparrow_{\hat{n}}\rangle$ and $|\downarrow_{\hat{n}}\rangle$ can, e.g., be the spin-up and spin-down states in the $\hat{n}$-direction of a quantum spin-$\frac{1}{2}$ system.

FIG. 1: About fishes, large and little. In any catch of fishes, the mesh would net large fishes and let out the little ones with the water. Likewise, the net for non-separable states lets out some quantum correlated states along with states that are deemed as having only "classical" correlations. "Little" fishes are by no means unimportant, as any fisherperson would swear. And, for example, one remembers that in the 1940s and later, a theater group evolved in India that was named "Little Theatre": they certainly weren't staging insignificant pieces. [The sketch is by Mahasweta Pandit.]

have led researchers to address the question whether entanglement is the only way to quantify quantum correlations present in a shared quantum state, and whether there are resources independent of entanglement that can be used to implement quantum protocols with nonclassical efficiencies. It turns out that the non-separability sieve can indeed be seen as leaving out some states that are quantum correlated in a different way. See figure 1. One can fine-grain the sieve, via several approaches, and conceptualize disparate measures of quantum correlations beyond the entanglement-separability paradigm [41–45]. Reviewing such quantum correlation measures and the ensuing implications is the main objective of this survey.

One of the first among such approaches was discovered around 2000, when Ollivier and Zurek [46, 47] and Henderson and Vedral [48] proposed a measure of quantum correlations, known as quantum discord (QD), by quantizing concepts from classical information theory [49]. Around the same time, several other measures were introduced including quantum work deficit [50–53], quantum deficit [54, 55], measurement-induced nonlocality [56], etc. Interestingly, there appeared in this way, quantum states of two or more parties that are not entangled, and yet quantum correlated. The non-vanishing of quantum discord for separable states may be contrasted with the fact that there exists an entanglement measure called distillable entanglement [57, 58], which is vanishing for certain entangled states, viz. the bound entangled states[4] [60].

Sec. II reviews definitions of quantum correlation beyond entanglement and some general properties. This is followed by strategies for detection and the computational complexities of these measures which we briefly review in Secs. III and IV respectively. Some attention is given to the class of states having vanishing QD in Sec. V. Understanding this set is useful for classifying the set of bipartite quantum states according to these quantum correlation measures.

Quantum information processing tasks in which QD or discord-like measures are expected to be important are discussed in Sec. VI. QD can be an interesting tool to detect cooperative phenomena like quantum phase transition and disorder-induced-order in quantum spin systems. This is discussed in Sec. VII. The relation of QD with open quantum system is taken up in Sec. VIII.

In Secs. II to VIII, investigations are restricted, in the main, to bipartite states. We move on to discuss QD for multipartite states in the succeeding sections. The constraints on the sharability of quantum correlations between different parts of a multiparty quantum system has been referred to as the monogamy of quantum correlations. Different aspects of this concept are considered in Secs. IX, X and XI. Definitions of a few multiparty quantum correlation measures are considered in Sec. XII. Some miscellaneous items are collected in Sec. XIII. A short conclusion is presented in Sec. XIV.

II. MEASURES OF QUANTUM CORRELATIONS

Quantification of quantum correlation (QC) present in any quantum state is one of the primary tasks related to the understanding and efficient utilization of the state for various quantum information processing schemes. In this review, we are mainly interested in QC measures which are different from the ones conceptualized within the entanglement-separability paradigm. Quantum discord (QD) is a prominent example of such a measure. In this section, we first provide definitions of these QC measures in three categories: A. Measurement-based QD (Subsec. II A), B. Distance-based QD (Subsec. II B) and C. Other QC measures (quantum discord-like measures) (Subsec. II C).

A. Measurement-based quantum discord

There are several ways that lead to the concept of QD of a bipartite quantum system. These can be classified

[4] There exists a physical quantity called shared purity that can be zero for certain entangled states and non-zero for certain separable states [59].

into two broad categories of which one is based on measurement in any one of the subsystems, which we will discuss now. The other category consists of the distance-based measures which is discussed in the succeeding subsection.

1. Quantum discord

Consider two classical random variables X and Y, for which the joint probability distribution of getting outcome $X = x$ and $Y = y$ is $p_{x,y}$. A measure of mutual interdependence of any of the variables on the other one is the classical mutual information [49] between the variables, which can be written as

$$I(X:Y) = H(X) + H(Y) - H(X,Y), \tag{1}$$

where $H(X)$ and $H(Y)$ are the Shannon entropies[5] of the marginal distributions $p_{x,.}$ and $p_{.,y}$, with dots indicating variables that have been summed over and $H(X,Y)$ is the Shannon entropy of the joint distribution $p_{x,y}$. The same quantity in Eq. (1) can be expressed as

$$I(X:Y) = H(X) - H(X|Y), \tag{3}$$

where the conditional entropy, $H(X|Y)$, is defined as

$$H(X|Y) = \sum_{y\in Y} p_y H(X|Y=y) = H(X,Y) - H(Y). \tag{4}$$

A sleight-of-hand equivalence of these two definitions of mutual information can also be observed from Venn diagram representations of the entropic quantities.

These definitions of classical mutual information can be taken over to the quantum domain [46–48]. It was proposed that the quantum version of the first definition, the quantum mutual information, can be obtained by replacing Shannon entropies by von Neumann entropies[6] [3] in Eq. (1). For a bipartite quantum state ρ_{AB}, shared between two parties, A and B, usually referred to as Alice and Bob, possibly situated in two distant locations, the quantum mutual information is defined as

$$I_{AB} = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{5}$$

where $\rho_i = \mathrm{tr}_j(\rho_{AB})$ ($\{i,j\} \in \{A,B\}, i \neq j$) are local density matrices of ρ_{AB}. One may similarly try to quantize the concept of conditional entropy, which would then lead us to a quantization of classical mutual information, as defined via Eq. (3). However, replacing Shannon entropy to von Neumann [3] in Eq. (4) leads to a quantity which can be positive as well as negative [62–65]. The quantum conditional entropy of ρ_{AB} was argued to be given by

$$S_{A|B} = \min_{\{\Pi_k^B\}\in\mathcal{M}^B} \sum_k p_k S(\rho_{A|k}), \tag{6}$$

where the minimization is taken over all quantum measurements, $\{\Pi_k^B\}$, performed on the system B, and $\mathcal{M}^B$ forms the set of all such measurements. Here, $\{p_k, \rho_{A|k}\}$ is the post-measurement ensemble that is formed at Alice's side, where $\rho_{A|k} = \mathrm{tr}_B(\mathbb{I}_m^A \otimes \Pi_k^B \rho_{AB} \mathbb{I}_m^A \otimes \Pi_k^{B\dagger})/p_k$, with $p_k = \mathrm{tr}_{AB}(\mathbb{I}_m^A \otimes \Pi_k^B \rho_{AB} \mathbb{I}_m^A \otimes \Pi_k^{B\dagger})$, and with $\mathbb{I}_m^A$ being the identity operator on the Hilbert space of Alice's subsystem[7] with dimension m. Therefore, the second form of the classical mutual information, as given in Eq. (3), when quantized in the way mentioned above, gives us the quantity

$$J_{A|B} = S(\rho_A) - S_{A|B}. \tag{7}$$

It can be shown that in general, $I_{AB} \geq J_{A|B}$. However, the inequality can be strict, and indeed it was noticed that they are unequal for almost all two-party quantum states [66]. Moreover, I_{AB} and $J_{A|B}$ are argued to quantify total correlations [67] and classical correlations [48] respectively of a bipartite state ρ_{AB}. Therefore, for a given two-party quantum state, ρ_{AB}, the difference between these two quantities, given in Eqs. (5) and (7) was proposed to be a measure of QC and was called as quantum discord (QD) [46, 47], given by

$$\mathcal{D}^{\leftarrow}(\rho_{AB}) = I_{AB} - J_{A|B}. \tag{8}$$

The notation "$\leftarrow$" in the superscript of QD denotes that the measurement has been performed in the subsystem 'B' while $\mathcal{D}^{\rightarrow}$ denotes QD for the measurement in the first subsystem, i.e. in 'A'. Unless defined otherwise, we will henceforth consider the quantum discord $\mathcal{D}^{\leftarrow}$, and denote it for convenience[8] as $\mathcal{D}$. The definition of QD also provides a justification for considering a maximization in the definition of $J_{A|B}$, since to obtain the amount of QC present in the state, one must pump out all the classical correlations from the total correlations, assuming that total correlations contain only classical and quantum correlations, and that the constituents are additive. Although we will predominantly be dealing with the case when the measurement in the definition

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[5] Let A be a classical random variable, which takes the value a with probability p_a. The Shannon entropy of A is then given by

$$H(A) = -\sum_a p_a \log_2 p_a. \tag{2}$$

[6] The von Neumann entropy [61] of a density matrix σ is given by $S(\sigma) = -\mathrm{tr}(\sigma \log_2 \sigma)$, which reduces to $-\sum_i \lambda_i \log_2 \lambda_i$, where λ_i are the eigenvalues of σ.

[7] Throughout the review, we consider bipartite states on $\mathbb{C}^m \otimes \mathbb{C}^n$, except when considering continuous variable systems.

[8] Since we are using 2 as the base of the logarithm, in the definition of the von Neumann entropy, the unit of QD will be "bits".

is a projective-valued (PV) one, positive-operator valued measurements[9] (POVMs) have also been considered for defining QD. Indeed, POVMs are already present in the definition of classical correlation, $J_{A|B}$ in Ref. [48]. In general, a definition of QD that utilizes POVMs is useful in relating the quantity to other information-theoretic quantities like accessible (classical) information [49] through the Holevo bound [16] and the entanglement of formation (see Appendix XV A 1) through the Koashi-Winter relations [68]. Performing a POVM, however, may render a physical system open and, therefore, has to be cautiously used while providing thermodynamic interpretation of QD and related quantitites [50–52, 69–73]. It is interesting to note here that projective measurements are shown to be optimal among all POVMs for rank-2 bipartite quantum states [74]. On the other hand, there exist states already for two-qubits, for which projective measurements are not optimal [74–78]. See also Ref. [79].

Let us begin here by enumerating some properties of QD, which come to the mind rather immediately, or which are used more frequently later in the review.

a) $\mathcal{D}(\rho_{AB}) \geq 0$, since $I_{AB} \geq J_{A|B}$.

b) QD is not symmetric, i.e., in general, $\mathcal{D}^{\leftarrow}(\rho_{AB}) \neq \mathcal{D}^{\rightarrow}(\rho_{AB})$. This is clearly visible, as conditional entropy is not symmetric for all states. They, of course, coincide for states which are symmetric under interchange of the two parties (cf. [80]).

c) QD is invariant under local unitary transformations, i.e., $\mathcal{D}(\rho_{AB}) = \mathcal{D}[(U_A \otimes U_B)\rho_{AB}(U_A \otimes U_B)^\dagger]$, for arbitrary unitaries U_A and U_B on the subsystems A and B. One of the important characteristics of von Neumann entropy is that it is invariant under unitary transformations, and hence I_{AB} is invariant under local unitaries. Consider now the effect of a local unitary transformation $U_A \otimes U_B$, acting upon the state ρ_{AB}, on the quantum conditional entropy. Suppose that the minimum in Eq. (6) is reached in the measurement $\{\tilde{\Pi}_k^B\}$, for the state ρ_{AB}. For the local unitarily transformed state $(U_A \otimes U_B)\rho_{AB}(U_A \otimes U_B)^\dagger$, a measurement $\{\Pi_k^B\}$ leads to the ensemble $\{p'_k, \rho'_{A|k}\}$, where $\rho'_{A|k} = U_A \mathrm{tr}_B(\mathbb{I}_m^A \otimes \Pi'^B_k \; \rho_{AB} \; \mathbb{I}_m^A \otimes \Pi'^{B\dagger}_k) U_A^\dagger / p'_k$, $p'_k = \mathrm{tr}_A[U_A \mathrm{tr}_B(\mathbb{I}_m^A \otimes \Pi'^B_k \; \rho_{AB} \; \mathbb{I}_m^A \otimes \Pi'^{B\dagger}_k) U_A^\dagger]$, $\Pi'^B_k = U_B^\dagger \Pi_k^B U_B$. Thereby, the optimization of the local unitarily transformed state is reached in the measurement $\{\tilde{\Pi}'^B_k = U_B^\dagger \tilde{\Pi}_k^B U_B\}$, and leads to the same value of the quantum conditional entropy as of ρ_{AB}.

d) QD is zero if and only if their exists a local measurement on B that does not disturb the quantum system [47, 66, 81].

e) For a bipartite pure state, QD reduces to entanglement, i.e., von Neumann entropy of the local density matrices.

f) QD is upper bounded by the von Neumann entropy of the measured subsystem[10] B i.e. $\mathcal{D}^{\leftarrow}(\rho_{AB}) \leq S(\rho_B)$ [86, 87], while $J_{A|B} \leq \min\{S(\rho_A), S(\rho_B)\}$ [88].

While QD and entanglement coincide for pure states, by considering mixed states, it can be shown that QD is different than entanglement. Specifically, it is non-vanishing for some separable states. An example which illustrates this is the class of Werner state [89], given by

$$\rho_W = \frac{1-p}{4}\mathbb{I}_2 \otimes \mathbb{I}_2 + p|\psi^-\rangle\langle\psi^-| \tag{10}$$

with $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ being the singlet state. Here $\mathbb{I}_n$ denotes the identity operator on the n-dimensional complex Hilbert space. It is separable when $p \leq \frac{1}{3}$. However, $\mathcal{D}(\rho_W) > 0$ in the entire range of p except at $p = 0$ [47, 90] (see figure 2).

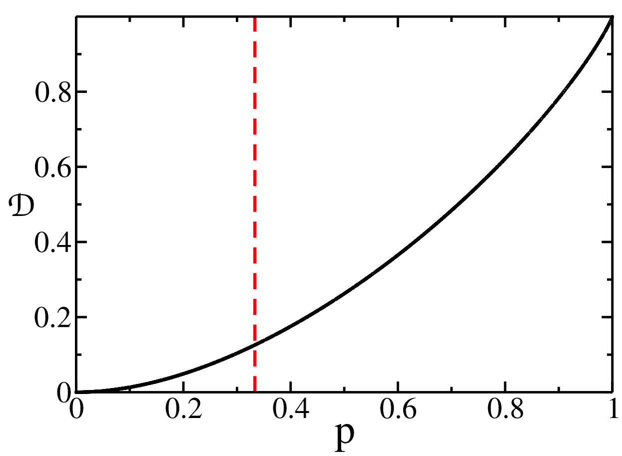

FIG. 2: Quantum discord for the Werner states $\rho_W = \frac{1-p}{4}\mathbb{I}_2 \otimes \mathbb{I}_2 + p|\psi^-\rangle\langle\psi^-|$. The red dashed line corresponds to $p = 1/3$ below which the state is unentangled. [Adapted from Ref. [47] with permission. Copyright 2001 American Physical Society.]

[9] A positive operator valued measure (POVM) [3] is a set of generalized measurement operators $\{\mathcal{A}_i\}$, which are positive semidefinite, and acts on a quantum state ρ in the following way:

$$\rho \to \rho_i = \mathcal{A}_i \rho \mathcal{A}_i^\dagger / p_i, \text{ with } p_i = \mathrm{tr}(\mathcal{A}_i \rho \mathcal{A}_i^\dagger), \tag{9}$$

where $\sum_i \mathcal{A}_i^\dagger \mathcal{A}_i = \mathbb{I}$, and p_i is the probability of obtaining the post-measurement state ρ_i.

[10] The Authors in Ref. [82] have given a necessary and sufficient condition for saturation of this upper bound of QD, by using the conditions for equality of the Araki-Lieb inequality [83–85].

2. Gaussian quantum discord

The concept of QD has been extended to continuous-variable systems, specifically to the case of two-mode Gaussian states [91–102]. When the measurement involved in QD is restricted only to the set of Gaussian measurements [103, 104], it is called Gaussian QD, which is an upper bound of QD of continuous-variable systems. Note that these measurements can be implemented by linear optics and homodyne detection.

Gaussian QD was first evaluated for squeezed thermal states [103, 104] and then further extended to arbitrary two-mode Gaussian states [104]. It has been shown [103, 104] that almost all two-mode Gaussian states have non-zero Gaussian QD. Moreover, squeezed thermal states are entangled if $\mathcal{D}_{Gauss}(\rho_{AB}) > 1$. However, if $\mathcal{D}_{Gauss}(\rho_{AB}) \leq 1$, conclusive identification of entangled state is as yet not possible.

Quantum correlation in continuous variable systems beyond Gaussian states has also been investigated. For a particular type of non-Gaussian two-mode Werner states [105], which is obtained by mixing a two-mode squeezed state with the vacuum, QD has been computed analytically. See also [106]. Giorda *et al.* [107] asked whether non-Gaussian measurements can be optimal for obtaining QD for Gaussian states. To address this query, two-mode squeezed thermal states and mixed thermal states have been studied by considering a range of experimentally feasible non-Gaussian measurements. It is observed that Gaussian measurements always provide the optimal value of Gaussian QD [107]. Moreover, there are numerical evidences which also reveal that QD for Gaussian states require only Gaussian measurements [107, 108]. Pirandola *et al.* [109] connected the Gaussian QD with the result that the minimum von Neumann entropy at the output of a bosonic Gaussian channel is achieved by Gaussian input states [110, 111] (see also [112]). The Authors showed that the solution of the minimization problem for the bosonic Gaussian channel implies the optimality of QD by using Gaussian measurements for a large family of Gaussian states. It is important to note that several experiments have been performed and proposals for the same given to detect and measure Gaussian QD [113–116].

3. Symmetric quantum discord

The original QD [47, 48] in Eq. (8) is not symmetric under the exchange of A and B [80]. However, by performing von Neumann measurements $\{\Pi_i^A \otimes \Pi_j^B\}$ on the entire system, a symmetric version of QD [117] can be defined. Before presenting the definition of the symmetric version of QD, it is useful to rewrite the original QD in the following way. Note first that the quantum mutual information of a bipartite quantum state can be expressed in the following way:

$$I(\rho_{AB}) = S(\rho_{AB}||\rho_A \otimes \rho_B), \tag{11}$$

where ρ_A and ρ_B are local density matrices of ρ_{AB}. The relative entropy between the two quantum states σ and ξ is given by

$$S(\sigma||\xi) = \mathrm{tr}(\sigma \log \sigma - \sigma \log \xi). \tag{12}$$

Clearly, it is not a symmetric function of its arguments, and therefore does not conform to the usual notion of a distance. However, time and again, this "non-standard" distance turns up in different formulae and notions in many areas including in quantum information. Furthermore, one can see that for rank-1 PV measurements, $J_{A|B}(\rho_{AB}) = \max_{\{\Pi_k^B\}\in\mathcal{M}^B} S(\phi_B(\rho_{AB})||\rho_A \otimes \phi_B(\rho_B))$. A symmetric version of QD can now be defined as

$$\begin{aligned}\mathcal{D}_{sym}(\rho_{AB}) = \min_{\{\Pi_i^A\otimes\Pi_j^B\}} [S(\rho_{AB}||\rho_A \otimes \rho_B) - \\ S(\phi_{AB}(\rho_{AB})||\phi_A(\rho_A) \otimes \phi_B(\rho_B))].\end{aligned} \tag{13}$$

Here

$$\begin{aligned}\phi_{AB}(\rho_{AB}) &= \sum_{i,j} (\Pi_i^A \otimes \Pi_j^B)\rho_{AB}(\Pi_i^A \otimes \Pi_j^B), \\ \phi_B(\rho_{AB}) &= \sum_k \mathbb{I}_m^A \otimes \Pi_k^B \rho_{AB} \mathbb{I}_m^A \otimes \Pi_k^B, \\ \phi_\alpha(\rho_\alpha) &= \sum_k \Pi_k^\alpha \rho_\alpha \Pi_k^\alpha, \ \alpha = A, B.\end{aligned} \tag{14}$$

One can rewrite Eq. (13) in terms of quantum mutual information I as [118]

$$\mathcal{D}_{sym}^{mutual}(\rho_{AB}) = \min_{\{\Pi_i^A\otimes\Pi_j^B\}} [I(\rho_{AB}) - I(\phi_{AB}(\rho_{AB}))]. \tag{15}$$

It expresses the minimal amount of correlations which are lost due to the measurements [120]. A similar interpretation is possible for the original QD, but for measurement performed only on one party [119, 120]. The symmetric version of QD has also been considered for the case when POVMs are used for the measurements at the two parties [121, 122]. $\mathcal{D}_{sym}$ is equivalent to what has been termed as measurement-induced disturbance (MID) [55], if instead of considering the minimization, the measurement is performed in the eigenvectors of the reduced density matrices of each part. Since MID does not consist of any optimization over the local measurements, it usually returns an overestimation of the amount of nonclassical correlations compared to the symmetrized version of QD [123]. An analytical formula of the symmetric version of QD has been discussed in Ref. [124] for the Bell-diagonal (BD) states, given by

$$\rho_{AB} = \frac{1}{4}\left(\mathbb{I}_2 \otimes \mathbb{I}_2 + \sum_{i=x,y,z} T_{ii}\sigma^i \otimes \sigma^i\right), \tag{16}$$

where T_{ii} are reals with $-1 \leq T_{ii} \leq 1$ $\forall i$. The T_{ii}'s must also satisfy the additional condition coming from the constraint that the state is positive semidefinite. σ^i, $i = x, y, z$, are the Pauli spin-1/2 operators. The Authors in Ref. [125] presented an experimental implementation of a witness operator for the symmetric version of QD in a composite system.

The symmetric version of QD can also be expressed as

$$\mathcal{D}^f_{sym}(\rho_{AB}) = \min_{\{\Pi^A_i \otimes \Pi^B_j\}} [S(\rho_{AB}||\phi_{AB}(\rho_{AB})) - S(\rho_A||\phi_A(\rho_A)) - S(\rho_B||\phi_B(\rho_B))]. \quad (17)$$

We will discuss the extensions of some of these forms to the multiparty domain. One of these extensions will give rise to the concept of global QD, discussed in Sec. XII A. Note that Eq. (17) can be seen as the difference between two terms, one of which is $S(\rho_{AB}||\phi_{AB}(\rho_{AB}))$, that can be interpreted as the "global distance" of the state ρ_{AB} from the resultant state after local measurements have been carried out. This global distance can be seen as the quantum correlations in ρ_{AB} except that there can be local contributions to this distance in the form of $S(\rho_A||\phi_A(\rho_A))$ and $S(\rho_B||\phi_B(\rho_B))$, and the sum of these two expressions forms the second term, which is subtracted from the global distance to obtain the symmetric version of QD.

Another symmetrized version of QD is the "two-way quantum discord", defined as [126]

$$\mathcal{D}^{\leftrightarrow}(\rho_{AB}) = \max\{\mathcal{D}^{\leftarrow}(\rho_{AB}), \mathcal{D}^{\rightarrow}(\rho_{AB})\}. \quad (18)$$

Other versions of symmetric QD are discussed in Refs. [127, 128].

B. Distance-based quantum discord

We have until now tried to conceptualize QD by quantizing certain concepts in classical information theory. Since such definitions of QD involve optimization over sets of local measurements, the computation of which is in general a challenging task. Moreover, while dealing with the theory of entanglement, we have realized that the quantifications of entanglement originating from different concepts lead to new insights in quantum information.

In this subsection, we are going to discuss the distance-based formulations of QD. The minimization involved in this definition, can often be performed explicitly and hence it becomes a convenient tool for analyzing QC associated with the system. In general, the distance between two quantum states can be defined in several ways [129]. Here, we consider two broad directions by which distance measures are defined, namely, the relative entropy and the norm distance.

In the preceding subsection, we have seen that the original information-theoretic version of QD can be written as the difference between two relative entropy distances. The relative entropy-based QD that is considered in this subsection is a qualitatively different one, and is akin to the relative entropy of entanglement[11] and geometric measures of entanglement. The idea here is to consider a set of states that are devoid of quantum correlations in some sense. Quantum correlation of a given state is then defined as the minimal distance of the state from that set.

1. *Relative entropy-based discord*

The concept of entanglement has led to the realization that there is a class of states, the separable states[12], which are "useless" for certain tasks and have zero entanglement. This in turn has been used to quantify entanglement by measuring the shortest distance of entangled state to the set of separable states [130–132]. In similar vein, one is led to the set of "quantum-classical"(q-c) states having the form

$$\chi^{\text{q-c}}_{AB} = \sum_i p_i \rho_i \otimes |\phi_i\rangle\langle\phi_i| \quad (20)$$

with $p_i \geq 0$, $\sum_i p_i = 1$, $\langle\phi_i|\phi_j\rangle = \delta_{ij}$, and ρ_i's belonging to the subsystem A. Clearly, for the q-c state, there exists a von Neumann measurement on the subsystem B that does not perturb the state. They form the class of "useless" states for tasks where $\mathcal{D}^{\leftarrow}$ is predicted to be a resource. The relative entropy-based QD with distance being considered from the q-c states (with the set of q-c states being denoted below as "q-c"), for a state ρ_{AB} is given by [133]

$$\mathcal{D}^{\text{q-c}}_{rel}(\rho_{AB}) = \min_{\chi^{\text{q-c}}_{AB} \in \text{q-c}} S(\rho_{AB}||\chi^{\text{q-c}}_{AB}). \quad (21)$$

Note that the role of A and B will be exchanged for "classical-quantum" (c-q) states, which are of the form

$$\chi^{\text{c-q}}_{AB} = \sum_i p_i |\phi_i\rangle\langle\phi_i| \otimes \rho_i, \quad (22)$$

with the same conditions stated above, except that ρ_i's belong to the subsystem B. These are exactly the set of "useless" states for tasks for which $\mathcal{D}^{\rightarrow}$ is considered to be useful. One can now define a $\mathcal{D}^{\text{c-q}}_{rel}$ using the c-q states.

[11] See Appendix XV A 4 for a definition of the relative entropy of entanglement.

[12] A separable state is of the form

$$\eta_{AB} = \sum_i p_i \eta^i_A \otimes \eta^i_B, \quad (19)$$

where η^i_j is a density matrix of the j^{th} site and $p_i \geq 0$ with $\sum_i p_i = 1$. These are exactly those states that can be prepared by LOCC between the sites.

We will now briefly discuss the relative entropy-based QD where the distance is taken from the bipartite "classical-classical" (c-c) states $\chi_{AB}^{\text{c-c}}$, given by

$$\chi_{AB}^{\text{c-c}} = \sum_i p_i |\phi_i\rangle\langle\phi_i| \otimes |\psi_i\rangle\langle\psi_i|, \tag{23}$$

with $\langle\phi_i|\phi_j\rangle = \delta_{ij}$ and $\langle\psi_i|\psi_j\rangle = \delta_{ij}$. Mathematically, the measure can be expressed as

$$\mathcal{D}_{rel}(\rho_{AB}) = \min_{\chi_{AB}^{\text{c-c}} \in C} S(\rho_{AB}||\chi_{AB}^{\text{c-c}}). \tag{24}$$

Here C denotes the set of all c-c states.

It is important to mention here that the set of q-c, c-q and c-c states are all subsets of the set of separable states, which form a convex set, while the formers do not.

One may now define a classical correlation based on relative entropy distance of the state ρ_{AB}, as

$$J_{rel}^{\text{q-c}}(\rho_{AB}) = S(\chi_{\rho_{AB}}^{\text{q-c}}||\Pi_{\chi_{\rho_{AB}}^{\text{q-c}}}), \tag{25}$$

where $\chi_{\rho_{AB}}^{\text{q-c}}$ and $\Pi_{\chi_{\rho_{AB}}^{\text{q-c}}}$ are respectively the closest q-c state of ρ_{AB} and the closest product state[13] of $\chi_{\rho_{AB}}^{\text{q-c}}$, with respect to the relative entropy distance. Interestingly, it was found that $I - (\mathcal{D}_{rel}^{\text{q-c}} + J_{rel}^{\text{q-c}}) = -\mathcal{L}$ where $\mathcal{L} = S(\Pi_{\rho_{AB}}||\Pi_{\chi_{\rho_{AB}}^{\text{q-c}}})$ [133] and I is the quantum mutual information given in Eq. (11). Here $\Pi_{\rho_{AB}}$ is the closest product state of ρ_{AB}. A similar relation among the same quantities, but by using a linearized variant of relative entropy has also been addressed in Ref. [134]. Note here that the above concept of relative entropy-based QD can also be extended to the multipartite domain [133]. See Sec. XII B.

2. *Geometric quantum discord*

In this subsection, we consider the quantification of quantum correlation again by using a distance to the set of q-c, c-q, or c-c states, but here the distance is defined via a norm on the relevant space of quantum states. Such quantifications are generally referred to as geometric quantum discord (GQD).

Let us begin with the definition of GQD of a bipartite state ρ_{AB}, as proposed by Dakić *et al.* [66], based on the Hilbert-Schmidt distance[14]. It is given by

$$\mathcal{D}_G(\rho_{AB}) = \min_{\chi_{AB}^{\text{q-c}} \in \text{q-c}} ||\rho_{AB} - \chi_{AB}^{\text{q-c}}||^2, \tag{26}$$

where the minimization is performed over the set of all quantum states with vanishing $\mathcal{D}^{\leftarrow}$. See Eq. (20). One of the utilities of the above definition lies in the fact that for a general two-qubit quantum state, one can show that Eq. (26) has the closed analytical form given by

$$\mathcal{D}_G(\rho_{AB}) = \frac{1}{4}\sum_i\sum_j(||x_i||^2 + ||T_{ij}||^2 - k_{\max}), \tag{27}$$

where ρ_{AB} is expressed using one- and two-point classical correlators as

$$\begin{aligned}\rho_{AB} &= \frac{1}{4}\Big(\mathbb{I}_2 \otimes \mathbb{I}_2 + \sum_i x_i \sigma^i \otimes \mathbb{I}_2 + \sum_i y_i \mathbb{I}_2 \otimes \sigma^i \\ &+ \sum_{ij} T_{ij}\sigma^i \otimes \sigma^j\Big),\end{aligned} \tag{28}$$

with $T_{ij} = \text{tr}(\rho_{AB}\ \sigma^i \otimes \sigma^j)$ being the two-point classical correlators forming a 3×3 correlation matrix T, while $x_i = \text{tr}(\rho_{AB}\ \sigma^i \otimes \mathbb{I}_2)$ and $y_i = \text{tr}(\rho_{AB}\ \mathbb{I}_2 \otimes \sigma^i)$, $i, j \in \{x, y, z\}$. $k_{\max}$ is the largest eigenvalue of the matrix $K = TT^T + xx^T$, where x is a column vector of the magnetizations x_i. Using this, one can show that for two-qubits, the states with maximal $\mathcal{D}_G$ are the singlet state and states connected to it by local unitaries. Among separable states, the states exhibiting maximum GQD are given by

$$\sigma_{i_1 i_2 i_3} = \frac{1}{4}\left(\mathbb{I}_2 \otimes \mathbb{I}_2 + \frac{1}{3}\sum_{k=1}^{3}(-1)^{i_k}\sigma^k \otimes \sigma^k\right), i_k = \pm 1. \tag{29}$$

Further generalizations in this direction have been carried out by Luo and Fu [119]. An arbitrary bipartite quantum state ρ_{AB} on $\mathbb{C}^m \otimes \mathbb{C}^n$ can be expressed as

$$\rho_{AB} = \sum_{ij} c_{ij}\ X_i \otimes Y_j, \tag{30}$$

where $\{X_i, i = 1, 2, \ldots, m^2\}$ and $\{Y_j, j = 1, 2, \ldots, n^2\}$ are sets of Hermitian operators, forming orthonormal bases in the space of Hermitian operators on $\mathbb{C}^m$ and $\mathbb{C}^n$ respectively, with the inner product and so does the operator $X_i \otimes Y_j$ on $\mathbb{C}^m \otimes \mathbb{C}^n$. By using Eq. (30), another form of GQD in terms of state parameters can be obtained and is given in the following theorem:

Theorem 1 [119]: *The analytical form of GQD for an arbitrary bipartite state ρ_{AB} on $\mathbb{C}^m \otimes \mathbb{C}^n$ can be expressed as*

$$\mathcal{D}_G(\rho_{AB}) = \text{tr}(\tilde{C}\tilde{C}^T) - \max_A \text{tr}(A\tilde{C}\tilde{C}^T A^T), \tag{31}$$

where $\tilde{C} = (c_{ij})$, $c_{ij} = \text{tr}(\rho_{AB}\ X_i \otimes Y_j)$, and the maximization is performed over $A = (a_{kl})$, with $a_{kl} = \text{tr}(|k\rangle\langle k|\ X_l^\dagger)$. Here $k = 1, 2, \ldots, m$, $l = 1, 2, \ldots, m^2$ and $\{|k\rangle\}$ is an orthonormal basis in $\mathbb{C}^m$.

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[13] A product state of two parties is of the form $\tilde{\eta}_A \otimes \tilde{\eta}'_B$.

[14] The Hilbert-Schmidt norm and the trace norm are special cases of the Schatten p-norm, which, for an arbitrary operator X, is defined as

$$||X||_p = \left[\text{tr}\big((X^\dagger X)^{\frac{p}{2}}\big)\right]^{\frac{1}{p}}.$$

The Hilbert-Schmidt norm and the trace norm are obtained for $p = 2$ and $p = 1$ respectively.

From the above form of $\mathcal{D}_G(\rho_{AB})$, one obtains a lower bound on $\mathcal{D}_G(\rho_{AB})$, namely

$$\mathcal{D}_G(\rho_{AB}) \geq \mathrm{tr}(\tilde{C}\tilde{C}^T) - \sum_{i=1}^{m} \lambda_i = \sum_{i=m+1}^{m^2} \lambda_i, \quad (32)$$

where λ_i's are the eigenvalues of $\tilde{C}\tilde{C}^T$ in a non-increasing order.

Motivated by the original definition of QD (see Eq. (8)), a "modified" GQD can be defined as [119]

$$\tilde{\mathcal{D}}_G(\rho_{AB}) = \min_{\{\Pi_k^B\}} ||\rho_{AB} - \phi_B(\rho_{AB})||^2, \quad (33)$$

where the minimization is performed over the set of projective measurements $\{\Pi_k^B\}$ performed by B and the definition of $\phi_B(\rho_{AB})$ is given in Eq. (14), and it turns out that $\mathcal{D}_G(\rho_{AB}) = \tilde{\mathcal{D}}_G(\rho_{AB})$. Instead of the Hilbert-Schmidt distance, the above concept of the modified GQD has also been generalized by considering the trace norm distance [135–138].

In subsequent years, several attempts have been made to obtain tighter lower bounds of the above expression of GQD given in Eq. (27) [139–156]. In particular, Hassan *et al.* [146] showed that the lower bound on GQD obtained in Eq. (32), can further be improved to

$$\mathcal{D}_G(\rho_{AB}) \geq \frac{2}{m^2 n}(||\vec{x'}||^2 + \frac{2}{n}||T'||^2 - \sum_{j=1}^{m-1} \eta_j), \quad (34)$$

where $\eta_j, j = 1, 2, \ldots, m^2 - 1$ are the eigenvalues of the matrix $(\vec{x'}\vec{x'}^T + \frac{2T'T'^T}{n})$, arranged in non-increasing order. Here $x'_i = \mathrm{tr}(\rho_{AB}\mathcal{L}_i \otimes \mathbb{I}_n)$ and $T'_{ij} = \mathrm{tr}(\rho_{AB}\mathcal{L}_i \otimes \mathcal{L}'_j)$ with $\mathcal{L}_i$ and $\mathcal{L}'_j$ being the generators of $SU(m)$ and $SU(n)$ respectively. The lower bound in Eq. (34) is tighter than that in Eq. (32) and this can be illustrated by two examples, viz. $\rho_{AB}(p) = p|e_1\rangle\langle e_1| + \frac{1}{9}(1-p)\mathbb{I}_3 \otimes \mathbb{I}_3$, and $\rho'_{AB}(p) = (1-p)|e_1\rangle\langle e_1| + p|e_2\rangle\langle e_2|$, for any p, where $|e_1\rangle = \frac{1}{\sqrt{6}}(|22\rangle + |33\rangle + |21\rangle + |12\rangle + |13\rangle + |31\rangle)$, $|e_2\rangle = \frac{1}{2}(|11\rangle + |22\rangle + \sqrt{2}\,|33\rangle)$ with $0 \leq p \leq 1$ (see figures 1 and 2 in Ref. [146]). Additionally, the lower bound obtained in Eq. (34) becomes exact for a $\mathbb{C}^2 \otimes \mathbb{C}^n$ system.

Furthermore, GQD for an arbitrary state ρ_{AB} on $\mathbb{C}^2 \otimes \mathbb{C}^n$ has also been derived by Vinjanampathy *et al.* [147] and Luo *et al.* [148]. Moreover, in Ref. [149], a tight measurement-based upper bound of GQD where the distance is calculated from the c-c states has been found for two-qubit quantum states by considering the Hilbert-Schmidt distance. In addition to this, nonclassical correlations of some well known bipartite bound entangled states (on $\mathbb{C}^2 \otimes \mathbb{C}^4, \mathbb{C}^3 \otimes \mathbb{C}^3$ and $\mathbb{C}^4 \otimes \mathbb{C}^4$) have been calculated by using GQD [21, 150, 157–159]. A relation between QD and GQD for two-qubit systems has further been proposed in Ref. [143]. Moreover, in subsequent works, a relation between negativity (for defintion, see Appendix XV A 3) and GQD has also been conjectured [160–162].

The original definition of QD involved one-sided measurements. Subsequently, certain symmetric versions of QD, involving measurements on both sides were defined. See Sec. II A 3. Within the span of distance-based measures of QD, $\mathcal{D}_{rel}$ in Eq. (24) is such a symmetric version of QD. A symmetric version of GQD involving two-sided measurements was defined in Refs. [141, 149, 151] as

$$\mathcal{D}_G^{sym}(\rho_{AB}) = \min\ ||\rho_{AB} - \phi_{AB}(\rho_{AB})||^2, \quad (35)$$

where $\phi_{AB}(\rho_{AB})$ is given in Eq. (14) and the minimization is carried out over the set of all two-sided independent local measurements. A lower bound, similar to the one in Eq. (32), can also be obtained in this case.

Down the avenue, several works were reported where questions have been raised regarding the validity of the above formulation of GQD [163–165]. In case of conventional QD, as expressed in Eq. (8), it is known that the value of QD can be increased by applying some local operations on the part on which measurement has to be performed, although it can not be increased by performing any operations on the unmeasured part. In contrast, it was shown [163, 164, 166] that GQD in Eq. (26) is not monotonic when the operations are performed even on the unmeasured subsystem of ρ_{AB}. In particular, if one considers the map on the unmeasured part say A, as $\tau : X \to \sigma \otimes X$, i.e. adding an ancilla at A, then the Hilbert-Schmidt norm of the state, after this action, is given by

$$||X||_2 \to ||X||_2\sqrt{\mathrm{tr}(\sigma^2)}, \quad (36)$$

using the property of the norm under tensor product. In other words, the value of GQD becomes a function of the purity of the local ancilla upon addition of an ancillary system.

In this regard, a possible remedy has also been suggested in Ref. [163]. Specifically, the definition in Eq. (26) can be modified as

$$\mathcal{D}_G^{mod}(\rho_{AB}) = \max_{\Lambda_A} \mathcal{D}_G(\Lambda_A \rho_{AB}), \quad (37)$$

where the maximization is taken over all quantum channels acting on part A. However, such introduction of another maximization makes the computation of the resulting quantity difficult. It was also pointed out that the inherent non-monotonicity present in the GQD, in principle can still lead to unwanted results [165–168]. It has been found that highly mixed states containing non-zero and even near-maximal quantum correlation as measured by QD may have negligible GQD. This is at least partly due to the fact that the Hilbert-Schmidt distance is highly sensitive to the purity of the state in its argument. Attempts have also been made to define GQD by using other distance measures such as the trace norm [165], Bures distance [169, 170], Hellinger distance [137, 171], etc. See also [172]. In this regard, Bai *et al.* [173] have shown that for a class of symmetric two-qubit "X-states"[15], GQD using the trace norm [176] serves as a lower bound for the same using the Hilbert-Schmidt distance. See also Ref. [177].

C. Other quantum correlation measures

Apart from QD, several other measures of quantum correlation beyond entanglement have been introduced. Below, we briefly discuss some of them, specifically, quantum work deficit (WD) [50–52], quantum deficit [54], and measurement-induced non-locality (MIN) [56].

It is important to mention that there are further measures that have been put forward in the last fifteen years or so. These include the ones that have been proposed [134, 178–184] based on Rényi and Tsallis entropies [185–191]. Further examples include Refs. [59, 192–205].

1. Quantum work deficit

Quantum work deficit (WD) [50] was introduced to quantify quantum correlation by exploring the connection between thermodynamics and information [69–72, 206]. It is defined as the information, or work, that cannot be extracted from a bipartite quantum state when the two parties are in distant locations, as compared to the case when the same are together. Just as in any thermodynamical consideration for extracting work, one must be careful in setting up the stage with respect to the allowed operations for the work extraction. The set of allowed operations for work extraction for the bipartite quantum state when the two parties are at the same location is termed as "closed operations (CO)". The same set in the distant laboratories paradigm is called "closed local operations and classical communication (CLOCC)" [50–53, 207–210]. Here, closed operations are formed by (i) global unitary operations, and (ii) dephasing operation on the bipartite state by a projective measurement on the entire Hilbert space of the two-party system. On the other hand, CLOCC is constituted of (i) local unitary operations, (ii) dephasing by local measurements on either subsystem, and (iii) communicating the dephased subsystem to the other one, by using a noiseless quantum channel. For a bipartite quantum state ρ_{AB} on $\mathbb{C}^m \otimes \mathbb{C}^n$, it was shown that the works extractable by CO and CLOCC are respectively I_{CO} and I_{CLOCC}, given by

$$I_{CO}(\rho_{AB}) = \log_2 d - S(\rho_{AB}), \tag{38}$$

$$I_{CLOCC}(\rho_{AB}) = \log_2 d - \min_{\{\Pi_i^B\}} S(\rho'_{AB}), \tag{39}$$

where $\rho'_{AB} = \sum_i \mathbb{I}_m^A \otimes \Pi_i^B \ \rho_{AB} \ \mathbb{I}_m^A \otimes \Pi_i^B$ is the locally dephased state, assuming that CLOCC involved dephasing on $\mathbb{C}^n$, and $d = mn$. Here, the minimization is performed over all projective measurements on the system at B. We have ignored here a multiplicative term, viz. $k_B T$, in the definitions of work, where T represents the temperature of the heat bath involved, and k_B is the Boltzmann constant. The difference between I_{CO} and I_{CLOCC} is defined as the "one-way work deficit", given by

$$\mathcal{WD}^{\leftarrow}(\rho_{AB}) = I_{CO}(\rho_{AB}) - I_{CLOCC}(\rho_{AB}). \tag{40}$$

Note that like in the definition QD in Eq. (8), " $\leftarrow$ " in the superscript indicates the subsystem B as the dephased party. Moreover, WD also reduces to von Neumann entropy of the local density matrices for pure bipartite states. WD is similar to QD for states whose marginal states are maximally mixed [211]. See also [212] in this regard.

If the dephasing process in CLOCC does not include any communication between the subsystems and both the parties completely dephase their subsystems by closed local operations, the corresponding work deficit is called zero-way work deficit. On the other hand, if the dephasing protocol in CLOCC followed by the two parties involves several communication rounds between them, the corresponding quantity is known as the two-way work deficit. Note that the relative entropy-based QD turns out to be zero-way work deficit when the distance is taken from the set of c-c states, whereas one-way work deficit is equal to relative entropy-based QD when the distance is considered from c-q or q-c states, whichever is relevant [52, 213]. The definitions of extractable work are related to the concept of Maxwell's demon [69–72, 206, 214–218]. Indeed, for each bit of information obtained, an amount of work equal to $k_B T$ can be performed. This however does not violate the second law of thermodynamics, as an equal amount of work is needed to erase the memory corresponding to the information. For this and further discussions on this issue, see [50–53, 73, 77, 207–210, 219–223].

2. Quantum deficit

Another measure of quantum correlation, introduced by Rajagopal and Rendell, has been called quantum deficit [54, 224]. It is defined as the closeness of a given quantum state to its decohered classical counterpart. More precisely, for a bipartite quantum state ρ_{AB}, it is given as the relative entropy distance between ρ_{AB} and its decohered density operator ρ_{AB}^d:

$$\mathcal{R}(\rho_{AB}) = S(\rho_{AB} || \rho_{AB}^d). \tag{41}$$

[15] A bipartite state is called an X-state [174, 175] if in the computational basis, it has non-zero entries only in its diagonal and anti-diagonal positions, so that the state looks like the letter "X".

The quantum deficit uses the decohered density matrix

$$\rho_{AB}^d = \sum_{a,b} p_{ab}|a\rangle\langle a| \otimes |b\rangle\langle b|, \tag{42}$$

where $\{|a\rangle\}$ and $\{|b\rangle\}$ are eigenbases of the reduced density matrices ρ_A and ρ_B respectively of ρ_{AB}. Here, $p_{ab} = \langle a| \otimes \langle b|\rho_{AB}|a\rangle \otimes |b\rangle$ are the diagonal elements of ρ_{AB}. Let λ_i be the eigenvalues of ρ_{AB}. Eq. (41) then reduces to

$$\mathcal{R}(\rho_{AB}) = \sum_i \lambda_i \log_2 \lambda_i - \sum_{a,b} p_{ab} \log_2 p_{ab}. \tag{43}$$

It is important to observe that no optimization is required for the evaluation of quantum deficit. Also, unlike QD and one-way WD, this measure is symmetric with respect to the subsystems.

3. *Measurement-induced nonlocality*

"Measurement-induced nonlocality (MIN)" is another measure of quantum correlation that is defined by using a distance to a set of states deemed as "classical" [56]. It is to be noted that the "nonlocality" in the name does not have any direct relation with the Einstein-Podolsky-Rosen argument [225] or the Bell's theorem [226, 227]. For a bipartite quantum state ρ_{AB}, we first consider arbitrary projective measurements $\{\Pi_k^B\}$ on the party B, that keeps the reduced density matrix ρ_B invariant if we forget the measurement outcome, i.e. $\sum_k \Pi_k^B \rho_B \Pi_k^B = \rho_B$. The MIN is then defined as the highest Hilbert-Schmidt distance between the pre- and post-measured states:

$$M_N(\rho_{AB}) = \max_{\{\Pi_k^B\}} ||\rho_{AB} - \phi_B(\rho_{AB})||^2. \tag{44}$$

The optimization over the $\{\Pi_k^B\}$ is required only when the spectrum of ρ_B is degenerate and the definition of $\phi_B(\rho_{AB})$ is given in Eq. (14). For the non-degenerate case, the only allowed measurement is on the eigenbasis of ρ_B. An analytical formula of MIN for arbitrary-dimensional pure states has been found, and for $|\psi_{AB}\rangle = \sum_i \sqrt{\mu_i}|i_A\rangle|i_B\rangle$, the MIN is given by

$$M_N(|\psi_{AB}\rangle) = 1 - \sum_i \mu_i^2, \tag{45}$$

where $\sqrt{\mu_i}$ are the Schmidt coefficients. Moreover, for mixed states on $\mathbb{C}^m \otimes \mathbb{C}^n$, there exists a tight upper bound of MIN, namely $M_N(\rho_{AB}) \leq \sum_{i=1}^{m^2-m} \lambda_i$ where $\{\lambda_i, i = 1, 2, \ldots, m^2 - 1\}$ are the eigenvalues of TT^T in non-increasing order, with T being the correlation matrix. Comparing the symmetric version of GQD as defined in Eq. (35), with MIN, one notices that they are complementary.

III. COMPUTABILITY OF QUANTUM DISCORD

For a general quantum state, calculation of QD involves an optimization over measurements, which makes it difficult to obtain a closed analytical expression. In particular, for calculating $S_{A|B}$ in Eq. (6), the minimum has to be taken over a certain set of measurements on the subsystem with B. This set can, for example, be the set of all PV measurements or all generalized measurements described by POVMs. As shown in Refs. [79, 228], the number of elements in the extremal POVM need not be more than the square of the dimension of the system, and hence for states on $\mathbb{C}^2 \otimes \mathbb{C}^2$, the optimization in the classical correlation does not need consideration of POVMs whose elements number more than four [229]. Moreover, it was argued that on $\mathbb{C}^m \otimes \mathbb{C}^m$, at most $\frac{m(m+1)}{2}$ POVM elements are required for the optimization [230], implying that in $\mathbb{C}^2 \otimes \mathbb{C}^2$, a 3-element POVM is sufficient. It is evident that for an arbitrary bipartite quantum state in arbitrary dimension, the optimized measurement setting over the set of PV measurements or POVMs for classical correlation is generally hard to perform, both analytically as well as numerically.

In this direction, Huang [231] showed that the time required to compute QD grows exponentially with the increase of the dimension of the Hilbert space, implying that computation of QD is NP-complete [3].

In finite dimensions, a closed formula of QD is known only for specific classes of states. However, an analytic expression of the Gaussian QD can be obtained for continuous variable systems, as seen in Sec. II A 2. Furthermore, as discussed in Sec. II B 2, GQD can be evaluated analytically for arbitrary two-qubit systems [232].

A. Qubit systems

In the two-qubit scenario, POVMs with rank-1 elements are sufficient to optimize the QD [229]. A compact form of QD for arbitrary rank-2 states on $\mathbb{C}^2 \otimes \mathbb{C}^2$ is obtained in Ref. [229], after performing the optimization over all POVMs where Koashi-Winter relation [68] has been used. We will discuss the latter in Sec. X. It was shown [233] that a PV measurement is optimal for QD in this case while it is conjectured that 3-element POVM is required to obtain QD for states with rank more than 2. Let us for a while focus our attention on X-states. The reason for such a choice is partly because for such states, there has been some progress towards numerical and analytical tractability of a closed form of QD [234, 235]. Another reason is that X-states often appear in physical systems of interest. In particular, for a Hamiltonian, H, having $\mathbb{Z}_2$-symmetry on $\otimes_i \mathbb{C}_i^2$, the two-qubit reduced density matrix, ρ_{AB}, of the ground state, ρ, boils down to a X-state. The argument runs as follows:

$$[H, \otimes_i \sigma_i^z] = 0 \implies [\rho, \otimes_i \sigma_i^z] = 0 \implies [\rho_{AB}, \sigma_A^z \otimes \sigma_B^z] = 0$$
$$\implies \rho_{AB} = \begin{bmatrix} a & 0 & 0 & e \\ 0 & b & f & 0 \\ 0 & f^* & c & 0 \\ e^* & 0 & 0 & d \end{bmatrix}, \tag{46}$$

where a, b, c, d are real and non-negative with $a+b+c+d = 1$. The positivity of ρ_{AB} is ensured by $|e|^2 \leq ad$ and $|f|^2 \leq bc$. In general, e and f may be complex numbers, although they can be made real and non-negative by local unitary transformations. Hence, without loss of generality, one can take $e, f \geq 0$. To perform the optimization involved in Eq. (6), if we restrict ourselves to PV measurements, we can parametrize the measurement basis $\{\Pi_k = |k'\rangle\langle k'|\}$ by two angles $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$:

$$\begin{aligned} |0'\rangle &= \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \\ |1'\rangle &= \sin\frac{\theta}{2}|0\rangle - e^{i\phi}\cos\frac{\theta}{2}|1\rangle. \end{aligned} \tag{47}$$

The original definition of QD in Eq. (8) can be rewritten as the difference between the conditional entropy of the post- and pre-measured quantum states ρ'_{AB} and ρ_{AB}, respectively and is given by

$$\mathcal{D}(\rho_{AB}) = S_{A|B} - S'_{A|B}, \tag{48}$$

where $S_{A|B}$ is the conditional entropy of the post-measured state, given in Eq. (6) while $S'_{A|B} = S(\rho_{AB}) - S(\rho_B)$ is the pre-measured conditional entropy which can be exactly obtained in closed form. It can be seen that $S_{A|B} = \min_{\{\Pi_k^B\}}[S(\rho'_{AB}) - S(\rho'_B)]$, $\rho'_{AB} = \sum_k p_k \rho_{A|k} \otimes \Pi_k^B$, where ρ'_B is a reduced density matrix of the average post-measured state ρ'_{AB}, and $\{p_k, \rho_{A|k} \otimes \Pi_k^B\}$ is the post-measured ensemble. Therefore,

$$S_{A|B} = \min_{\theta,\phi}[\Lambda_+ \log_2 \Lambda_+ + \Lambda_- \log_2 \Lambda_- - \sum_{i=1}^{4} \lambda_i \log_2 \lambda_i], \tag{49}$$

where the eigenvalues of ρ'_B are $\Lambda_\pm = (1 \pm (a-b+c-d)\cos\theta)/2$ and the same of ρ'_{AB} are given by

$$\begin{aligned} \lambda_{1,2} &= \{1 + (a-b+c-d)\cos\theta \\ &\quad \pm[(a+b-c-d+(a-b-c+d)\cos\theta)^2 \\ &\quad +4(e^2+f^2+2ef\cos 2\phi)\sin^2\theta]^{1/2}\}/4, \\ \lambda_{3,4} &= \{1 - (a-b+c-d)\cos\theta \\ &\quad \pm[(a+b-c-d-(a-b-c+d)\cos\theta)^2 \\ &\quad +4(e^2+f^2+2ef\cos 2\phi)\sin^2\theta]^{1/2}\}/4. \end{aligned} \tag{50}$$

To obtain $S_{A|B}$, we need to minimize the quantity over the parameters θ and ϕ. The concavity of Shannon entropy ensures that minimization over ϕ happens at $\cos 2\phi = 1$, although the extremum points over θ has not be exactly located analytically. Assuming that the optimal measurement basis is either the eigenstates of σ^z or those of σ^x has been found to provide a close estimate. See Refs. [236–241] in this regard. For the states satisfying the above assumption, we have

$$\mathcal{D}(\rho_{AB}) \stackrel{?}{=} \min\{\mathcal{D}_{\{\sigma^x\}}(\rho_{AB}), \mathcal{D}_{\{\sigma^z\}}(\rho_{AB})\}, \tag{51}$$

where $\mathcal{D}_{\{\sigma^\alpha\}}(\rho_{AB})$ is the QD with the measurement basis being the eigenbasis of σ^α with $\alpha = x, z$. Here, the measurement in QD has been restricted to PV ones. The question-mark is kept on the equality to indicate that the relation is not true in general. For a subset of X-states, namely for Bell-diagonal states (for which $a = d, b = c$), Eq. (51) is valid [90, 242]. Even for symmetric X-states (i.e., with $b = c$) [236], Eq. (51) is not always valid. It was proven that optimal measurement for QD is $\{\sigma^z\}$, if $(|e| + |f|)^2 \leq (a-b)(d-c)$, while the optimal measurement will be $\{\sigma^x\}$ when $|\sqrt{ad} - \sqrt{bc}| \leq |e| + |f|$ [26, 243]. Let us mention here that for the two-parameter family of X-states within the specific regions mentioned in the previous sentence, QD (that contains an optimization over all POVMs) is obtained from a POVM with 3 elements, confirming the conjecture of Ref. [229].

Beyond X-states, recent studies in this direction reveal that for a large majority of two-qubit states, an optimal measurement is among the eigenstates of σ^x, σ^y, and σ^z, and very small errors persist for the states which do not minimize on the aforementioned sets [235, 244, 245]. Motivated by these observations and the error analysis for the X-states, QD has been considered for different restricted classes of measurements, and the general term, "constrained QD", has been used to identify them [246]. The differences of the original QD and such constrained QDs have been investigated for Haar uniformly generated bipartite two-qubit as well as two-qutrit states with different ranks, including some positive partial transpose (PPT[16]) bound entangled states [60]. In particular, for the X-states, the maximal absolute error is 0.0029. It was found that the error decreases very rapidly with increase of size of the restricted measurement set. These restricted classes of projectors were chosen in several ways over the space of projection measurements. Moreover, it was also shown that for the quantum transverse XY spin chain of finite length, constrained QD exactly matches with the actual QD and hence can detect the quantum phase transition (QPT) in that system resulting the same scaling exponent [246]. Similar analysis has also been carried out for quantum WD for the same restricted classes of measurements.

[16] A bipartite quantum state will be called PPT [247, 248] if it remains positive under partial transposition.

B. Higher dimensional systems

Due to the optimization involved in computing QD, most of the studies therein are limited to $\mathbb{C}^2 \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \mathbb{C}^n$ systems, where measurements are considered in the qubit part, and only PV measurements are allowed, so that a relatively easy parametrization is possible, as discussed in the preceding subsection. This is no more true for higher dimensional systems. For example, to study QD of two spin-1 systems, one requires six parameters to completely specify a general PV measurement. In general, for a spin-s system, $n(n-1)-1$ parameters are required to define the complete set of PV measurements, where $n = 2s+1$. If the system possesses some special type of symmetry like parity symmetry, the number of free parameters can get reduced. For example, for two-qutrit states with S_z-parity symmetry [249], it is enough to consider the class of bases given by

$$\begin{aligned}
|1_{\vec{r}}\rangle &= \cos\beta(e^{-i\phi_0}\cos\alpha|1\rangle + e^{i\phi_0}\sin\alpha|-1\rangle) - \sin\beta\; e^{-i\gamma}|0\rangle,\\
|0_{\vec{r}}\rangle &= \sin\beta(e^{-i\phi_0}\cos\alpha|1\rangle + e^{i\phi_0}\sin\alpha|-1\rangle) + \cos\beta\; e^{-i\gamma}|0\rangle,\\
|\text{-}1_{\vec{r}}\rangle &= -e^{-i\phi_0}\sin\alpha|1\rangle + e^{i\phi_0}\cos\alpha|-1\rangle, \qquad (52)
\end{aligned}$$

where $\vec{r} = (\alpha, \beta, \gamma)$ and $\tan\phi_0 = \tan\gamma\ \tan(\frac{\pi}{4} - \alpha)$.

Interestingly, for bound entangled states in $\mathbb{C}^3 \otimes \mathbb{C}^3$ given in Refs. [157, 250], it was observed that the error between the actual QD, obtained by considering arbitrary PV measurements in $\mathbb{C}^3$, and the QD by using standard spin measurement bases corresponding to S^x, S^y, and S^z is very low, thereby indicating the importance of constrained QD.

IV. WITNESSING QUANTUM DISCORD

In entanglement theory, witness operators [248, 251, 252] play an important role in detecting entangled states, especially in the laboratory. Its immense importance lies, at least partly, on the fact that it is a tool to find out whether a state is entangled or not without state tomography [253–256] and by performing a lower number of local measurements than in other methods.

The concept of witness operators is based on the Hahn-Banach theorem. The Hahn-Banach theorem [257] in functional analysis guarantees the existence of a linear functional, $f : \mathbb{B} \to \mathbb{R}$, from a Banach space $\mathbb{B}$ to the set of real numbers $\mathbb{R}$, such that for any convex and compact subspace $\mathcal{M} \subset \mathbb{B}$ and for any $x \in \mathbb{B}$ but $x \notin \mathcal{M}$, one has

$$f(\mathcal{M}) = 0, \quad f(x) \neq 0. \qquad (53)$$

Since the state space in quantum mechanics does form a Banach space and the set of separable states, $\mathcal{S}$, is convex and compact [258], the existence of an operator which can distinguish an entangled state from the set of separable states is guaranteed by the Hahn-Banach theorem. More precisely,

$$\begin{aligned}
&\forall\rho \notin \mathcal{S},\ \exists\, W \text{ s.t. } \mathrm{tr}(W\rho) < 0\\
&\quad \text{while } \mathrm{tr}(W\sigma) \geq 0\ \forall\sigma \in \mathcal{S}, \qquad (54)
\end{aligned}$$

where W is a Hermitian operator, and is referred to as an entanglement witness (EW). It is important to note here that given an entangled state, finding an optimal witness operator is still a challenging task (see [251, 259–261]). Let us also mention here that the Bell inequalities [226, 227] can also be thought as witnesses of quantum entanglement, albeit non-optimal.

In a similar spirit, one may wish to find a witness operator which can distinguish the set of zero discord states from a discordant state. From the definition of an EW operator, in Eq. (54), one may be tempted to replace σ by a zero discord state. However, the set of states with vanishing discord do not form a compact set and neither it is convex, and hence a direct use of the Hahn-Banach theorem in this case is not possible. In this regard, it was shown [262, 263] that to detect discord-like nonclassical correlation, a non-linear witness operator, $\mathcal{W} : \mathcal{B}(\mathbb{C}^m \otimes \mathbb{C}^n) \to \mathbb{R}$, can be defined[17], such that for any c-c state, χ

$$\mathcal{W}\chi \geq 0 \text{ and } \mathcal{W}\rho < 0, \qquad (55)$$

where ρ is any non-c-c state, and

$$\mathcal{W}\tilde{\rho} = c - \mathrm{tr}(\tilde{\rho}A_1)\mathrm{tr}(\tilde{\rho}A_2)\ldots\mathrm{tr}(\tilde{\rho}A_m), \qquad (56)$$

for an arbitrary quantum state $\tilde{\rho}$, with $c \geq 0$ and $A_1, A_2, \ldots, A_m$ being positive Hermitian operators. Moreover, the following theorem can be proven.

Theorem 2 [262]: *A linear witness map cannot detect nonclassical correlation of a separable state.*

Proof: Suppose $\mathcal{W}_{linear}$ is a linear witness operator which can detect c-c states i.e. $\mathrm{tr}(\chi\mathcal{W}_{linear}) \geq 0$. Therefore, $\mathrm{tr}(\sum_k p_k\chi_k\mathcal{W}_{linear}) \geq 0$, where $\{p_k, \chi_k\}$ is any ensemble of c-c states. Now an arbitrary bipartite separable state σ_{AB}, can always be written as a convex combination of product states [89], and hence convex combination of c-c states. This implies $\mathrm{tr}(\sigma_{AB}\mathcal{W}_{linear}) \geq 0$. ■

The proof of Theorem 2 considers "nonclassical" correlation as that in non-c-c state. However, the proof also goes through if one considers the same as that in non-q-c or non-c-q states. It is worth mentioning that non-linear entanglement witness operators have also been investigated [264–266], and it was shown that non-linearities help to make the detection process more efficient.

The constant c and the positive operators A_i in Eq. (56) can be determined from the nonclassical state ρ. The Hermitian operators $A_1, A_2, \ldots, A_m$ are constructed by taking the projections of the eigenvectors of ρ [262] and $c = \sup_{\tilde{\rho}} \mathrm{tr}(\tilde{\rho}A_1)\mathrm{tr}(\tilde{\rho}A_2)\ldots\mathrm{tr}(\tilde{\rho}A_m)$, where $\tilde{\rho}$ is any

[17] $\mathcal{B}(\cdot)$ denotes the set of bounded linear operators on its argument.

quantum state which has a bi-orthogonal product eigenbasis. For example, consider the mixed state

$$\tilde{\sigma}_{AB} = \frac{1}{2}\Big(|00\rangle\langle 00| + |1+\rangle\langle 1+|\Big), \tag{57}$$

where $|+\rangle = \big(|0\rangle + |1\rangle\big)/\sqrt{2}$. The above state is a c-q state having non-zero QD if subsystem B performs the measurement. To successfully detect the state, it was found that one can assume $A_1 = |00\rangle\langle 00|$ and $A_2 = |1+\rangle\langle 1+|$, and $c = 0.182$. The above choice of course leads to $\mathcal{W}\tilde{\sigma}_{AB} < 0$, while $\mathcal{W}\chi^{\text{q-c}} \geq 0 \;\forall$ q-c states $\chi^{\text{q-c}}$. One should note here that the witness operator proposed here can be implemented when multiple copies of the state are not available [260, 267]. Another non-linear witness operator has been proposed by Maziero *et al.* [268], to identify two-qubit states having non-vanishing QD. The states for which the witness is provided is given in Eq. (28), with all off-diagonal elements of the correlation matrix, T_{ij} $(i \neq j)$, being zero. It was shown that for these two-qubit states, the proposed form of the witness operator is given by[18]

$$\mathcal{W}\rho_{AB} = \sum_{i=1}^{3}\sum_{j=i+1}^{4} |\langle\hat{O}_i\rangle_\rho\langle\hat{O}_j\rangle_\rho|, \tag{58}$$

where $\hat{O}_i = \sigma^i \otimes \sigma^i$ for $i = 1,2,3$ and $\hat{O}_4 = \sum_i x_i\sigma^i \otimes \mathbb{I}_2 + \sum_{i=1}^{3} y_i \mathbb{I}_2 \otimes \sigma^i$, with $\sum_i x_i^2 = \sum_i y_i^2 = 1$ and $\langle\hat{O}_i\rangle_\rho = \text{tr}(\rho_{AB}\hat{O}_i)$. It was shown that $\mathcal{W}\rho_{AB} = 0$ for states having either (i) all T_{ii} are vanishing or (ii) all the $x_i = 0 = y_i$ $\forall i$ and all T_{ii} except any one are vanishing. This implies that such states are c-c states. For the Bell-diagonal states, for which the magnetizations x_i and y_i are vanishing, the witness operator $\mathcal{W}\rho_{AB}$ turns out to be necessary and sufficient to detect the states with non-vanishing QD [268]. Moreover, it was proposed [269] that the witness operator can be implemented by the technique of nuclear magnetic resonance (NMR).

For arbitrary bipartite states on $\mathbb{C}^2 \otimes \mathbb{C}^n$, another method to identify states with positive QD, based on the PPT criterion [247, 248] was proposed [270]. In particular, it was shown that all c-q states belong to a new subclass of PPT states, which was called strong PPT (SPPT) states[19] i.e., $\mathcal{D}^{\rightarrow}(\rho_{AB}) = 0 \implies$ the state is SPPT on $\mathbb{C}^2 \otimes \mathbb{C}^n$.

In Ref. [272, 273], unlike the witness operator described in Eq. (58), a single observable of QD witness was introduced which turns out to be invariant under local unitary (LU) operations. Such witness operator can detect an arbitrary bipartite quantum state ρ_{AB} of arbitrary dimensions (i.e., $\mathbb{C}^m \otimes \mathbb{C}^n$) having positive QD, provided four copies of the state are available. The witness operator in this case is given by [272]

$$\mathcal{W} = u_1 - u_3 - \frac{2}{m}(u_2 - u_4), \tag{59}$$

where

$$\begin{aligned} u_1 &= V_{14}^A V_{23}^A V_{12}^B V_{34}^B, \;\; u_2 = V_{14}^A V_{12}^B V_{34}^B, \\ u_3 &= V_{12}^A V_{34}^A V_{12}^B V_{34}^B, \;\; u_4 = V_{12}^A V_{12}^B V_{34}^B. \end{aligned} \tag{60}$$

Here $V_{ij}^{A,B} = \sum_{k,l} |kl\rangle\langle lk|_{ij}$ is the swap operator on the i^{th} and the j^{th} copies of the subsystem A or B. It was shown that $\text{tr}(\mathcal{W}\rho_{AB}^{\otimes 4}) = 0 \implies \mathcal{D}^{\rightarrow}(\rho_{AB}) = 0$ in $\mathbb{C}^m \otimes \mathbb{C}^n$. When $m = 2$, the above theorem becomes necessary and sufficient. The treatment also provides a lower bound on GQD. Moreover, for two-qubit states, quantum circuit of the above witness operator by using local measurements have also been proposed.

In addition to this, other attempts have been made to detect the nonclassical correlations in a quantum state, as quantified by distance-based measures, without full-state tomography. In Ref. [153], Jin *et al.* reported that the exact GQD for an arbitrary unknown two-qubit state can be obtained by performing certain projective measurements, and was shown to be advantageous in comparison to tomography. In particular, it was shown that the method proposed requires measurements of three parameters which are three moments of the matrix $K = TT^T + xx^T$ (see Sec. II B 2), while in quantum state estimation [274], 15 parameters have to be obtained. However, the former scheme needs more copies (not more than six [153]) of states in each round compared to the latter one. In the two-qubit case, it was found that a quantity, proposed to be related to GQD, can be estimated by six or seven measurements on four copies of ρ_{AB} [152]. For further studies in the direction of discriminating quantum states with non-zero QD from those with vanishing values of the same, see [275, 276].

V. VOLUME OF STATES WITH VANISHING QUANTUM DISCORD

With respect to the entanglement-separability problem, and for definiteness, considering the bipartite case, the entire state space can be divided into two sets, viz. those consisting of entangled and separable states. An important question in this regard is about the "relative volume" of these two sets [258]. A similar question can be asked in the context of QD. Specifically, in this section, we will be discussing about the volume of set of states having vanishing QD.

Before discussing the division of the space of density operators into segments with zero and non-zero QD

[18] For convenience of notation, we will interchangeably use 1, 2, 3 for x, y, z.

[19] An arbitrary bipartite $\mathbb{C}^2 \otimes \mathbb{C}^n$-dimensional quantum state $\rho_{AB} = \mathbf{X}^\dagger\mathbf{X}$ with $\mathbf{X} = \begin{pmatrix} X_1 & SX_1 \\ 0 & X_2 \end{pmatrix}$ is SPPT iff there is a canonical conjugate $\mathbf{Y} = \begin{pmatrix} X_1 & S^\dagger X_1 \\ 0 & X_2 \end{pmatrix}$, such that $\rho_{AB}^{T_A} = \mathbf{Y}^\dagger\mathbf{Y}$. Here X_1, X_2 and S are $n \times n$ dimensional matrices [271].

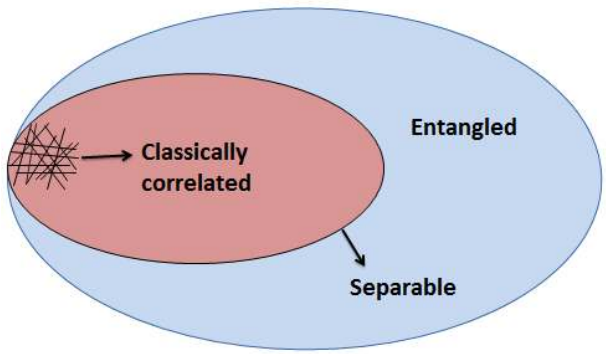

FIG. 3: Classification of quantum states of separated systems with respect to their entanglement and QD. Clearly, separable states contain the classically correlated states i.e. zero-discord states. Depending on the definition of QD utilized, the "classically correlated" states can be q-c, c-q or c-c states.

states, we notice that in a complex Hilbert space, separable pure states[20] have vanishing volume in the subspace of all pure states. QD coincides with entanglement in case of pure states and hence "almost all"[21] pure states have non-vanishing QD. Therefore the question about volume of zero QD states remains non-trivial only for mixed states.

The Authors in Refs. [258, 279] showed that the volume of separable states is non-zero. The result was independent of the dimension of the Hilbert spaces involved and the number of subsystems. This result initiated a series of research works, among which is the work by Szarek [280], where the radius of the separable ball was estimated for an arbitrary number of subsystems. An earlier result by Braunstein *et al.* [281] showed that such estimates on the radius have implications for experiments using NMR.

We now try to see whether the set of all states having vanishing QD, which is a proper subset of the set of separable states, also has a non-zero volume. For a given state ρ_{AB}, $\mathcal{D}(\rho_{AB}) = 0$ iff the state is q-c. Ferraro *et al.* [282] proved that

$$\mathcal{D}(\rho_{AB}) = 0 \implies [\rho_{AB}, \mathbb{I}_A \otimes \rho_B] = 0. \qquad (62)$$

Note that this is equivalent to $[\rho_{AB}, \mathbb{I}_A \otimes \rho_B] \neq 0 \implies \mathcal{D}(\rho_{AB}) > 0$. The set of states with zero QD is surely a subset of the set which satisfies the equation on the right-hand-side of (62). It was proven [282] that the bigger set has measure zero. Furthermore, an arbitrarily small perturbation on a zero-discord state leads to a state having strictly positive QD. This is in sharp contrast to the situation of states having vanishing entanglement. Indeed, while there are separable states of non-full rank that can be made entangled by a small perturbation, full-rank separable states are submerged in the interior of the separable states and do not become entangled if the perturbation is sufficiently weak. For a schematic diagram, see figure 3.

Instead of focusing on the volume of zero QD states, we can try to understand methods for knowing whether a state has zero QD. A method for this purpose was provided in Ref. [66], which works for bipartite states of arbitrary dimensions. To obtain this method, we consider the singular value decomposition $U\tilde{C}W^T = [c_1, c_2, \ldots, c_L]$ of a bipartite state ρ_{AB} on $\mathbb{C}^m \otimes \mathbb{C}^n$ written out in Eq. (30). Here, U and W are $m^2 \times m^2$ and $n^2 \times n^2$ orthogonal matrices, and diag$[c_1, c_2, \ldots, c_L]$ is an $m^2 \times n^2$ matrix. In the new basis, ρ_{AB} takes the form $\rho_{AB} = \sum_{k=1}^{L} c_k S_k \otimes F_k$, where $L = \text{rank}(\tilde{C})$. A necessary and sufficient condition for vanishing QD ($\mathcal{D}^{\leftarrow}$) is then the mutual commutativity of the F_k ($k = 1, 2, \ldots, L$). It was also underlined in [66] that this necessary and sufficient condition is more efficient than state tomography. Another necessary and sufficient criterion for zero QD of a bipartite quantum state was obtained in [283] based on whether the corresponding density matrix can be written in a block form with the blocks being normal and mutually commuting. See also [284].

The geometric pictures of the sets of states with zero and non-zero QD [285, 286] and GQD [241, 242, 285, 287, 288] have also been investigated, especially for two-qubit states. Note that mixing of two positive-discord states can lead to a zero-discord state, as also mixing two zero-discord states can lead to a positive-discord state.

The proposals that relate the vanishing of QD between a system and its environment with the complete positivity of the corresponding evolution of the system will be considered in Sec. VIII.

VI. ARE QUANTUM CORRELATED STATES WITHOUT ENTANGLEMENT USEFUL?

The early development of quantum information theory, especially in quantum communication [289–291], strongly suggests that entanglement shared between two or more parties is an important resource necessary for achieving efficiencies that cannot be reached by states without entanglement. However, about a decade ago, a prominent divergence from this line of thought has begun to emerge and researchers have started to ask: Is quantum entanglement the only correlation-like resource for performing tasks with nonclassical efficiencies? In this section, we are going to address this question. At the outset, let us mention that there exists, for example, the Bennett-Brassard

[20] An N-party separable pure state is defined as

$$|\psi\rangle_{12\ldots N} = |\chi_{A_1}\rangle \otimes |\chi_{A_2}\rangle \ldots \otimes |\chi_{A_l}\rangle, \qquad (61)$$

where $2 \leq l \leq N$, $\cup_j A_j = \{1, 2, \ldots, N\}$ and $A_i \cap A_j = \emptyset\ \forall i, j$. Note that such states can be fully separable ($l = N$), bi-separable ($l = 2$), etc.

[21] The phrase "almost all" is used to indicate that a certain property holds for all members of a space except for a set of measure zero [277, 278].

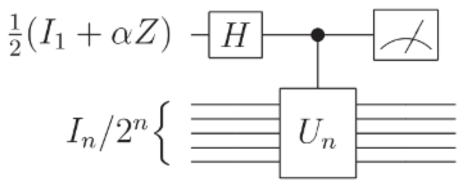

FIG. 4: Schematic diagram of the DQC1 circuit, comprised of a single-qubit system in a mixed state of polarization α, together with a N-qubit bath in which each of the qubit is in a maximally mixed state $\mathbb{I}_2$. In order to compute the normalized trace of an arbitrary unitary operator, the single-qubit system is subjected to a Hadamard gate, which is followed by a controlled unitary U_N on the qubits those belong to the N-party bath. N is represented as n in the figure. [Reprinted from Ref. [320] with permission. Copyright 2008 American Physical Society].

1984 quantum key distribution protocol [292], that deals with only product states, at least in the ideal case, that is secure against even quantum adversaries, provided we do not require device-independent security [293–297]. Let us also remember that there exists the Bernstein-Vazirani algorithm [298–300] of quantum computation that again uses product states at all stages of the protocol. However, the Bernstein-Vazirani algorithm requires a controlled-unitary operation that acts on a large number of qubits, which has product states as input and output. It is possible that the implementation of this unitary by breaking it up into single- and two-qubit unitaries [301] will generate states having QC in the intermediate steps. We will see that a similar situation appears in the deterministic quantum computation with a single qubit (DQC1) [13] protocol. Below we consider some QIP tasks in which, it is claimed that the states required in the process possess non-zero amount of QD, while they do not have any or a significant amount of entanglement. We warn the potential readers that some parts of this section are currently contested in the community. The protocols that we are going to discuss about are deterministic quantum computation with a single qubit, remote state preparation, and local broadcasting, with emphasis on whether the resource involved can be identified as QD.

Apart from the above mentioned schemes, QD has been claimed to be useful for several other QIP tasks. These include, e.g. the quantum state merging protocol [63, 302, 303], identification of unitaries and quantum channels [304, 305], and quantum metrology [306, 307]. See also [307–312]. QD is also asserted to be useful in studying biological systems like photosynthesis in the light-harvesting pigment-protein complexes [313–316] and tunnelling through enzyme-catalysed reactions [317]. For further claims on the usefulness of QD in QIP tasks, see [307–312]. Cf. [281].

A. Deterministic quantum computation with single qubit

Let us first briefly illustrate the task and circuit of DQC1 [13]. We then discuss the QC in different partitions of the set-up, and ask whether the efficiency of the protocol is related to the QC.

The task of the DQC1 algorithm, as proposed by Knill and Laflamme [13], is to assess the normalized trace[22] of a unitary matrix which cannot be solved efficiently by any known classical algorithms [81, 318–320]. The set-up consists of $N+1$ qubits, and the initial state is

$$\rho^{in}_{N+1} = \big(\frac{1}{2}\mathbb{I}_2 + \alpha|0\rangle\langle 0| - \alpha|1\rangle\langle 1|\big)_1 \otimes \mathbb{I}_{2^N}/2^N, \quad (63)$$

with $\alpha \geq 0$. As schematically depicted in figure 4, the first qubit (called as "system") is subjected to a Hadamard gate[23] and is followed by a unitary operation on the entire set-up. The collection of N qubits other than the system is referred to as the "bath". The unitary on the entire set-up is a controlled-U_N, where U_N is a unitary operator on the bath. Hence, the initial state ρ^{in}_{N+1} would lead to the final state given by

$$\begin{aligned}\rho^{f}_{N+1} &= \frac{1}{2^{N+1}}(\mathbb{I}_{2^{N+1}} + \alpha|0\rangle_1\langle 1|_1 \otimes U_N^\dagger \\ &+ \alpha|1\rangle_1\langle 0|_1 \otimes U_N). \end{aligned} \quad (64)$$

It is interesting to study the behavior of QC of the final state to understand whether the nonclassical efficiencies of the algorithm are related to QC. To find out the trace of U_N, one can now calculate the expectation values of the observables σ^x and σ^y of the system. These are given by

$$\begin{aligned}\langle\sigma^x\rangle_1 &= \mathrm{tr}(\sigma^x\rho^f_1) = \frac{\alpha}{2^N}\mathrm{Re}\,[\mathrm{tr}(U_N)], \\ \langle\sigma^y\rangle_1 &= \mathrm{tr}(\sigma^y\rho^f_1) = \frac{\alpha}{2^N}\mathrm{Im}\,[\mathrm{tr}(U_N)], \end{aligned} \quad (65)$$

where $\rho^f_1 = \frac{1}{2}\mathbb{I}_2 + \frac{1}{2^{N+1}}\big(\alpha|0\rangle\langle 1|\,\mathrm{tr}(U_N^\dagger) + \alpha|1\rangle\langle 0|\,\mathrm{tr}(U_N)\big)$, as obtained from Eq. (64) by tracing out the N-qubit bath.

There is no known classical algorithm which can compute the trace of an arbitrary unitary operator in an efficient way [81, 318–320]. The circuit of DQC1 involves a controlled unitary gate which can be realized by several single- and two-qubit gates with polynomial resources. At this point, it is probably natural to expect that entanglement generated in the state is the key resource for

[22] The normalized trace of a matrix M on $\mathbb{C}^m$ is defined as $\frac{1}{m}\mathrm{tr}(M)$.

[23] The Hadamard gate is defined as the unitary operator that transforms $|0\rangle \to |+\rangle$ and $|1\rangle \to |-\rangle$, where $|0\rangle$ and $|1\rangle$ are eigenvectors of σ_z and $|+\rangle$ and $|-\rangle$ are eigenvectors of σ_x.

success of the process[24]. Surprisingly, it was found that the final state is separable in the system-bath bipartition for any U_N and for all $\alpha > 0$. This can be seen by putting $U_N = \sum_j e^{i\phi_j}|e_j\rangle\langle e_j|$ in Eq. (64), which gives the final state of the form $\rho^f_{N+1} = \frac{1}{2^{N+1}}\sum_j(|\psi_j\rangle\langle\psi_j| + |\psi'_j\rangle\langle\psi'_j|) \otimes |e_j\rangle\langle e_j|$, where $\{|e_j\rangle\}$ is an eigenbasis of the unitary U_N, ϕ_j are real, $|\psi_j\rangle = \cos\theta\ |0\rangle + e^{i\phi_j}\sin\theta\ |1\rangle$, and $|\psi'_j\rangle = \sin\theta\ |0\rangle + e^{i\phi_j}\cos\theta\ |1\rangle$, with $\sin 2\theta = \alpha$.

The above example seems to imply that there are quantum algorithms involving mixed states where the computational advantage over classical protocols does not depend on entanglement, and hence there exists a possibility of different quantum properties of the multipartite state, independent of entanglement, which behave as resources. To explore such a prospect, Datta *et al.* [320] computed QD in the splitting between the system qubit and the bath. As we have discussed in Sec. III, the main difficulty in computing QD lies in the fact that it is not easy to find the optimal measurement basis involved. To overcome the difficulty, a random unitary operator was generated, uniformly with respect to the Haar measure over the space of unitary operators on the Hilbert space of the system, and it was shown that the choice of the basis plays an insignificant role in the evaluation of QD across the system-bath bipartition. Hence, the result can be obtained by using a measurement basis chosen from the x-y plane. By choosing the optimal measurement basis as the eigenbasis of σ^x, for large N, QD can be approximated as

$$\mathcal{D}_{\text{DQC1}} = 2 - h\left(\frac{1-\alpha}{2}\right) - \log_2\left(1+\sqrt{1-\alpha^2}\right) - (1-\sqrt{1-\alpha^2})\log_2 e, \quad (66)$$

where $h(\alpha)$ is the Shannon binary entropy, defined as

$$h(\alpha) = -\alpha\log_2\alpha - (1-\alpha)\log_2(1-\alpha). \quad (67)$$

Note that the measurement involved in the definition is carried out on the Hilbert space of the system. Moreover, $\mathcal{D}_{\text{DQC1}}$ is independent of N, and to obtain Eq. (66), one assumes that for a typical unitary U_N, real and imaginary parts of $\text{tr}(U_N)$ are small. Therefore, for any $\alpha \geq 0$, QC, in the form of QD, is present in the system-bath bipartition (see figure 1 in Ref. [320]). The results indicate that the efficiencies in DQC1 may have a connection with QD, thereby providing an avenue towards establishing QD as resource.

This work leads to several theoretical [324–328] (see also [168, 169]) and experimental studies [168, 170, 329–332] (see also [169]) that explored the possibility of identifying QD as a resource in DQC1.

[24] It was shown that a large amount of entanglement does not ensure increase of speed-up in an algorithm [321]. The question however is whether entanglement or other QC are a necessary ingredient (see e.g. [300, 322, 323]).

The main criticism of the above result is that implementation of the controlled-unitary operation, which would typically be simulated by several single-and two-qubit quantum gates [301], may generate entanglement as well as QD in the intermediate steps of the process [333]. Another counter-argument [66] was found by using a condition on the final state to possess non-vanishing QD. First notice that Eq. (64) can alternatively be re-written as

$$\rho^f_{N+1} = \frac{1}{2^{N+1}}\big(\mathbb{I}_2 \otimes \mathbb{I}_{2^N} + \frac{1}{2}\sigma^x_1 \otimes (U_N + U_N^\dagger) + \frac{1}{2i}\sigma^y_1 \otimes (U_N - U_N^\dagger)\big). \quad (68)$$

By using the necessary and sufficient condition of QD discussed in Sec. III, it was shown that QD vanishes across the system-bath bipartition of the state ρ^f_{N+1} in Eq. (68) iff $U_N^\dagger = k\,U_N$ [66]. Such unitaries exist, as seen by choosing $U_N = e^{i\phi}A$ where $A^2 = \mathbb{I}_{2^N}$. Moreover, it is believed that the trace of this unitary operator cannot be simulated by a classical algorithm with polynomial resources. Therefore, this example opens up a debate on the results in [320] about the identification of QD as a resource in DQC1 (cf. [334, 335]).

Recently, it was also shown that the trace of any unitary operator and the complexity of the DQC1 circuit are connected to the notion of "entangling power" [336].

B. Remote state preparation

Remote state preparation (RSP) [337–339] (see also [34–36], and see Refs. [340–350] for experimental developments) is a quantum communication scheme, related to the quantum teleportation protocol [291], for sending a partially unknown qubit. Like in teleportation, the RSP scheme also requires a shared state between a sender, Alice, and a receiver, Bob. Suppose Alice wants to send $|\Phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)$, $0 \leq \phi < 2\pi$ to Bob, and they share a singlet state. The set $\{|0\rangle + e^{i\phi}|1\rangle : 0 \leq \phi < 2\pi\}$ is referred to as the equatorial qubit. Bob knows that the sent qubit is equatorial. Alice knows further: She knows even the value of the ϕ of the equatorial qubit that she intends to send to Bob. Notwithstanding her knowledge of ϕ, since ϕ is a real number in $[0, 2\pi)$, to send it via a classical communication channel, say phone call, Alice will need an infinite amount of communication, if the shared entangled state is not used. In case the entangled state is used, a measurement by Alice in the $\{|\Phi\rangle, |\Phi^\perp\rangle\}$ basis[25] - this is why Alice needs to know ϕ - and one bit of classical communication from Alice to Bob can help Bob to get his part of the singlet state in the input state $|\Phi\rangle$.

[25] Here, $|\Phi^\perp\rangle = \frac{1}{\sqrt{2}}(|0\rangle - e^{i\phi}|1\rangle)$.

One can generalize this protocol to the case when Alice and Bob share an arbitrary state ρ_{AB}, and Alice's aim is to send a qubit, with Bloch vector $\vec{s}$, which is perpendicular to a given unit vector $\vec{\beta}$. Alice knows $\vec{s}$, but Bob just has the knowledge of $\vec{\beta}$. After performing a local generalized measurement at her side, Alice sends a bit of classical communication to Bob. The task of Bob is to perform a suitable quantum operation such that the fidelity between the output and input states, averaged over the unit circle on the Bloch sphere made by all the vectors in the plane perpendicular to $\vec{\beta}$ and passing through the center of the sphere is maximized.

There have been claims that there may be separable states whose RSP fidelity is higher than that of certain entangled states, leading to the possibility of identifying QD as a resource in RSP [66] (cf. [351–355]). The claims however have been countered [356] (cf. [164, 355]). In particular, it has been shown that the fidelity of RSP, when carefully defined, gives a higher value for any entangled state than all unentangled ones.

C. Connection with local broadcasting

Quantum mechanical postulates prohibit copying of an unknown pure quantum state, and even two nonorthogonal pure states, by a single machine, a result known as the no-cloning theorem [357, 358]. In a general setting, an ensemble of mixed quantum states $\{p_i, \rho^i\}$ is provided and the question is whether it is possible to find a quantum operation Λ such that $\text{tr}_S\Lambda(\rho^i_S \otimes \sigma_E) = \text{tr}_E\Lambda(\rho^i_S \otimes \sigma_E) = \rho^i$ where Λ is independent of i. Such an operation, called broadcasting of states, exists if and only if the states $\{\rho_i\}$ in the ensemble $\{p_i, \rho_i\}$ are mutually commuting [359]. The above procedure of broadcasting has been generalized by Piani *et al.* [121] for shared bipartite states, and named as local broadcasting. A bipartite state ρ_{AB} is locally broadcastable (LB), if there exists local operations $\Lambda_{AA'}$ and $\Lambda_{BB'}$ such that

$$\begin{aligned} & \text{tr}_{AB}\Lambda_{AA'} \otimes \Lambda_{BB'}(\rho_{AB} \otimes \sigma_{A'} \otimes \sigma'_{B'}) \\ = & \ \text{tr}_{A'B'}\Lambda_{AA'} \otimes \Lambda_{BB'}(\rho_{AB} \otimes \sigma_{A'} \otimes \sigma'_{B'}) \\ = & \ \rho_{AB}. \end{aligned}$$

Note that in LB, no classical communication is allowed. Communication of quantum states is certainly not allowed. It is also worth mentioning that entangled states are not LB [360–368]. The question is whether separable states having non-zero QD are suitable for LB. In this regard, the following theorem [121] states that this is not the case.

Theorem 3 [121]: *A state ρ_{AB} is LB if and only if it is a classical-classical state.*

The above theorem gives an operational interpretation of c-c states (for other variations of the LB theorem, see Refs. [369–371]).

The no-cloning and no-broadcasting theorems tell us about which states cannot be cloned and broadcast by global quantum engines, and it is known that such states are useful in quantum technologies [372]. It may similarly be hoped that the results on no local-cloning and no local-broadcasting by local quantum engines will be useful for applications in quantum process (see [373] in this regard).

VII. QUANTUM DISCORD IN QUANTUM SPIN SYSTEMS

Quantum correlations, in both entanglement as well as discord-like avatars, have turned out to be important for understanding QIP schemes that are more efficient than their classical analogs [2, 42]. In order to achieve such tasks, one requires to identify certain realizable physical systems - substrates - in which they can be implemented in the laboratory. Interacting spin models [374, 375], which can naturally be found in solid-state systems [376, 377], are one of the potential candidates for such realizations. With currently available technology, it is also possible to realize such systems in optical lattices [10, 378–382], trapped ions [8, 11, 383], superconducting qubits [384–386], NMR [387], etc. Therefore, along with its fundamental importance, investigating QC in these spin models is also important from the perspective of applications.

Over the years, it was shown that a change in the behavior of correlations can indicate occurrence of certain co-operative phenomena. In particular, at zero temperature, certain variations in the correlation functions or their derivatives can infer rich phenomena like quantum phase transitions (QPT) [388]. In a pair of seminal papers, Osterloh *et al.* [389], and Osborne and Nielsen [390] showed that the first derivative, with respect to the control parameter, of nearest-neighbor bipartite entanglement, as quantified by concurrence (see Appendix XV A 2, for a definition), of the zero-temperature state in the one-dimensional (1D) quantum transverse Ising model can capture the signature of QPT present in this model. Furthermore, it was demonstrated that there are quantum many-body systems in which "localizable entanglement length" diverges while the classical correlation length remains finite [391, 392]. QPTs are traditionally uncovered by the divergence of "length" of classical correlation functions [393]. It has also been realized that it is useful to understand the role of entanglement in classical simulation of quantum many-body systems [394–396]. These have led to a significant amount of effort being given to the analysis of the behavior of entanglement, mainly bipartite, of zero-temperature states in isotropic Heisenberg rings [397–399] and in various other quantum many-body systems [42, 378, 400] (see also [401–413]) which include both ordered as well as disordered quantum spin-$\frac{1}{2}$ models with nearest-neighbor, next-nearest-neighbor as well as long range interactions [414–420]. Similar studies have also been carried out in higher-dimensional many-body systems [378, 400]. In 2003, Vidal *et al.* [421] went beyond bipartite entanglement and investigated the behavior of entanglement entropy between two disjoint blocks of a spin chain (block entanglement), which was later extended to several other systems [400]. It was found that block entanglement tends to follow an "area law" in gapped systems [422].

Apart from the zero-temperature states, bipartite as well as multipartite entanglement have also been used to investigate thermal equilibrium states in different spin models either by analytical or numerical techniques. It has in particular been found that entanglement can sometimes be nonmonotonic with the increase of temperature [397, 423–428], which is in contrast to the fragile nature of entanglement in the presence of environment.

In all the above works, tools from quantum information theory have been employed to understand, mainly, equilibrium co-operative phenomena present in quantum many-body systems. However, realizing QIP tasks in these systems normally demand investigation of trends of entanglement with time, both bipartite as well as multipartite, in the time-evolved state. Such studies have led to an important area in quantum computation, called one-way quantum computer [429, 430] which has been extensively investigated, both theoretically and experimentally. Moreover, statistical mechanical properties like the question of ergodicity of bipartite entanglement was investigated in XY and XYZ spin systems [211, 424, 426, 431–436]. The dynamics of entanglement has further been explored in Refs. [437–441] for different types of quenches. See also [442, 443]. The dynamical behavior of block entropy after a sudden quench was considered by Calabrese and Cardy [444] in the transverse Ising chain and then later investigated in various other models [422].

As argued in this review, QC are not limited to entanglement. It is interesting to check whether the behavior of QC beyond entanglement can also identify the key phenomena of these systems. In this section, we outline the works in this direction.

A. Models

Let us first briefly review the quantum spin systems in which QD has been investigated in recent years. Interacting systems of localized spins provide a paradigm where QD is capable of detecting natural phenomena like QPT, ground state factorization, ergodicity, etc. So far, most of the studies of QD in critical systems are limited to 1D spin systems. Similar to entanglement, non-analyticity of the derivative of QD near the critical point can indicate the QPT in the system.

The Hamiltonian of a 1D nearest-neighbor "XYZ spin model" with transverse magnetic field can be written as

$$H = J\sum_{\langle i,j\rangle}[(1+\gamma)S_i^x S_j^x + (1-\gamma)S_i^y S_j^y + \Delta S_i^z S_j^z] + h_z \sum_i S_i^z, \quad (69)$$

where $\langle \cdot,\cdot \rangle$ denotes the sum over nearest-neighbor spins and S_i^α ($\alpha = x, y, z$) are spin operators of appropriate dimension at the i^{th} site of the system. J and γ are respectively the exchange coupling and the anisotropy parameter in the x-y plane. Δ and h_z are the coupling constant and the strength of external magnetic field in the z-direction, respectively. Here, J and h_z have the unit of energy while Δ and γ are dimensionless. When $J > 0$ the model is antiferromagnetic, while $J < 0$ corresponds to a ferromagnetic system. We assume $1 \leq i, j \leq N$. On top of that, periodic boundary condition requires $S_{N+1} = S_1$. The thermodynamic limit can be obtained by taking the $N \to \infty$ limit.

For spin-$\frac{1}{2}$ systems, S_i^α ($\alpha = x, y, z$) are proportional to the Pauli spin matrices. Though the Hamiltonian, even for the spin-$\frac{1}{2}$ case, is not solvable in general, it can be diagonalized exactly in certain special cases in 1D. When $\Delta = 0$ and $\gamma \neq 0$, the model reduces to the "transverse XY spin model", whose eigenenergies and eigenvectors can be obtained exactly by using successive Jordan-Wigner, Fourier and Bogoliubov transformations [445–448]. Similar method can also be employed to find the entire spectrum of the above Hamiltonian with $\gamma = \Delta = 0$, known as the "XX model". The case when $h_z = 0$ and $\Delta \neq 0$, known as the "XXZ model" without magnetic field can also be diagonalized analytically by using thermodynamic Bethe ansatz [449].

B. Statics

If the Hamiltonian does not have any explicit time dependence, and we are interested with static states of the system such as the ground or thermal states, we refer to the analysis as the "static" case. If the system is at zero temperature, its properties, including any change of phase, are completely driven by quantum fluctuations. However, at any finite temperature, this is not the case. In particular, a thermal state is a mixture of the ground state as well as all the excited states, with appropriate probabilities which are fixed by the temperature, and hence the properties of a thermal equilibrium state is driven by the interplay between quantum and thermal fluctuations. When the system reaches high enough temperature, only the thermal fluctuations dominate. Below we briefly discuss the properties of ground and thermal states by using QD in some of the well studied spin models.

1. *Spin-$\frac{1}{2}$ systems*

Let us first concentrate on the Hamiltonian in Eq. (69) for the spin-$\frac{1}{2}$ case. To study QD between the i^{th} and $(i+r)^{\text{th}}$ sites of a state, we first need to calculate the two-site reduced density matrix, $\rho_{i,i+r}$, by tracing out all the sites except $i, i+r$ from the ground or thermal state of the system. Let us also assume the periodic boundary condition which implies that all reduced density matrices are the same. As discussed in Sec. III, systems having $\mathbb{Z}_2$-symmetry, enjoy some simplifications and the two-site reduced density matrix of such Hamiltonians can then be written as

$$\rho_{i,i+r} = \frac{1}{4}\Big[\mathbb{I}_4 + \langle\sigma^z\rangle(\sigma_i^z \otimes \mathbb{I}_2 + \mathbb{I}_2 \otimes \sigma_{i+r}^z) + \sum_{\alpha=x,y,z} \langle\sigma_i^\alpha \sigma_{i+r}^\alpha\rangle \sigma_i^\alpha \sigma_{i+r}^\alpha\Big], \quad (70)$$

where $\langle\sigma^\mu\rangle = \mathrm{tr}(\sigma^\mu \rho_i)$, with ρ_i being the single site reduced density matrix, denotes the magnetization of the system and $\langle\sigma_i^\mu \sigma_{i+r}^\nu\rangle = \mathrm{tr}(\sigma^\mu\sigma^\nu \rho_{i,i+r})$ are the elements of the correlation tensor, as defined after Eq. (28), with $\mu, \nu = \{x, y, z\}$. The above state is the "symmetric X" state (i.e., the state in Eq. (46) with $b = c$). If the ground state is degenerate, one may consider the equal mixture of all the degenerate ground states which can be called the symmetry-unbroken ground state or the zero-temperature thermal state, and is given by

$$\rho_{\mathrm{eq}} = \lim_{\beta\to\infty} \frac{e^{-\beta H}}{Z}, \quad (71)$$

where $Z = \mathrm{tr}\big[\exp(-\beta H)\big]$ is the partition function and $\beta = 1/k_B T$ with k_B being Boltzmann constant and T being the absolute temperature. Such mixtures retain the form of the reduced two party state as in Eq. (70). In particular, the magnetizations in the x- and y-directions still vanish. The same properties can be retained in certain symmetric pure superpositions of the degenerate ground states. On the other hand, when one considers the symmetry-broken state, the magnetizations in the x- and y-direction remain non-zero.

***XXZ* chain ($\gamma = 0$ and $h_z = 0$):** It is known that the XXZ model undergoes QPTs at $\Delta = \pm 1$ [449]. For $J > 0$, when the system crosses $\Delta = -1$ from $\Delta < -1$, a ferromagnetic-to-XY (spin flopping) transition occurs, while at $\Delta = 1$, the system undergoes an XY-to-antiferromagnetic transition. It is known that the former is an infinite-order QPT, whereas the latter is a first-order one. The $\Delta = -1$ transition is detected by the discontinuity in the derivative of QD, while it is the discontinuity of QD that itself detects the transition at $\Delta = 1$ [450–452]. Recently, Huang [453] provided an analytical expression of QD between two distant neighbors of the system. In case of entanglement, the transitions at $\Delta = -1$ and $+1$ are detected respectively by the change of entanglement from vanishing to non-vanishing and by its being maximal [454, 455]. QD, however, can detect the QPT at $\Delta = -1$ until some finite temperature with $k_B T \leq 3$ [456]. Such study has also been carried out for the XXZ chain with an external magnetic field and has been shown that QD is a faithful critical point detector also for this system at zero as well as finite temperatures [457].

Transverse field Ising and *XY* chains: In Eq. (69), if we consider $\Delta = 0$, $\gamma \neq 0$, the Hamiltonian then

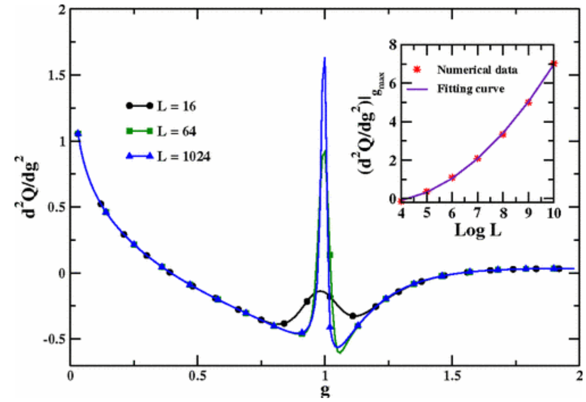

FIG. 5: Quantum discord in the transverse Ising model. Behavior of the second derivative of QD is plotted against g ($= h_z/J$ in our notation) in the transverse Ising model. In the figure, quantum discord is denoted by Q, while it is $\mathcal{D}$ in our notation. Also the system size is L here while it is N in the text. The vertical axes are in bits while the horizontal ones are dimensionless. [Reprinted from Ref. [451] with permission. Copyright 2009 American Physical Society.]

describes a system, which is known as the XY model. By setting $\gamma = 1$, it further reduces to the transverse Ising model. Dillenschneider [450] was among the first to study QD in the transverse Ising model to identify the QPT present in this model[26] at $h_z/J = 1$. It was shown that the next-nearest-neighbor QD (but not the nearest-neighbor QD) has its maximum value near the critical point, where the monogamy bound for concurrence squared is conjectured to be saturated [390]. However, unlike quantum entanglement, both the nearest-neighbor and next-nearest-neighbor QD are maximal in the region close to the QPT, but not exactly at the quantum critical point. It was shown that although nearest and next-nearest-neighbor QD are continuous, the first derivative of the QD of nearest-neighbor spins shows an inflexion, while, interestingly, the first derivative of the latter has divergence at $h_z/J = 1$ [451]. It was also pointed out in the same work that the second derivative of QD of the nearest-neighbor sites has quadratic logarithmic divergence, and the corresponding scaling analysis has also been performed (see figure 5).

The Ising QPT at $h_z/J = 1$ in the anisotropic XY model is marked by a divergence in the derivative of the nearest-neighbor QD with respect to the external field [425]. For the symmetry-broken state, this divergence is present in the entire Ising universality class ($0 < \gamma \leq 1$), while for the thermal ground state, it holds for all γ except $\gamma = 1$ [458]. At $\gamma = 1$, as discussed above,

[26] The Ising transition point at $h_z/J = 1$ separates the antiferromagnetic (AFM, $J > 0$) or ferromagnetic (FM, $J < 0$) phase from the paramagnetic (PM) one, while the anisotropy transition separates the AFM or FM order along the x-direction from the same along the y-direction.

instead of the first derivative, the second derivative of the nearest-neighbor QD diverges [451]. It is worthwhile to mention here that in the case of entanglement, the Ising QPT is always characterized by a divergence of the first derivative of bipartite entanglement for the entire Ising universality class ($\gamma \in (0,1]$) including the Ising model ($\gamma = 1$). This is expected because the Ising transition is seen for the entire Ising universality class which includes the Ising model. The reason behind the different behavior of QD seen for the Ising QPT in the Ising model is still not clear.

Apart from the quantum criticalities, viz. the Ising and the anisotropy transitions, it has been revealed that in the XY model, there exists a point in which entanglement, both bipartite as well as multipartite, vanishes, with the corresponding point being known as the factorization point, given by $h_z = h_z^f = J\sqrt{1-\gamma^2}$ [459]. The factorization point and its neighborhood refer to a region where entanglement is low, which is an important information for possible implementation of QIP in this system.

Up to now, we were discussing about the role of bipartite QD in physical phenomena of quantum many-body systems. We will now discuss whether discord length, i.e. the behavior of QD between two sites, with increasing lattice distance between the sites, has significance in physical phenomena of these systems. Note that entanglement vanishes for pairs which are farther than next-nearest-neighbors in the transverse field XY model, and this is independent of whether the system is at the factorization point. Interestingly this is not the case for QD. Specifically, in Ref. [425], the Authors showed that just like nearest-neighbor QD, QD between farther neighbors can still characterize QPTs. In Refs. [453, 460, 461], five regions in the parameter space of XY model have been identified where scaling of two-site QD with the distance between the sites are different. They are $h_z/J > 1, h_z/J = 1, \sqrt{1-\gamma^2} < h_z/J < 1, h_z/J = \sqrt{1-\gamma^2}$ and $0 < h_z/J < \sqrt{1-\gamma^2}$.

At the factorization point, $h_z^f = J\sqrt{1-\gamma^2}$, the ground state is doubly degenerate [459]. If we take the thermal state in the $T \to 0$ limit, the two-site QD becomes scale-invariant, i.e. the QD between the i^{th} and $(i+r)^{\text{th}}$ spins, denoted by $\mathcal{D}_r$, remains constant for any r, which leads to violation of monogamy for QD [462, 463]. We will discuss the issue of monogamy of quantum correlations in Sec. IX. However, the situation changes if one takes the symmetry-broken ground state. Tomasello *et al.* [458] showed that if one considers a symmetry-broken state, as obtained by a negligible perturbation of longitudinal field (h_x), all the two-site QDs, $\mathcal{D}_r$, vanish at the factorization point for all system sizes. Moreover, it was numerically found that in the symmetry-broken phase, close to the factorization point, the two-site QD between the i^{th} and $(i+r)^{\text{th}}$ sites scales as

$$\mathcal{D}_r \sim (h_z - h_z^f)^2 \times \left(\frac{1-\gamma}{1+\gamma}\right)^r. \qquad (72)$$

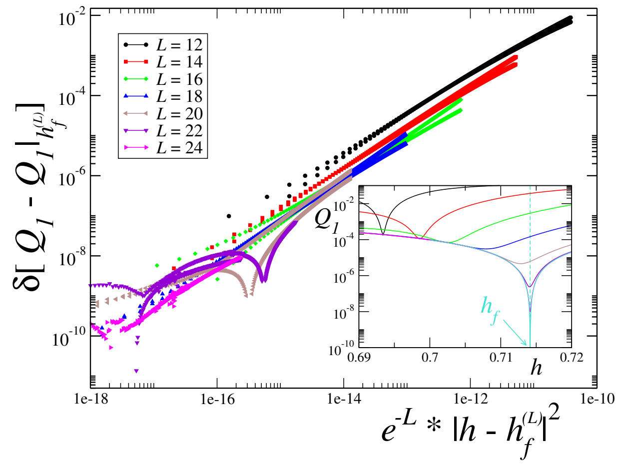

FIG. 6: Scaling of nearest-neighbor QD (denoted by Q_1 in the figure) is analyzed close to the factorization point for $\gamma = 0.7$. The system size is L here while it is N in the text. It is observed that $Q_1^{(L)}$, which is the value of Q_1 for a system of size L, converges in the thermodynamic limit as $e^{-\alpha L}(h - h_f^{(L)})$, $\alpha \approx 1$. Here h replaces h_z/J, and $h_f^{(L)}$ is the value of h at the factorization point for a system of size L. The quantity plotted in the vertical axis is $\left(Q_1^{(L)} - Q_1^{(L)}\Big|_{h=h_f^{(L)}}\right) - \left(Q_1^{(L\to\infty)} - Q_1^{(L\to\infty)}\Big|_{h=h_f^{(L\to\infty)}}\right)$. Due to the extremely fast convergence to the asymptotic value, differences with the thermodynamic limit are comparable with density matrix renormalization group [464, 465] accuracy, already at $L \sim 20$. Inset: Raw data of Q_1 as a function of h. The cyan line is for $L = 30$ for which, up to numerical precision, the system behaves as being at the thermodynamic limit. The vertical axes are in bits, while the horizontal ones are dimensionless. [Reprinted from Ref. [458] with permission. Copyright 2011 IOP Publishing.]

The scaling of the symmetry-broken QD near the factorizing point is plotted in figure 6, which is consistent with the results obtained in Ref. [466].

The temperature-dependence of nearest-neighbor QD of the XY model have been studied in Refs. [425, 457, 467, 468]. Like entanglement [397], non-monotonicity of QD with the increase of temperature have also been reported [425]. It was shown that the nearest-neighbor QD is a better indicator of the Ising transition ($h_z/J = 1$) than the two-site entanglement at finite temperature. On the other hand, at low temperatures the anisotropy transition ($\gamma = 0$) can be correctly detected both by entanglement and QD. With the increase of temperature, QD turns out to be a better physical quantity to identify the Ising transition point than pairwise entanglement [457].

Dhar *et al.* [469] studied long range QD between the non-interacting end spins of an open quantum XY spin chain, with the end spins weakly coupled to the bulk of the chain. It was shown that when the end couplings are adiabatically varied below a certain threshold, QD between the end spins remains frozen. The interval of the freezing can detect the anisotropy transition in the chain.

Other models: The behavior of QD has recently been investigated in an alternating field XY model [427] where the external magnetic field is not uniform for all the sites but has an alternating nature. Interestingly, with the introduction of variations of local transverse fields, it was found that apart from the AFM/FM to PM transition, the system undergoes a dimer to AFM/FM transition. Both the transitions are shown to be detected by the divergence of first derivatives of the nearest-neighbor QD. The effect of thermal fluctuation on QD has also been studied in this system and nonmonotonic behavior of QD with respect to temperature is found in the AFM/FM and PM phases while the dimer phase does not show any non-monotonic behavior.

Patterns of QD in several other 1D quantum spin systems have been carried out. The systems include XY spin chain [470] with three-spin interaction [471, 472] and with Dzyaloshinskii-Moriya (DM) interaction [473–476], XYZ model with inhomogeneous interaction [477], symmetric spin trimer and a tetramer [478], Dicke model, and the Lipkin-Meshkov-Glick model [479].

QD has also been studied in the the quenched disordered quantum XY model [467] where the coupling constant is chosen randomly from a Gaussian distribution. The disorder is assumed to be quenched which imply that the time scale of the dynamics of the system is much shorter than the equilibration time of the disorder. Although disorder may intuitively seem to suppress physical quantities of the system, it turns out that QD can be enhanced with the introduction of disorder - an instance of the "order-from-disorder" phenomena [463, 467, 480–489]. The disorder-induced enhancement is observed both at zero and finite temperatures. Moreover, it was shown that in some parameter regimes, thermal fluctuation interfere constructively to generate a more pronounced order-from-disorder in QD. It was also shown that the long-range behavior of QD can be improved by introducing disorder in the XY spin chain [463]. However, the scale invariant behavior of QD at the factorization point of the ordered system is absent in its quenched disordered counterpart.

2. Spin-1 systems

As already discussed in Sec. III, computation of QD of higher-dimensional states, is difficult and hence most of the studies on the behavior of QD in spin models are limited to systems consisting of spin-$\frac{1}{2}$ particles. However, there are some methods (see Sec. III B) which can be employed to deal with two-qutrit states, originating say, from spin-1 systems. QD in the ground state of the spin-1 XXZ chain and a spin-1 bilinear quadratic chain has been studied [490]. For optimizing over the projective measurements, generation of random unitary matrices is employed as an initial step [491, 492]. The Hamiltonian of the spin-1 XXZ model can be obtained from Eq. (69) by setting $\gamma = h_z = 0$ and by taking the S_i's as spin-1 operators. The model is known to have several quantum critical points with respect to the strength of the zz-interaction Δ as we walk from low to high Δ: (i) $\Delta = \Delta_{c_1} \equiv -1$: FM $\rightarrow$ XY phase as in the spin-$\frac{1}{2}$ XXZ chain; (ii) $\Delta = \Delta_{c_2} \approx 0$: $XY \rightarrow$ Haldane; (iii) $\Delta = \Delta_{c_3} \approx 1.185$: Haldane $\rightarrow$ Néel phase [493–495]. The first and third transitions are respectively 1st and 2nd order while the second one is a Kosterlitz-Thouless (KT) transition of infinite order. The behavior of QD against Δ within $-1 < \Delta < 1.5$ is shown in figure 7 [490]. While QD seemingly fails to capture the infinite order KT transition (and the situation is the same with other QC measures), it can accurately detect the second order Haldane-Néel phase transition. The QD indeed shows an inflection point at $\Delta_{c_3} \approx 1.185$ which results in a kink in the derivative of QD. Moreover, the model has a SU(2) symmetry point at $\Delta = 1$ which can also be observed from the sudden change of QD, happening due to the change of the optimal measurement basis.

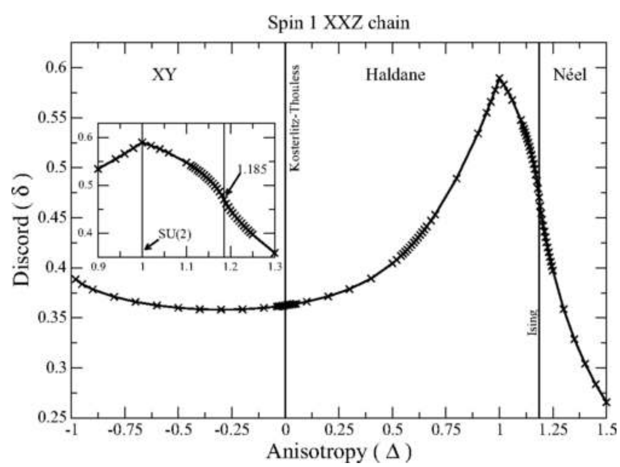

FIG. 7: Quantum discord detects a Haldane - Néel transition. The figure shows QD versus the zz-interaction strength in the 1D spin-1 XXZ model. In the figure, QD and zz-interaction strength are respectively denoted by δ and Δ, while these are denoted by $\mathcal{D}$ and Δ/J in the text, respectively. Different phases, transition points, and the $SU(2)$ symmetry point are shown. The vertical axes are in bits, while the horizontal ones are dimensionless. [Reprinted from Ref. [490] with permission. Copyright 2016 American Physical Society.]

Another model considered in Ref. [490] is a 1D spin-1 bilinear biquadratic model. The Hamiltonian in this case is given by

$$H_{\rm BB} = \sum_{\langle i,j \rangle} \Big[\cos\theta (\mathbf{S}_i \cdot \mathbf{S}_j) + \sin\theta (\mathbf{S_i} \cdot \mathbf{S}_j)^2 \Big], \qquad (73)$$

where $\theta \in [0, 2\pi)$ is an angle that modulates the coupling strength of the nearest-neighbor spins. By tuning θ, the system undergoes four different kinds of QPTs - a KT transition at $\theta_{c1} = 0.25\pi$ from Haldane to trimerized phase, a first order transition at $\theta_{c2} = 0.5\pi$ from trimerized to ferromagnetic, and another first order transition at $\theta_{c3} = 1.25\pi$ from ferromagnetic to dimerized phase, and finally a second order transition at $\theta_{c4} = 1.75\pi$ from trimerized to Haldane phase. There is difference in opinions about other transitions which have been suggested for this model. Like the XXZ spin-1 chain, this model also has a special SU(3) symmetry point at $\theta = 0.25\pi$. In this case, QD has been computed for system of up to 12 spins with open boundary conditions. Despite the small system size, QD can actually detect the critical points at θ_{c2} and θ_{c3}. However, it is failed to identify the KT transition and the second order transition from dimerized to Haldane phase. Moreover, like the XXZ model, a sudden change in QD occurs, due to a drastic change of measurement basis, at the SU(3) symmetry points. For further attempts to calculate QD and related measures for two-qutrit spin systems with different magnetic fields, see Refs. [496–498].

Another spin-1 Hamiltonian where QD has been studied is given by [499]

$$H_{\mathrm{UF}} = \sum_{\langle i,j \rangle} S_i^x S_j^x + S_i^y S_j^y + + S_i^z S_j^z + U \sum_i (S_i^z)^2, \quad (74)$$

where U is the strength of the uniaxial field which is the same for all lattice sites. The ground state of the Hamiltonian is known to have three phases, namely, a Néel AFM phase ($U < -0.315$), a Haldane phase ($-0.315 \leq U \leq 0.968$) and a "large-D" phase ($U > 0.968$) [500–502]. Note that U is a dimensionless quantity. These three phases have been studied by the block entropy and entanglement spectrum [440, 503–506]. In Ref. [499], QD of the reduced density matrix of the two central spins of the zero-temperature state of the Hamiltonian in Eq. (74) with open boundary condition has been analyzed by using density matrix renormalization group. The quantities calculated here are symmetric QD (see Sec. II A 3 and global QD (see Sec. XII A). Taking into account the symmetry of the Hamiltonian, it was argued that the optimization over measurements, required for estimating the global QD, can be made efficient by reducing the number of parameters over which the optimization is performed [249, 507]. See the discussion in Sec. III B in this regard. See also [508, 509].

Figure 8 depicts the variation of the symmetric QD, $\mathcal{D}_{sym}$) with U. The Néel AFM-Haldane phase transition, a second order QPT, is signalled by a discontinuity of the first derivative of symmetric QD of the zero-temperature state and scaling analysis predicts the transition point to be at $U = -0.3156$, which is consistent with result obtained in Ref. [504] from the analysis of entanglement in this system. However, the Haldane - large-D transition at $U = 0.968$ [505] is known to be Gaussian, a third-order transition, and is hard to detect. By performing the second derivative of the symmetric QD, this transition is predicted to be at $U = 0.994$, and the critical exponent is found to be 1.6. Both the results are in good agreement with previous calculations [505] with 20000 spins. It was

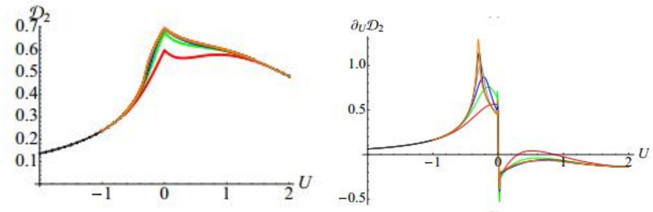

FIG. 8: (Left panel) Néel AFM - Haldane transition by using symmetric QD between nearest-neighbor sites, and (right panel) its derivative for the reduced state of the two central spins of an open-ended chain, described by the Hamiltonian in Eq. (74) of lengths 8 (red), 16 (green), 32 (blue), 64 (gray), 128 (black), and 256 (orange) going from bottom to top. The symmetric QD in the vertical axis is denoted by $\mathcal{D}_2$ in the figure while it is $\mathcal{D}_{sym}$ in the text. The vertical axes are in bits while the horizontal ones are dimensionless. [Reprinted from Ref. [499] with permission. Copyright 2015 American Physical Society.]

argued that the results obtained by using symmetric QD are with at most 256 spins, and hence can be improved substantially by considering larger system sizes.

C. Dynamics

Let us now move on to discuss the behavior of QD in the time-evolved state of different systems. The considerations are often for time-dependent Hamiltonians, and the initial state that is usually considered is the canonical equilibrium state at the initial time[27], denoted by $\rho_{\mathrm{eq}}(t = 0)$. For example, the dynamics of entanglement has been studied after a sudden quench in the transverse field of a 1D quantum XY model [424, 431, 443]. The transverse field is given by

$$\begin{aligned} h_z(t) &= a \text{ (constant) } \text{ for } t \leq 0, \\ &= b \ (\neq a) \text{ for } t > 0. \end{aligned} \quad (75)$$

In this case, evaluation of the time-evolved state does not require a time-ordered integral, since the Hamiltonian after $t = 0$ becomes time-independent. Putting $b = 0$ [424] and the initial temperature $\to 0$, the behavior of entanglement, as quantified by logarithmic negativity [516], $\mathcal{L}$ (for definition, see Appendix XV A 3), has been investigated with respect to the initial field and time. For fixed (relatively) short times, entanglement shows several collapses and revivals with the increase of the initial transverse field - dynamical phase transitions. Such revivals cannot be seen for larger times. It was found that

[27] For the behavior of entanglement in the time-evolved state in the system described by the time-independent quantum transverse XY model, with the evolution starting off from a non-thermal state, see Refs. [442, 510–515].

the behavior of nearest-neighbor QD can predict such collapse and revival of entanglement [517] (see also Ref. [518]). Specifically, it was observed that at the vicinity of collapse, if QD is increasing i.e. if the slope of QD with respect to a is positive, then entanglement will revive for a certain larger value of the initial field. Mathematically,

$$\tilde{a}\frac{\partial\mathcal{D}(\rho_{i,i+1}(t))}{\partial\tilde{a}}\Big|_{\tilde{a}_c} > 0 \Rightarrow \mathcal{L} > 0 \text{ for some } |\tilde{a}| > |\tilde{a}_c|, \tag{76}$$

where $\tilde{a} = a/J$ and $\tilde{a}_c$ is the value of the transverse field where $\mathcal{L}$ vanishes for any fixed time $\tilde{t} = t/J$. At $t > 0$, instead of switching off the magnetic field, one can also quench the system by fixing the magnetic field to some other constant value, b, where $b \neq a$. The effect of such quench in QD has recently been investigated [468]. In the XY Hamiltonian, given in Eq. (69) with $\Delta = 0$, if the transverse field at the i^{th} site is replaced by $h_1(t) + (-1)^i h_2(t)$ where $h_1(t)$ and $h_2(t)$ respectively possess a non-zero value and then both are switched off at a latter time, it was shown that QD also undergoes several revivals and collapses with the system parameters $h_1(t)/J$ and $h_2(t)/J$ for relatively short times [427]. However, the nature and count of the revivals and collapses depend on the initial values of the alternating fields. In the XXZ models, the dynamics of QD has also been investigated after a sudden quench in the zz-interaction strength [519]. Similar to the Ising and XY models, QD is found to be oscillating initially and finally saturating to a constant value.

Instead of taking a step-function-like quench, given in Eq. (75), the quench can also be taken as a linear ramp [520–525] driven across the quantum critical point. The ramp-like quench through the Ising transition point at a finite and steady rate is considered previously in Refs. [520, 522, 524] and can be written as

$$h_z(t) = t/\tau, \tag{77}$$

where τ is related to the characteristic time-scale for the rate of quenching and t is varied from $-\infty$ to ∞. In the 1D transverse XY model with a linear quench in the magnetic field, QD vanishes for both the limits $\tau \to -\infty$ and ∞, but has a peak at an intermediate value of the inverse quenching rate τ [526, 527]. It was found that both entanglement as well as QD behave similarly and exhibit a power-law scaling with the slow variation of τ. QD has also been studied with quenching of the field in the transverse Ising model with three-spin interactions [527].

We now consider the situation when the evolution time is large enough, so that statistical-mechanical questions like ergodicity can be asked. A physical quantity is said to be ergodic if the time-average of the quantity is equal to its ensemble-average. More precisely, a physical quantity $\mathbb{A}$ is said to be ergodic if the following two values match. One of these is the value of $\mathbb{A}$ in the time-evolved state at large time, where the evolution starts off from

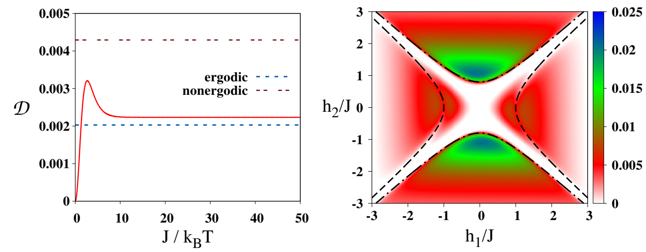

FIG. 9: Ergodicity of quantum discord of 1D alternating transverse field XY model. The Hamiltonian in this case is the usual 1D transverse-field XY model, with the transverse field being of the form $h_1(t) + (-1)^i h_2(t)$ at site i. Left panel: The red solid line represents the trends of QD for the canonical equilibrium state of the Hamiltonian at large time against J/k_BT. The blue dashed and black double-dashed lines correspond to QD of the time-evolved states of the same Hamiltonian at large time, where the initial states are chosen to be the thermal equilibrium states of the initial-time Hamiltonian with $h_1(t=0)/J = 0.0$, $h_2(t=0)/J = 0.15$ and $h_1(t=0)/J = 2.5$, $h_2(t=0)/J = 1.0$ respectively. Here $\gamma = 0.8$, the temperature of the initial state is given by $J/k_BT = 100$, and the transverse fields $h_1(t)$ and $h_2(t)$ are switched off for $t > 0$. QD of the evolved state matches with that of the thermal state for some temperature in the case of the blue dashed line, implying an ergodic nature of QD, while in the other case (black double-dashed line), a nonergodicity of QD is obtained. The vertical axis is in bits while the horizontal axis is dimensionless. Right panel: Map of ergodic regions on the $(\frac{h_1}{J}, \frac{h_2}{J})$ plane of the same Hamiltonian. The white regions are ergodic, as quantified by the ergodicity score, given by $\eta^{\mathcal{D}}(\frac{h_1}{J}, \frac{h_2}{J}) = \max\left\{0, \mathcal{D}_\infty\left(T, \frac{h_1(0)}{J}, \frac{h_2(0)}{J}\right) - \max_{T'}\mathcal{D}_{eq}\left(T', \frac{h_1(\infty)}{J}, \frac{h_2(\infty)}{J}\right)\right\}$, where $\mathcal{D}_\infty$ and $\mathcal{D}_{eq}$ denote the quantum discords of the time-evolved and the canonical equilibrium states respectively at large time. A nonzero ergodicity score implies nonergodicity of QD. The temperature of the canonical state, from which the evolution starts off, is given by $J/k_BT = 100$. The anisotropy γ and the nature of the driving field remain the same as in the left panel. Both the axes in the right panel are dimensionless. [Adapted from Ref. [427] with permission. Copyright 2016 American Physical Society.]

the canonical equilibrium state[28] at the initial time with a temperature T. The other is the value of $\mathbb{A}$ in the equilibrium state of the large-time Hamiltonian at some temperature T' [211, 426, 427, 431, 432, 435, 436, 446–448, 468, 528–530]. The difference of these two quantities has been denoted by $\eta^{\mathbb{A}}$ and called the ergodicity score, where a maximization over T' has already been carried out [436]. Often, T' is constrained to be within an order of magnitude of T [211, 426]. Sometimes the states being compared have been required to lie on the same

[28] There is of course a quenching in some physical parameter, e.g. in the magnetic field, at the initial or some intermediate time before the "large" time.

energy surface [431]. In Ref. [446], it was shown that the transverse magnetization of the transverse XY model is nonergodic. The case of quantum correlations was taken up in Refs. [211, 426, 427, 431, 436, 468]. In particular, for the transverse XY model with the transverse field being given by Eq. (75), it was shown that while bipartite entanglement is always ergodic (within the numerical accuracy used), QD can be ergodic as well as nonergodic [436]. It was further found [468] that for the same model, if a and b are chosen in such a way that the system is quenched from the antiferromagnetic to deep inside the paramagnetic phase, QD is enhanced, while it gets faded out during the paramagnetic to antiferromagnetic quench. Moreover, a quench within same phase was found to cause enhancement of QD. In Ref. [426], the Authors extended the results of the XY model to the XYZ model with the time-dependent magnetic field in the z-direction as given in Eq. (75), in 1D, ladder (quasi-two), and 2D lattices. It was shown that tuning the interaction strength can initiate a nonergodic to ergodic transition of QD. For the 1D alternating field XY model, QD can also exhibit ergodic-nonergodic transitions with the variations of the system parameters (see figure 9) [427].

D. Geometric quantum discord in many-body systems

After the success of QD in describing cooperative quantum phenomena, in following years it was seen that geometric formulations of QD can also characterize the properties of various interacting systems [249, 531–537]. In particular, in Ref. [531], the XXZ model with an external field and the XXX model with DM interaction were considered, and the dependencies of GQD on the system parameters were studied. Similar work in this direction has also been reported by Cai *et al.* [533] where the DM interaction has been included along with an XXZ interaction. In addition to this, the Authors of Ref. [532] employed the quantum renormalization group method in the XXZ and the anisotropic XY models, and showed with several iterations of the renormalization that QD as well as GQD can faithfully detect the phase transition points present in the systems. Ground state properties of a 1D Heisenberg system with next-nearest-neighbor interaction has been characterized by using GQD in Ref. [535], and was shown, for 4-site and 6-site systems, that there exists a one-to-one connection between the energy spectrum and GQD. In the cyclic XX chain with uniform transverse magnetic field [536], it has been shown that at $T = 0$, GQD possesses a non-zero value for all pair-separations, $r = |i - j|$, if the external field, h_z, lies below a certain critical value, h_z^c, and decaying only as r^{-1} for large r. On the other hand, it remains non-zero for all temperatures, decaying as T^{-2r} for sufficiently high T. The topological quantum phase transition observed in the ground state of Kitaev's 1D p-wave spinless quantum wire model has also been detected by using GQD [538]. In particular, it has been reported that the derivative of GQD is nonanalytic at the critical point, in both zero and finite temperature cases. GQD has also been studied in the atom-cavity system modeled by the Jaynes-Cummings (JC) model [539], and found that it persists in the atom versus cavity partition while entanglement vanishes [540, 541] (cf. [542, 543]). See also [544–546] in this regard. Several other studies have been conducted along these lines, which have shown that the study of GQD can provide important insight into cooperative physical phenomena [540, 541, 547, 548].

VIII. QUANTUM DISCORD AND OPEN QUANTUM SYSTEMS

Until now, we have either considered the ideal scenario of an isolated system, i.e. a system that is not affected by the environment and the properties of the system only depend on its own parameters, or a system at which one looks only at a given instant of time without considering how it arrived to that instant. The general situation is however far richer, and naturally leads one to consider the dynamics of open quantum systems [549–553]. Literature on QD in open quantum systems include Refs. [554–587].

An open system consists of a system S, and an environment E. The Hilbert space of the composite system, $S + E$, is the tensor product space $\mathbb{C}^m \otimes \mathbb{C}^n$, where $m = \dim(S)$ and $n = \dim(E)$. Typically, the environment is considered to be very large compared to the system, and it is not always possible to have access to the entire environment. The physical state of the composite system is denoted by the density matrix ρ_{SE}, whereas the system state can be obtained by tracing out the environment i.e. $\rho_S = \mathrm{tr}_E \rho_{SE}$.

In general, the composite system $S + E$ can be described by the Hamiltonian

$$H_{SE} = H_S \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E + H_{int}, \tag{78}$$

where $H_{S(E)}$ is the Hamiltonian of the system (environment) and H_{int} denotes the Hamiltonian describing the interaction between the system and the environment. Below we briefly discuss the formalism to study the evolution of ρ_S in presence of the environment E.

A. Dynamical maps

The system-environment state, which can together form an isolated system, is considered to be in a joint initial state $\rho_{SE}(0)$. Since the dynamics of an isolated quantum system is predicted by the Schrödinger equation, the time evolved state reads

$$\rho_{SE}(t) = U_{SE}(t)\ \rho_{SE}(0)\ U_{SE}^{\dagger}(t), \tag{79}$$

where $U_{SE}(t)$ is the unitary operator acting both on the system and the environment.

The evolved state $\rho_S(t)$, at time t, can now be expressed as

$$\rho_S(t) = \mathrm{tr}_E[\rho_{SE}(t)] = \mathrm{tr}_E[U_{SE}(t)\rho_{SE}(0)U_{SE}(t)^\dagger], \quad (80)$$

which is obtained by tracing out the environment part from the joint state ρ_{SE}. If the initial density matrix is of the form $\rho_{SE}(0) = \rho_S \otimes |0\rangle\langle 0|_E$, then the final state can be expressed as $\rho_S(t) = \sum_i \langle i|U_{SE}|0\rangle \ \rho_S(0) \ \langle 0|U_{SE}|i\rangle_E$ with $\{|i\rangle\}$ being an orthonormal basis of the environment. It leads to the introduction of a linear map Φ_t, given by [588–594]

$$\rho_S(t) = \Phi_t^S(\rho_S) = \sum_i \mathcal{K}_i \ \rho_S(0) \ \mathcal{K}_i^\dagger, \quad (81)$$

where the Kraus operators $\mathcal{K}_i$ satisfy $\sum_i \mathcal{K}_i^\dagger \mathcal{K}_i = \mathbb{I}_m^S$ with $\mathbb{I}_m^S$ being the identity operator of the Hilbert space $\mathbb{C}^m$. The dynamical map providing the evolution of the system due to the interaction with environment satisfies certain properties like linearity, hermiticity, positivity, and trace preservation and on top of that they are completely positive[29] (CP). The complete positivity of the system is guaranteed by the assumption of an uncorrelated product initial state of the system and environment. The presence of classical correlation as well as QC may lead to non-complete positivity of the system [595–600]. Specifically, further investigations in this direction reveal that initially entangled system-bath states can lead to non-CP maps [595, 601–603]. In subsequent years, it was found that there exists nonclassical correlations other than entanglement which, when existing between system and environment, can also result in non-CP dynamical maps [604].

In recent works [604–610], efforts have been made to describe properties of the initial system-environment duo that can assure CP-ness of the reduced dynamics. In particular, it was proven that a dynamical map is CP if the initial system-environment state is a *c-c* state [605], which, of course, have vanishing QD. However, this does not necessarily imply that a non-zero QD in the initial system-environment state will lead to non-CP dynamical map of the system. Indeed, Brodutch *et al.* [607] constructed a separable state with non-vanishing QD, that when considered as a initial state of the system-environment pair, can be written in the Kraus representation from (Eq. (81)), so that the dynamical map of the system is CP. Buscemi [608] followed this up by constructing an example of a class of maps which are CP, and for which it is possible for the system-environment states to be entangled.

[29] A map Φ^S acting on density matrices on $\mathbb{C}^m$ is said to be completely positive if any possible extension, $\Phi_t^S \otimes \mathbb{I}_n^E$, of Φ^S to a bigger Hilbert space $\mathbb{C}^m \otimes \mathbb{C}^n$ is also positive.

	Kraus operators
BF	$E_0 = \sqrt{1-p/2}\, I, E_1 = \sqrt{p/2}\, \sigma_1$
PF	$E_0 = \sqrt{1-p/2}\, I, E_1 = \sqrt{p/2}\, \sigma_3$
BPF	$E_0 = \sqrt{1-p/2}\, I, E_1 = \sqrt{p/2}\, \sigma_2$
GAD	$E_0 = \sqrt{p}\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix}, E_2 = \sqrt{1-p}\begin{pmatrix} \sqrt{1-\gamma} & 0 \\ 0 & 1 \end{pmatrix}$
	$E_1 = \sqrt{p}\begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix}, E_3 = \sqrt{1-p}\begin{pmatrix} 0 & 0 \\ \sqrt{\gamma} & 0 \end{pmatrix}$

TABLE I: Kraus operators for some well-known quantum channels: bit flip (BF), phase flip (PF), bit-phase flip (BPF), and generalized amplitude damping (GAD), where p and γ are decoherence parameters, with $0 \leq p, \gamma \leq 1$.

B. Prototypical open systems

Studying the patterns of QD under environmental effects is the main objective in this part of the review. An open quantum system can be modeled in different ways which may represent situations such as decoherence under dissipative environment, repeated quantum interactions, spin-boson models, etc.

We start the discussion with the dynamics of QD between subparts of a system under Markovian as well as non-Markovian noisy channels. When the system passes through a channel, channel acts as an environment. In this scenario, it may be natural to assume that the system and the given channel are in a product state, and hence Kraus representation is valid here. In Table I, we tabulate the Kraus operators for some well-known channels which will be relevant in this review.

1. *Correlation dynamics under decoherence*

QC in a system, in general, decreases while interacting with the environment. The fragile nature of QC with time is one of the main obstacles in the implementation of quantum information tasks. For example, entanglement disappears completely after a finite time, for many dynamical maps, a phenomenon referred to as sudden death of entanglement [554–562, 567, 582, 583]. On the contrary, QD, typically, asymptotically decays with time [236, 269, 282, 547, 611–637]. Moreover, there exists some special cases, when QD of the evolved state remains constant over a finite interval of time - a phenomenon known as *freezing* of QD. The dynamics of QD can also be such that it shows a kink in its profile which causes a finite discontinuity in its derivative, a phenomenon known as *sudden change* of QD. We briefly discuss below both these

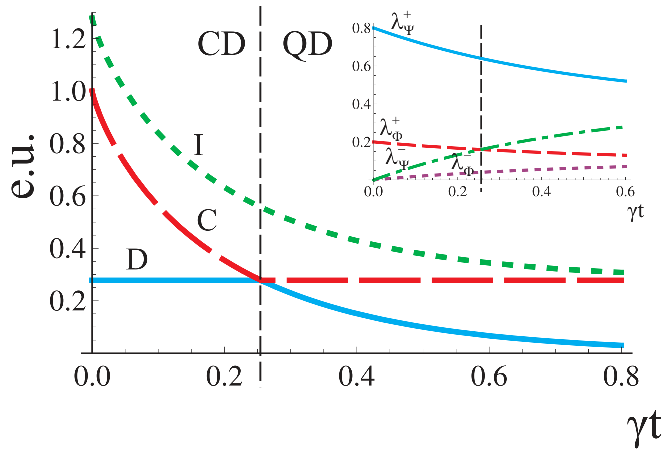

FIG. 10: Freezing of quantum discord. Dynamics of mutual information (green dotted line), classical correlation (red dashed line), and QD (blue solid line) as functions of γt under the conditions $T_{11}(0) = 1$, $T_{22}(0) = -T_{33}$ and $T_{33} = 0.6$. In the inset, the eigenvalues λ_Ψ^+ (blue solid line), λ_Ψ^- (green dash-dotted line), λ_Φ^+ (red dashed line), and λ_Φ^- (violet dotted line) are plotted as functions of γt for the same parameter values. In the figure, "CD" and "QD" represent regimes of "classical decoherence" and "quantum decoherence" respectively. "e.u." stands for "entropic units". The horizontal axes are dimensionless. The vertical axis of the inset is also dimensionless. [Reprinted from Ref. [616] with permission. Copyright 2010 American Physical Society.]

phenomena, and the conditions on the states and channels leading to these events.

a. *Freezing of quantum discord*

In 2010, Mazzola *et al.* [616] discovered that for certain Bell-diagonal states[30], QD does not decay for a finite time interval in presence of a noisy environment. More precisely, when the input state is subjected to local PF channels, given in Table I, the time evolved state is given by

$$\rho_{AB}(t) = \lambda_{\psi^+}(t)|\psi^+\rangle\langle\psi^+| + \lambda_{\phi^+}(t)|\phi^+\rangle\langle\phi^+| + \lambda_{\phi^-}(t)|\phi^-\rangle\langle\phi^-| + \lambda_{\psi^-}(t)|\psi^-\rangle\langle\psi^-|, \quad (82)$$

which is of the form $\frac{1}{4}(\mathbb{I}_4 + \sum_i T_{ii}\sigma_i \otimes \sigma_i)$. Here,

$$\lambda_{\psi^\pm}(t) = \frac{1}{4}[1 \pm T_{11}(t) \mp T_{22}(t) + T_{33}(t)],$$
$$\lambda_{\phi^\pm}(t) = \frac{1}{4}[1 \pm T_{11}(t) \pm T_{22}(t) - T_{33}(t)], \quad (83)$$

where $T_{11}(t) = T_{11}(0)(1-p)^2$, $T_{22}(t) = T_{22}(0)(1-p)^2$, $T_{33}(t) = T_{33}(0) \equiv T_{33}$. The channel parameter, p, of the PF channel (see Table I) is related to the elapsed time by the relation $p = 1 - \exp(-\gamma t)$, where γ is referred to as the phase damping rate. Now under the conditions $T_{11}(0) = \pm 1$, $T_{22}(0) = \mp T_{33}$, $|T_{33}| < 1$, the mixture of four Bell states is a mixture of two Bell states. Using that as the initial state sent through the local phase damping channel, the QD for $t < t' = -\frac{1}{2\gamma}\ln(|T_{33}|)$ is given by

$$\mathcal{D}(\rho_{AB}(t)) = \sum_{j=1}^{2} \frac{1 + (-1)^j T_{33}}{2} \log_2[1 + (-1)^j T_{33}]. \quad (84)$$

This is independent of time and we remember that it is valid only for $t < t'$. This is known as freezing of QD (see figure 10). Figure 10 shows another interesting feature - QD is constant and classical correlation $J_{A|B}$, decays for $t < t'$ while QD decays and classical correlation does not change with time for $t > t'$. Moreover, this behavior of QD has been observed experimentally using photonic [617] and NMR two-qubit states [269, 632].

A necessary and sufficient condition for obtaining the freezing phenomenon of QD with the Bell-diagonal state as the input to local PF channels is provided in Ref. [638], and given in the following theorem.
Theorem 4 [638]: *The Bell-diagonal states given in Eq. (16) can exhibit freezing of QD under local PF channels if and only if λ_i's either satisfy*

$$\lambda_1\lambda_4 = \lambda_2\lambda_3, (\lambda_1 - \lambda_4)(\lambda_2 - \lambda_3) > 0 \quad (85)$$

or,

$$\lambda_1\lambda_2 = \lambda_3\lambda_4, (\lambda_1 - \lambda_2)(\lambda_4 - \lambda_3) > 0. \quad (86)$$

It was also shown that there exists a form of non-Markovian dynamics under which QD remains invariant for all time [630]. Importantly, multiple intervals of recurring frozen QD [639–641] can also be observed when the dynamics is considered in non-Markovian regime. In another work [640], the initial Bell-diagonal state passes through local channels, where each channel modeled by an interaction of the corresponding qubit with a classical field. It was found that both entanglement and QD show collapse and revival, and that QD exhibits multiple freezing intervals (see figure 11). For an experimental demonstration, see Ref. [642]. It was noticed that when QD is frozen, classical correlation is oscillating and vice versa (cf. [643]) and was also argued that revival of QC is related to the non-Markovian nature of the evolution.

For certain channels like BF, PF, BPF, a necessary and sufficient condition for freezing of QD was provided [245] for bipartite as well as multipartite states under local noisy channels. In this regard, "canonical initial (CI)

[30] For Bell-diagonal states, see Eq. (16).

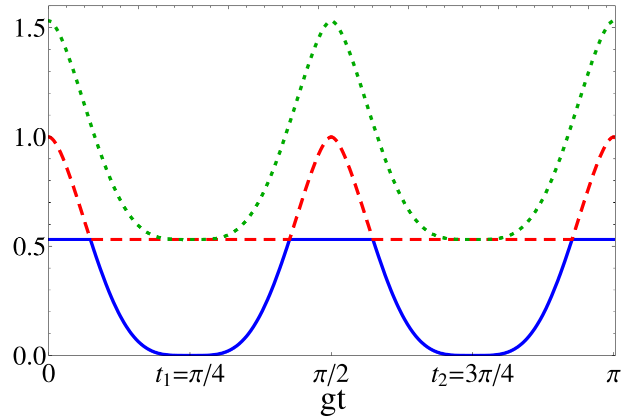

FIG. 11: Dynamics of quantum discord $\mathcal{D}$ (blue solid line), classical correlation J (red dashed line) and total correlation I (green dotted line) for an initial Bell-diagonal state of the form $\rho_{AB}(0) = \lambda_1(0)|\psi^+\rangle\langle\psi^+| + \lambda_2(0)|\psi^-\rangle\langle\psi^-| + \lambda_3(0)|\phi^+\rangle\langle\phi^+| + \lambda_4(0)|\phi^-\rangle\langle\phi^-|$ with $\lambda_1(0) = 0.9$, $\lambda_2(0) = 0.1$ and $\lambda_3(0) = \lambda_4(0) = 0$, passing through local channels, with each channel being modeled by an interaction between the corresponding qubit and a classical field. The interaction strength is given by $g\hbar$. The vertical axis is in bits while the horizontal axis is dimensionless. [Reprinted from Ref. [640] with permission. Copyright 2012 American Physical Society.]

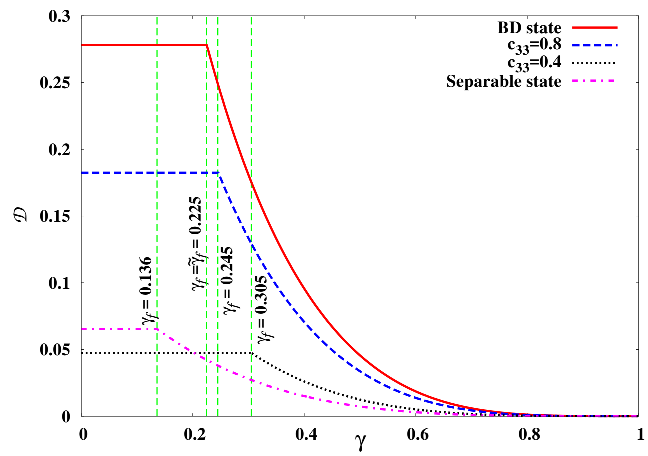

FIG. 12: Dynamics of quantum discord for two-qubit SCI states under local BF channels for $|T_{11}| = 0.6$ and $T_{33}^2 + y_1^2 = 1$. Note that a CI state reduces to a BD state under the assumption, $y_1 = x_1 = 0$. The red solid line represents the BD state with $|T_{22}| = 0.6$ and $|T_{33}| = 1$. The vertical axis is in bits, while the horizontal one is dimensionless. [Adapted from Ref. [245] with permission. Copyright 2015 American Physical Society.]

states" of the form[31]

$$\rho_{AB} = \frac{1}{4}\Big[\mathbb{I}_2\otimes\mathbb{I}_2 + \sum_{i=1}^{3} T_{ii}\sigma_A^i\otimes\sigma_B^i + \left(x_1\sigma_A^1\otimes\mathbb{I}_2 + y_1\mathbb{I}_2\otimes\sigma_B^1\right)\Big] \tag{87}$$

have considered to investigate the freezing phenomenon of QD. As discussed in Sec. III, for most two-qubit states among CI states, optimization of QD occurs in the eigenbases of σ^1, σ^2, or σ^3, and such states are called special CI (SCI) states. A necessary and sufficient criteria for freezing of QD for the two-qubit SCI states as inputs to local BF channels is given below.

Theorem 5 [245]: *A necessary and sufficient condition for freezing of QD of the output of a local BF channel where the input is a two-qubit SCI state, over a finite interval of time is given by any of the following sets of equations:*

$$\begin{cases} (i) & (T_{22}/T_{33}) = -(x_1/y_1) = -T_{11}, \\ (ii) & T_{33}^2 + y_1^2 \leq 1, \\ (iii) & F\left(\sqrt{T_{33}^2+y_1^2}\right) < F(T_{11}) + F(y_1) - F(x_1); \end{cases} \tag{88}$$

$$\begin{cases} (i) & (T_{33}/T_{22}) = -(x_1/y_1) = -T_{11}, \\ (ii) & T_{22}^2 + y_1^2 \leq 1, \\ (iii) & F\left(\sqrt{T_{22}^2+y_1^2}\right) < F(T_{11}) + F(y_1) - F(x_1). \end{cases} \tag{89}$$

Here $F(y) = 2\left(h(\frac{1+y}{2}) - 1\right)$ and $p = \gamma$ for the BF channel. Figure 12 exhibits the dynamics of QD for certain SCI states including BD states. The "freezing terminal" (p_f), representing the time at which the freezing behavior of quantum correlation in the decohering state vanishes, can be much larger for some CI states compared to the Bell-diagonal states. Moreover, a complementarity relation between the frozen value of the QD and the freezing terminal has been proposed. Importantly, it is possible to define a freezing index, quantifying the goodness of freezing for states having very slow decay rate of QC, that can also capture the QPT in the quantum XY spin model [245].

The trace norm and Hilbert-Schmidt-norm GQD under the effect of Markovian channels also exhibit freezing. See figure 13. The conditions on correlators T_{ij}, leading to the freezing of QD for the BF, PF, and BPF channels have been provided for BD states as initial states [631].

[31] An arbitrary two-qubit state, given in Eq. (28), reduces to

$$\rho_{AB} = \frac{1}{4}\Big[\mathbb{I}_2\otimes\mathbb{I}_2 + \sum_{i=1}^{3} T_{ii}\sigma_A^i\otimes\sigma_B^i + \sum_{i=1}^{3}\left(x_i\sigma_A^i\otimes\mathbb{I}_2 + \sum_{i=1}^{3} y_i\mathbb{I}_2\otimes\sigma_B^i\right)\Big],$$

up to local unitary transformations. Since the magnetizations other than x_1 and y_1 decay under the bit-flip channel, it is expected that they do not contribute to the freezing phenomenon involving the same channel, and hence they are set to zero in Eq. (87).

A necessary and sufficient condition for freezing of GQD has been provided for X-states as input under local dephasing noise [644]. Local filtering can remove the system's ability to have a frozen QD in evolution [645, 646].

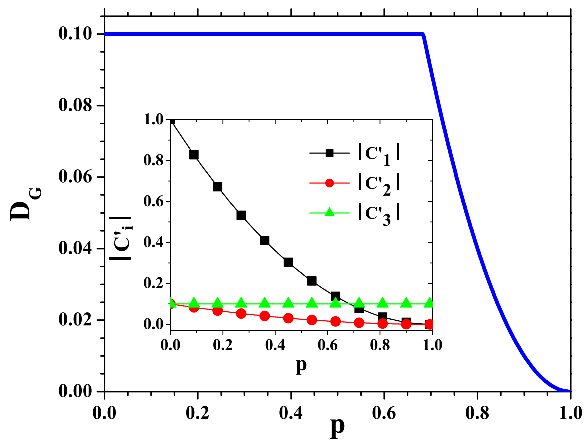

FIG. 13: Freezing behavior of trace norm GQD with the BD state given in Eq. (16) as the initial state with $T_{11} = 1$, $T_{22} = -0.1$ and $T_{33} = 0.1$ under the local PF channel. Here D_G represents the trace norm GQD. Inset: Absolute values of the correlators as functions of p. Here $|C_1'| = -|T_{11}|(1-p)^2$, $|C_2'| = -|T_{22}|(1-p)^2$, and $|C_3'| = |T_{33}|$. [Reprinted from Ref. [631] with permission. Copyright 2015 American Physical Society.]

The freezing behavior of global QD of a multiparty version of the BD state, given by

$$\rho = \frac{1}{2^N}\left(\mathbb{I}^{\otimes N} + \sum_{i=1}^{3} T_{ii}(\sigma^i)^{\otimes N}\right), \tag{90}$$

has been discussed in Ref. [647] under local PF channels. It has been found that a variety of discord-like QC measures, under certain conditions, and with Bell-diagonal state as initial state, exhibit freezing [648]. In recent years, Cianciaruso *et al.* [649] demonstrated the freezing phenomenon of Bures distance-based GQD for a specific class of BD states, each party of which is independently interacting with a non-dissipative decohering environment. The conditions for choosing a set of initial states to freeze QD, have also been investigated for other environmental conditions [650–652].

b. Sudden change phenomenon

We have seen that for certain classes of quantum states, despite the environmental effects, QD can remain fixed over a finite interval of time. Interestingly, the decay profile of QD may experience a sudden change, so that the derivative of QD has a finite discontinuity [612]. Such behavior of QD can be seen when an initial state is chosen to be a Bell-diagonal state, which is sent through a local PF channel. The conditions on the correlators of the initially prepared Bell-diagonal state for it to experience sudden change has also been provided [612]. This phenomenon has been realized using the polarization degrees of freedom of two photons [617] and also in NMR experiments [269, 653]. Considering a pure state as the initial state, for certain interactions with the bath, QD undergoes several sudden changes[32] [236, 654]. It was argued that abrupt change of QD occurs due to the change of optimal basis, required to compute classical correlation [625]. For a different variant of QD measure, namely, trace norm GQD, it has also been reported that when a Bell-diagonal state is sent through a local PF and or a local GAD channel, trace norm GQD changes twice while the associated classical correlation encounter only one sudden change in the decay process, as also observed in NMR experiments [631, 632].

2. System coupled with a spin-chain environment

The system-reservoir dynamics that we have considered up to now only deals with the map which describes the final state of the system after interaction. We will now consider a scenario where the bath consists of a collection of quantum spin-1/2 particles interacting according to some Hamiltonian, which represents a quantum spin model having quantum critical points. One may now study how QC between parts of the system gets affected by certain phenomena like QPT in the spin model environment, when we put on a system-environment coupling. Suppose that the initial state of the system-environment duo is unentangled i.e., $\rho_{SE}(0) = \rho_S(0)\otimes\rho_E(0)$. The Hamiltonian of the reservoir can, for example, be the XY spin chain, given in Eq. (69) with $\Delta = 0$. The total Hamiltonian in this case is given by $H = H_I + H_E$, where $H_I = \frac{1}{2}J(S_A^z + S_B^z)\sum_i \sigma_i^z$ is the Hamiltonian for the interaction, and H_E is the quantum XY spin model. A and B are the parts of the system, S_A^z and S_B^z are spin-operators of the system and J is proportional to the system-environment coupling strength. Suppose the system is initially prepared in a Werner state given in Eq. (10) and the total state ρ_{SE} evolves via H. The behavior of QD over finite time has been investigated in this case and it was observed that near the critical point of the spin model, QD gets minimized [655]. Interestingly, when the initial state does not possess any entanglement i.e. when $p \in [0, 1/3]$, entanglement, being zero, fails to detect any QPT of the environment, while QD can characterize it. In Ref. [656], for some special choice of initial state with vanishing QD and the trans-

[32] It is not yet clear whether pure inputs will be able to provide a frozen QD after passing through a noisy channel.

verse Ising model as environment, it has been reported that at the Ising transition point, QD rapidly increases from zero to a finite steady value, while it oscillates in the paramagnetic region, and in the ferromagnetic case, it saturates to a very low value. There are several other spin models like three-site interaction in spin chain, DM interaction in XY chain, isotropic Heisenberg chain, long-range Lipkin-Meshkov-Glick model, etc., that have been considered as environments, and their effects on QD of a pure as well as mixed state as initial states have been investigated [657–663].

External control, sometimes, is useful to extend the coherence of the system [664–666]. The role of a bang-bang pulse (a train of instantaneous pulses) on the quantum correlation of two non-interacting qubits coupled to independent reservoirs is investigated in Ref. [667]. In another scenario, the effect of quantum zeno and anti-zeno effects on two non-interacting qubits coupled to a common bosonic reservoir was considered in Ref. [668].

Later, Luo *et al.* investigated a slightly different system-bath scenario, called the two spin-star model, where two central qubits, initially prepared in an X-state, are coupled to their own spin baths that are of XY type [669]. There is no interaction between the two central qubits. Both spin baths are modeled by the ferromagnetic 1D transverse XY spin chain. The Hamiltonian for the entire setup is given by $H = H_S + H_E + H_I$ where

$$\begin{aligned} H_S &= \tau_A^z + \tau_B^z, \\ H_E &= -\frac{J}{2} \sum_{k=A',B'} \sum_{l=1}^{N} \Big((1+\gamma)\sigma_{l,k}^x \sigma_{l+1,k}^x \\ &\qquad + (1-\gamma)\sigma_{l,k}^y \sigma_{l+1,k}^y + 2\lambda \sigma_{l,k}^z \Big), \\ H_I &= J\delta \sum_{l=1}^{N} (\tau_A^z \otimes \sigma_{l,A'}^z + \tau_B^z \otimes \sigma_{l,B'}^z), \end{aligned} \tag{91}$$

where $\tau^z = |e\rangle\langle e| + |g\rangle\langle g|$ with $|e\rangle$ and $|g\rangle$ being the excited and the ground states of each qubit of the central two-qubit system. Here, A and B denote the qubits of the system while A' and B' represent the spin-baths which are taken to be periodic XY models coupled with respective qubits of the system. At the initial time $t = 0$, the state of the central two-qubits is taken to be a Bell-diagonal state, described in Eq. (16) with $T_{ii} \in [-1, 1]$. Since the XY model can be solved analytically, an exact expression for the reduced density matrix of the central two-qubit system can be obtained at any finite time t, and then QD of the same can be obtained with a measurement on qubit B. It was shown that a freezing phenomenon followed by a sudden transition can be observed for an appropriate choice of the initial state parameters. In particular, lowering the value of T_{33}, results in increasing the freezing time, but with a pay-off in the value of QD, which gets decreased when T_{33} is lowered. It was also argued that the sudden transition is closely related to the QPT of the XY model. Next, the Authors investigated the effect of a bang-bang pulse [664] (see also [665–667]) applied on the system to suppress the decoherence. As expected, the bang-bang pulse is shown to be useful to enhance the freezing time (related to what has been termed as "freezing terminal" [245]) and thereby delays the sudden change in time.

Quantum discord has also been calculated in various other prototypical models including spin-bosonic systems [670–673], detuned harmonic oscillators in a common heat bath [674], dissipative cascaded systems [675], qubits in a dissipative cavity [676], impurity qubits in BEC reservoir [677], continuous variable systems [678–683], etc.

Experimentally, in an explicit open system scenario, QD has been investigated in various substrates e.g. photons [617, 684–687], ions [688], NMR systems [689], open solid systems [690], etc.

Just like the usual quantum discord, the behavior of Gaussian QD has also been explored for various system-bath models like resonant harmonic oscillators coupled to a common environment [678, 691], non-resonant harmonic oscillators under weak and strong dissipation [692], two-mode Gaussian systems in a thermal environment [679, 681], two-mode squeezed thermal state in contact with local thermal reservoirs [693], bipartite Gaussian states in independent noisy channels [694], double-cavity opto-mechanical system [695], etc. Experimentally, the behavior of Gaussian QD has been investigated in Refs. [696–701].

C. Geometric quantum discord in open systems: Further issues

Investigations similar to those for QD in open quantum systems, as discussed above, have also been carried out using one-norm and two-norm GQDs. It was discovered that QD and GQD do not necessarily imply the same ordering for arbitrary two-qubit X-states [702]. That is, for a pair of such states, say ρ_{AB} and ρ'_{AB}, $\mathcal{D}(\rho_{AB}) \leq \mathcal{D}(\rho'_{AB})$ does not guarantee $\mathcal{D}_G(\rho_{AB}) \leq \mathcal{D}_G(\rho'_{AB})$. Such examples have been seen to be present in situations where ρ_{AB} and ρ'_{AB} are respectively the initial and final states of a system-bath duo, with the bath being either Markovian or non-Markovian [618, 703, 704].

As is the case for QD, it has been shown that there are instances for which GQD provides better understanding of the dynamics of the system than that by entanglement, when the system is subjected to environmental perturbation [288, 705–709]. Starting with a pure state, ways of protecting GQD, as measured by the Hellinger distance or the Bures distance, of the evolved state under non-Markovian structured bosonic reservoir have also been found [709].

IX. MONOGAMY OF QUANTUM CORRELATIONS

When a quantum state is shared between many parties, the amount of classical correlation between all pairs of parties can be maximal. Consider for example, a system composed of N spin-$\frac{1}{2}$ particles, in a state which is the equal mixture of all spin-up and all spin-down, in the z-direction. All two-particle states are then $\frac{1}{2}\left(|\uparrow_z\uparrow_z\rangle\langle\uparrow_z\uparrow_z| + |\downarrow_z\downarrow_z\rangle\langle\downarrow_z\downarrow_z|\right)$, which is certainly maximally classically correlated, independent of the value of N (> 2). In particular, for three-party system shared between Alice (A), Bob (B) and Charu (C), Alice can simultaneously be maximally classically correlated with Bob and Charu[33]. However, in a similar scenario, QC cannot be freely shared.

Let us again consider a tripartite scenario, where three parties, A, B, and C share a quantum state ρ_{ABC}, it can happen that Alice and Bob share a singlet and Alice and Charu share another singlet, so that Alice-Bob as well as the Alice-Charu pair share a maximally quantum correlated state. We are assuming here that the measure of quantum correlation being used is maximal in $\mathbb{C}^2 \otimes \mathbb{C}^2$ for the singlet state. This is true, for example for entanglement of formation [57, 710–713], quantum discord [47, 48], and quantum work deficit [50, 51]. Moreover, the system shared by Alice, Bob, and Charu is assumed to be in $\mathbb{C}^4 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. However, if A, B and C share a system in $\mathbb{C}^m \otimes \mathbb{C}^m \otimes \mathbb{C}^m$, a maximally quantum correlated state between A and B will imply, for all quantum correlated measures (satisfying a certain set of intuitively reasonable axioms), that A and B share a pure state. This in turn implies that the Alice-Bob pair must be as a product with the state of Charu, so that Alice cannot have any correlation, classical or quantum, with Charu [68, 289, 335, 403, 714–718]. This property of bipartite quantum correlation in the multiparty scenario has been termed as the monogamy of quantum correlation. As we see, it is a "qualitative" version of the monogamy. This qualitative version can and has been quantified in a seminal paper by Coffman, Kundu, and Wootters [403]. Unless stated otherwise, we will henceforth deal with monogamy only for states in $\mathbb{C}^m \otimes \mathbb{C}^m \otimes \mathbb{C}^m$ for some specific or arbitrary m.

There are several ways to quantify monogamy, and we will follow the one in Ref. [403]. For further discussions on this matter, see [718, 719]. Following Ref. [403] (see also [720–723]), for a given bipartite QC measure $\mathcal{Q}$, we call an arbitrary N-party quantum state $\rho_{12\ldots N}$, as "monogamous" if it satisfies the inequality

$$\mathcal{Q}_{1:\text{rest}} \geq \sum_{j=2}^{N} \mathcal{Q}_{1:j}, \tag{92}$$

where $\mathcal{Q}_{1:\text{rest}} \equiv \mathcal{Q}(\rho_{1:2\ldots N})$ in the 1:rest bipartition and $\mathcal{Q}_{1:j} \equiv \mathcal{Q}(\rho_{1j})$ denotes the QC between the parties 1 and j. Here "rest" comprises of all the other parties except the first one. If $\mathcal{Q}$ satisfies the above relation for all states, then $\mathcal{Q}$ is called a monogamous QC measure. Relation (92) is known as the monogamy inequality for a bipartite QC measure $\mathcal{Q}$. It is clear that in the relation (92), the party "1" has been given a special status since it reveals the sharability constraints of QC of party "1" with other constituent parties of the multipartite state. We call the party "1" as the "nodal" observer. In this review, we discuss all the results on monogamy using the party "1" as the nodal observer, unless stated otherwise.

It is now useful to define a quantity, known as monogamy score [403, 721–723] for any bipartite measure $\mathcal{Q}$ and any multiparty state, given by

$$\delta_{\mathcal{Q}} = \mathcal{Q}_{1:\text{rest}} - \sum_{j=2}^{N} \mathcal{Q}_{1:j}. \tag{93}$$

Since there exists certain bipartite QC measures [2, 42] which are computable, at least numerically, it is possible to compute $\delta_{\mathcal{Q}}$ for those measures, leading to computable multiparty QC measures for multipartite mixed states which is otherwise rare. Non-negativity of $\delta_{\mathcal{Q}}$ implies that the state is monogamous and vice-versa and $\mathcal{Q}$ is said to be monogamous iff $\delta_{\mathcal{Q}} \geq 0$ for all states for a fixed dimension.

There are several bipartite QC measures which satisfy the monogamy inequality, while there are plenty of measures that do not. Squared concurrence [710, 711], squared negativity [248, 516], squared entanglement of formation [57, 710, 712, 713], squashed entanglement [724] and one-way distillable entanglement [57, 725] satisfy relation (92) for three-qubit states [403, 715, 726, 727]. Concurrence and entanglement of formation violate the monogamy relation even for pure three-qubit states [716, 727–729]. See also Refs. [730–737] in this regard.

It is interesting to ask whether QC measures beyond entanglement satisfy or violate the monogamy relation. It was found that although squared QD, $(\mathcal{D}^{\leftarrow})^2$, satisfy monogamy for three-qubit pure states [717], there exists a class of three-qubit pure states for which QD violates monogamy relations, i.e. for those states[34], $\delta_{\mathcal{D}} < 0$ [716, 721]. The behavior of QD monogamy score can be useful in different quantum information protocols which we will discuss in Sec. XI. Since there are some measures which satisfy monogamy while there are some which violate the same, it is interesting to find properties related to monogamy that are true for all QC measures.

In this respect, Streltsov *et al.* [738] raised the following question: Does there exist any measure of QC

[33] Charu can be the name of a woman or man in parts of South Asia.

[34] States with negative monogamy score for QD exist, irrespective of the party in which the measurement is carried out.

which is non-zero for separable states, but still satisfy the monogamy relation for all states? The answer was found to be negative. Specifically, the following result was obtained.

Theorem 6 [738]: *Suppose a bipartite QC measure, $\mathcal{Q}$, possesses the following property: $\mathcal{Q}$ is (i) non-negative, (ii) local unitarily invariant and (iii) non-increasing under addition of a pure ancillary system. For it to satisfy monogamy, $\mathcal{Q}$ must be zero for all separable states.*

Proof: Let $\rho_{AB} = \sum_i p_i |\psi_i\rangle\langle\psi_i|_A \otimes |\phi_i\rangle\langle\phi_i|_B$ be an arbitrary separable state which can always be written as a convex combination of rank-1 projectors [89]. A special extension of ρ_{AB} in a tripartite state is given by

$$\rho_{ABC} = \sum_i p_i |\psi_i\rangle\langle\psi_i|_A \otimes |\phi_i\rangle\langle\phi_i|_B \otimes |i\rangle\langle i|_C, \qquad (94)$$

where $\langle i|j\rangle_C = \delta_{ij}$. It is local unitarily equivalent in the BC part with another state σ_{ABC}, given by

$$\sigma_{ABC} = \sum_i p_i |\psi_i\rangle\langle\psi_i|_A \otimes |0\rangle\langle 0|_B \otimes |i\rangle\langle i|_C. \qquad (95)$$

Now by using conditions (ii) and (iii), we have $\mathcal{Q}(\sigma_{AC}) \geq \mathcal{Q}(\sigma_{A:BC}) = \mathcal{Q}(\rho_{A:BC})$. Since $\mathcal{Q}$ satisfies monogamy relation, we have

$$\mathcal{Q}(\sigma_{AC}) \geq \mathcal{Q}(\rho_{AB}) + \mathcal{Q}(\rho_{AC}). \qquad (96)$$

From Eqs. (94) and (95), one can find that $\sigma_{AC} = \rho_{AC}$, which implies $\mathcal{Q}(\rho_{AB}) = 0$ (by using condition (i)). Since ρ_{AB} is an arbitrary separable state, $\mathcal{Q}$ vanishes and hence the proof. ■

It was also shown that the QC measures, which are non-monogamous for a certain state, can be made monogamous for that state by a proper choice of a monotonically increasing function of that measure [739]. More precisely, we have the following theorem.

Theorem 7 [739]: *If a bipartite QC measure $\mathcal{Q}$ is non-monogamous, for an N-partite quantum state $\rho_{12\ldots N}$ in arbitrary finite dimensions, i.e., $\mathcal{Q}_{1:rest} < \sum_{i=2}^{N} \mathcal{Q}_{1i}$, then there always exists a non-decreasing function $f : \mathbb{R} \to \mathbb{R}$ such that*

$$f(\mathcal{Q})_{1:\text{rest}} > \sum_{i=2}^{N} f(\mathcal{Q})_{1i}, \qquad (97)$$

provided that $\mathcal{Q}$ is monotonically non-increasing under discarding systems and under tracing out of subsystems, invariance happens only for states satisfying monogamy.

Proof: Since $\mathcal{Q}$ is non-increasing under discarding of subsystems and is non-monogamous, $\underbrace{\mathcal{Q}_{1:\text{rest}}}_{\tilde{x}} > \underbrace{\mathcal{Q}_{1i}}_{\tilde{y}_i} \geq 0 \ \forall i$ and $\mathcal{Q}_{1:\text{rest}} < \sum_i \mathcal{Q}_{1i}$. It implies that

$$\lim_{m\to\infty} \left(\frac{\tilde{y}_i}{\tilde{x}}\right)^m = 0 \ \forall i. \qquad (98)$$

Thus for every $\epsilon_i > 0$, however small, one must have positive integers $n_i(\epsilon_i)$, $i = 2, \ldots, N$, such that

$$\left(\frac{\tilde{y}_i}{\tilde{x}}\right)^m < \epsilon_i \ \forall m \geq n_i(\epsilon_i). \qquad (99)$$

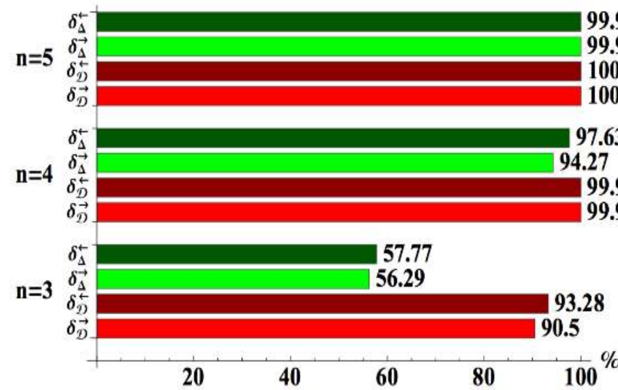

FIG. 14: Percentages of Haar uniformly generated states satisfying the monogamy relations for quantum discord and work deficit. The number of parties is denoted as "n" in the diagram. The monogamy scores for $\mathcal{D}^{\leftarrow}, \mathcal{D}^{\rightarrow}, \mathcal{WD}^{\leftarrow}$, and $\mathcal{WD}^{\rightarrow}$ are respectively denoted in the diagram by $\delta_{\mathcal{D}}^{\leftarrow}, \delta_{\mathcal{D}}^{\rightarrow}, \delta_{\Delta}^{\leftarrow}$, and $\delta_{\Delta}^{\rightarrow}$. [Reprinted from Ref. [735] with permission. Copyright 2015 American Physical Society.]

Choose $\epsilon_i < \frac{1}{N-1} \ \forall i$ and suppose $n = \max\{n(\epsilon_i)\}$, then for any integer $m \geq n$, one gets

$$\sum_{i=2}^{N} \left(\frac{\tilde{y}_i}{\tilde{x}}\right)^m < \sum_{i=2}^{N} \epsilon_i < 1 \Rightarrow \tilde{x}^m \geq \sum_{i=2}^{N} (\tilde{y}_i)^m. \qquad (100)$$

Hence the proof. ■

Note that if a QC measure is monotonically non-increasing under LOCC, its positive powers are also non-increasing under LOCC.

The monogamy property of QC measures also changes from non-monogamous to monogamous when the number of parties are increased [735]. Figure 14 depicts the percentages of states which satisfy the monogamy relations of QD and WD for a fixed number of parties up to five. The states are generated Haar uniformly. The figure clearly indicates the increase in the percentage of monogamous states as one moves from three-qubit to five-qubit quantum states [735].

The monogamy property of GQD has also been explored in the following years. Streltsov *et al.* [738] has shown that for a general tripartite pure quantum state, $|\psi_{ABC}\rangle$, GQD is monogamous, i.e. $\mathcal{D}_G(|\psi_{A:BC}\rangle) \geq \mathcal{D}_G(\rho_{AB}) + \mathcal{D}_G(\rho_{AC})$, where ρ_{AB} and ρ_{AC} are the reduced density matrices of $|\psi_{ABC}\rangle$. A possible extension of the monogamy relation for GQD in case of mixed quantum states has recently been reported by Daoud *et al.* [740], where the Authors considered two families of generalized three-qubit X-states. Furthermore, Cheng *et al.* [741] have proven a monogamy relation of GQD for a tripartite mixed quantum state ρ_{ABC} which reads as

$$\mathcal{D}_G(\rho_{AB}) + \mathcal{D}_G(\rho_{AC}) \leq \frac{1}{2}. \qquad (101)$$

X. CONNECTING ENTANGLEMENT WITH QUANTUM DISCORD-LIKE MEASURES

In this section, we will discuss about relations of QD and QD-like measures with entanglement measures. It turns out that such relations can be used to establish connections between discord monogamy score and bipartite as well as multipartite entanglement measures for multipartite states.

A. Links to entanglement of formation

As we have already noted, if any two parties, A and B, of a tripartite system in $\mathbb{C}^m \otimes \mathbb{C}^m \otimes \mathbb{C}^m$ in a pure state, possess maximal QC, then the state is nearly always of the form $|\psi_{ABC}\rangle = |\psi'_{AB}\rangle \otimes |\psi''_C\rangle$, thereby implying no correlation of party C with A as well as B. In particular, there is no classical correlation, e.g. quantified by $J_{A|C}$ between A and C. One may now ask the extent to which $J_{A|C}$ can increase for a non-maximal QC between A and B. Koashi and Winter [68] derive the following useful result.

Theorem 8 [68]: *For an arbitrary tripartite state ρ_{ABC},*

$$\mathcal{E}_{AB} + J_{A|C} \leq S_A, \tag{102}$$

where $\mathcal{E}_{AB}$ is the EOF of the reduced state ρ_{AB} while $J_{A|C}$ denotes the classical correlation of ρ_{AC} (introduced in Sec. XV A 1) with measurement being performed in C. S_A is the von Neumann entropy of the reduced density matrix ρ_A. Here, the equality holds only when the shared state is pure.

Proof: Let us first consider an arbitrary pure state $|\psi_{ABC}\rangle$ such that $\text{tr}_C(|\psi_{ABC}\rangle\langle\psi_{ABC}|) = \rho_{AB}$ and similarly for ρ_{AC}. Let us also assume that $\rho_{AB} = \sum_i p_i |\psi^i_{AB}\rangle\langle\psi^i_{AB}|$ where $|\psi^i_{AB}\rangle$'s form the minimum pure state decomposition required for EOF of ρ_{AB}. Let us denote the measurement at C that realizes this optimal ensemble by acting n the state $|\psi_{ABC}\rangle$ as $\{M_i\}$. Tracing out B, the same measurement on C leads to the ensemble on the A's part as $\{p_i, \text{tr}_B(|\psi^i_{AB}\rangle\langle\psi^i_{AB}|)\}$ [742], and hence from Eq. (7), we obtain

$$\begin{aligned} J_{A|C} &\geq S(\rho_A) - \sum_i p_i S\big(\text{tr}_B(|\psi^i_{AB}\rangle\langle\psi^i_{AB}|)\big) \\ &= S(\rho_A) - \mathcal{E}(\rho_{AB}). \end{aligned} \tag{103}$$

On the other hand, suppose that the optimum measurement performed on C and required for obtaining $J_{A|C}$ is $\{\tilde{M}_i\}$. It results in the output ensemble at A as $\{\tilde{p}_i, \tilde{\rho}_{A|i} = \text{tr}_{BC}(|\tilde{\psi}^i_{ABC}\rangle\langle\tilde{\psi}^i_{ABC}|)\}$. Thus

$$\begin{aligned} J_{A|C} &= S(\rho_A) - \sum_i \tilde{p}_i S(\tilde{\rho}_{A|i}) \\ &\leq S(\rho_A) - \mathcal{E}(\rho_{AB}), \end{aligned} \tag{104}$$

where the inequality arises from the fact that second term of $J_{A|C}$ is higher than or equal to the EOF of ρ_{AB} for all measurements[35]. From (103) and (104), we have $J_{A|C} + \mathcal{E}(\rho_{AB}) = S(\rho_A)$ for pure tripartite states. Now an arbitrary state, ρ_{ABC}, can be purified to form a pure four-party state $|\psi_{ABCD}\rangle$, such that $\rho_{ABC} = \text{tr}_D(|\psi_{ABCD}\rangle\langle\psi_{ABCD}|)$. Using the above relation for pure states and by taking CD as a single party, one gets $J_{A|CD} + \mathcal{E}(\rho_{AB}) = S(\rho_A)$. Note now that $J_{A|CD}$ is non-increasing under discarding the subsystem[36], i.e. $J_{A|CD} \geq J_{A|C}$. Combining the above results, we obtain Eq. (102) for arbitrary tripartite states. ■

For a tripartite state, ρ_{ABC}, a relation between QD of the reduced state ρ_{AB} and the classical correlation of ρ_{BC} can be obtained by using Eq. (102) and is given by [82]

$$\mathcal{D}(\rho_{AB}) + J_{C|B} \leq S(\rho_B), \tag{105}$$

where the equality holds for pure states. It is important to note here that the definition of quantum discord used in the Koashi-Winter result in Theorem 8 involves an optimization over POVMs, and not merely over PV measurements. This will remain true whenever the Koashi-Winter result is used.

For a tripartite quantum state ρ_{ABC}, we have [335]

$$\begin{aligned} \mathcal{D}(\rho_{AB}) &+ \mathcal{D}(\rho_{AC}) \\ &= S(\rho_A) - J_{A|B} + S(\rho_A) - J_{A|C} + \Delta \\ &\geq \mathcal{E}(\rho_{AB}) + \mathcal{E}(\rho_{AC}) + \Delta, \end{aligned} \tag{106}$$

where $\Delta = S(\rho_B) + S(\rho_C) - S(\rho_{AB}) - S(\rho_{AC})$, and where the inequality in (102) has been used. Strong subadditivity of von Neumann entropy gives $\Delta \leq 0$ and hence no definite relation can be established between the EOFs and the QDs in (106). However, for a pure state $|\psi_{ABC}\rangle$, $\Delta = 0$ since $S(\rho_B) = S(\rho_{AC})$ and $S(\rho_C) = S(\rho_{AB})$. Thus for a tripartite pure state, one has "conservation law" given by

$$\mathcal{D}(\rho_{AB}) + \mathcal{D}(\rho_{AC}) = \mathcal{E}(\rho_{AB}) + \mathcal{E}(\rho_{AC}). \tag{107}$$

B. Relating with multipartite entanglement

We now establish a connection between two multiparty QC quantifiers, namely, discord monogamy score and a genuine multiparty entanglement measure, known as generalized geometric measure (GGM) [743–745] (see

[35] For rank-1 $\{\tilde{M}_i\}$, it is clear that the output state in the A part is pure and hence, $\sum_i \tilde{p}_i S(\tilde{\rho}_{A|i}) = \sum_i \tilde{p}_i S\big(\text{tr}_B(|\tilde{\psi}^i_{AB}\rangle\langle\tilde{\psi}^i_{AB}|)\big) \geq \mathcal{E}(\rho_{AB})$. If the measurement is not of rank-1, $\tilde{M}_i = \sum_j \tilde{M}_{ij}$, for some rank-1 $\{\tilde{M}_{ij}\}$ with $\tilde{p}_{ij} = \text{tr}\big((\mathbb{I}^A \otimes \tilde{M}^C_{ij})\rho_{AC}\big)$ and $\tilde{\rho}_{A|ij} = \text{tr}_C(\mathbb{I}^A \otimes \tilde{M}^C_{ij}\rho_{AC}\mathbb{I}^A \otimes \tilde{M}^C_{ij})/p_{ij}$. Now one can also show that $\tilde{p}_i = \sum_j \tilde{p}_{ij}$ and $\tilde{p}_i\rho_{A|i} = \sum_j \tilde{p}_{ij}\rho_{A|ij}$. Thus from the concavity of von Neumann entropy, $\sum_i \tilde{p}_i S(\rho_{A|i}) \geq \sum_{ij} p_{ij} S(\rho_{A|ij}) \geq \mathcal{E}(\rho_{AB})$.

[36] See Appendix XVI for the proof.

also [746–748], see Appendix XV B for definition).

Theorem 9 [723]: *For all three-qubit pure states, $|\psi_{ABC}\rangle$, whose GGM are same as that of the generalized GHZ* (gGHZ) *state*[37], *$|gGHZ_3\rangle$, the discord monogamy score of $|\psi_{ABC}\rangle$ is bounded above by the modulus of the discord monogamy score of the gGHZ state, i.e.*

$$-\delta_{\mathcal{D}}(|gGHZ_3\rangle) \leq \delta_{\mathcal{D}}(|\psi_{ABC}\rangle) \leq \delta_{\mathcal{D}}(|gGHZ_3\rangle), \quad (109)$$

provided the maximum eigenvalue in GGM of the arbitrary state is obtained from the nodal : rest bipartition.

Proof: Without loss of generality, let us fix the party A as the nodal observer. For an arbitrary three-qubit pure state $|\psi_{ABC}\rangle$, $\delta_{\mathcal{D}}$ is given by

$$\delta_{\mathcal{D}}(|\psi_{ABC}\rangle) = S(\rho_A) - \mathcal{D}(\rho_{AB}) - \mathcal{D}(\rho_{AC}), \quad (110)$$

and the same for $|gGHZ_3\rangle$ is given by

$$\delta_{\mathcal{D}}(|gGHZ_3\rangle) = h(\alpha), \quad (111)$$

where $h(\alpha)$ is defined in Eq. (67). The GGM of these two states, $|\psi_{ABC}\rangle$ and $|gGHZ_3\rangle$, are respectively given by

$$\mathcal{G}(|\psi_{ABC}\rangle) = 1 - \max\{\lambda_A, \lambda_B, \lambda_C\}, \quad (112)$$

$$\mathcal{G}(|gGHZ_3\rangle) = 1 - \alpha, \quad (113)$$

where λ_i, $i = A,\ B,\ C$, are the largest eigenvalues of the reduced density matrices ρ_A, ρ_B, ρ_C respectively. Here we assume $\alpha \geq \frac{1}{2}$. Suppose now that the GGMs for these two states are equal which leads $\alpha = \max\{\lambda_A, \lambda_B, \lambda_C\} = \lambda_A$ as per the premises of the theorem. This immediately implies $\delta_{\mathcal{D}}(|\psi_{ABC}\rangle) \leq h(\lambda_A) = \delta_{\mathcal{D}}(|gGHZ_3\rangle)$, where we use the fact that $S(\rho_A) = h(\lambda_A)$, and $\mathcal{D} \geq 0$.

To obtain lower bound, we note that Eq. (106) reduces to $\mathcal{D}(\rho_{AB}) + \mathcal{D}(\rho_{AC}) = \mathcal{E}(\rho_{AB}) + \mathcal{E}(\rho_{AC})$ when $|\psi\rangle_{ABC}$ is pure and also the EOF ($\mathcal{E}$) of a bipartite state is bounded above by von Neumann entropies of the local density matrices[38]. Therefore $\mathcal{D}(\rho_{AB}) + \mathcal{D}(\rho_{AC}) \leq 2S(\rho_A)$, which implies $\delta_{\mathcal{D}}(|\psi_{ABC}\rangle) \geq -S(\rho_A) = -h(\lambda_A) = -h(\alpha) = -\delta_{\mathcal{D}}(|gGHZ_3\rangle)$. ■

XI. APPLICATIONS OF DISCORD MONOGAMY SCORE

Over the last few years, it has been found that the discord monogamy score can be efficiently used for analysis and applications in different multiparty quantum information tasks including state discrimination, distinguishing between noisy channels, classical information transfer between multiple senders and receivers and identifying different phases in many-body systems.

A. Quantum state discrimination

The set of three-qubit genuinely multiparty entangled pure states can be divided into two disjoint subsets with respect to transformation possible by using stochastic local operations and classical communication (SLOCC) [750]. Specifically, it was shown that states from one class cannot be converted into another at the single-copy level under LOCC with any non-zero probability. These two inequivalent classes are the "GHZ" and the "W" classes, arbitrary members of which can be expanded as

$$|GHZ^c\rangle = \sqrt{K}(\alpha_0|000\rangle + \beta_0 e^{i\phi}|\psi_1\psi_2\psi_3\rangle), \quad (114)$$

where $|\psi_j\rangle = \alpha_j|0\rangle + \beta_j|1\rangle$, with $K = \big(1 + 2\beta_0\Pi_{i=0}^3\alpha_i\cos\phi\big)^{-1}$ and

$$|W^c\rangle = \sqrt{a}|001\rangle + \sqrt{b}|010\rangle + \sqrt{c}|100\rangle + \sqrt{d}|000\rangle, \quad (115)$$

where $a,\ b,\ c,\ d$ are real numbers with $a+b+c+d = 1$. The three-party gGHZ state, $|gGHZ_3\rangle$, belong to the GHZ class, while the generalized W (gW) state, given by

$$|gW_3\rangle = \sqrt{a}|001\rangle + \sqrt{b}|010\rangle + \sqrt{c}|100\rangle, \quad (116)$$

is a subclass of $|W^c\rangle$. It can be easily shown that the discord monogamy score is negative for the entire class of gW states while it is non-negative for the gGHZ states [721]. Furthermore, it was shown that for states of the W class, $\delta_{\mathcal{D}} < 0$ [716, 721], although for states of the GHZ class, $\delta_{\mathcal{D}}$ can be both positive and negative (and zero). To prove the result for the W class, first notice that the monogamy score of squared concurrence vanishes, i.e. $\mathcal{C}^2_{AB} + \mathcal{C}^2_{AC} = \mathcal{C}^2_{A:BC}$, for all W-class states [403]. Since $\mathcal{E}$ (see Eq. (149)) is a concave function of $\mathcal{C}^2$ [711] and $\mathcal{E}, \mathcal{C} \in [0,1]$, $\mathcal{E}_{A:BC} < \mathcal{E}_{AB} + \mathcal{E}_{AC}$ for states of the W class[39]. Using the relation of Koashi-Winter given in

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[37] An N-qubit gGHZ state [749] is given by

$$|gGHZ_N\rangle = \sqrt{\alpha}|00\ldots0\rangle_N + \sqrt{1-\alpha}e^{i\phi}|11\ldots1\rangle_N, \quad (108)$$

with $\alpha \in [0,1]$, and ϕ being a phase factor.

[38] Suppose the optimal pure state decomposition of ρ_{AB}, is the ensemble $\{p_i, |\psi_i\rangle\}$. Thus from Eq. (149), $\mathcal{E}(\rho_{AB}) = \sum_i p_i S(\rho^i_X) \leq S(\sum_i p_i\rho^i_X) = S(\rho_X)$, where we use the concavity of von Neumann entropy. Here, $X = A, B$, $\rho^i_X = \mathrm{tr}_{\bar{X}}(|\psi_i\rangle\langle\psi_i|)$ with $\bar{X}$ being the complement to $X \in \{A, B\}$.

[39] For a concave function $f(x)$, with $f(0) = 0$, we can show that if $x = \sum_j y_j$, then $f(x) \leq \sum_j f(y_j)$, where equality holds when $y_j = 0$, $\forall j$ except some y_i. To show this, note here that for some $t \in [0,1]$, as f is concave, we have $f(tz) = f(tz + (1-t)0) \geq tf(z)$. So,

$$\begin{aligned}\sum_j f(y_j) &= \sum_j f\Big(\Big(\sum_i y_i\Big)\frac{y_j}{\sum_i y_i}\Big) \\ &= \sum_j f(xt_j) \geq \sum_j t_j f(x) = f(x),\end{aligned} \quad (117)$$

where $0 \leq t_j \leq 1$, and $\sum_j t_j = \sum_j y_j/(\sum_i y_i) = 1$. Equality holds only when $t_j = 0\ \forall j$ except one.

Eqs. (102), and (106), for states of the W-class, one finds

$$\mathcal{D}^{\leftarrow}_{AB} + \mathcal{D}^{\leftarrow}_{AC} = \mathcal{E}_{AB} + \mathcal{E}_{AC} > \mathcal{E}_{A:BC} = \mathcal{D}^{\leftarrow}_{A:BC}. \quad (118)$$

The inequality comes from the concavity of entanglement of formation with respect to concurrence squared. The inequality is strict, as (i) $\mathcal{C}_{AB} = 0$ or $\mathcal{C}_{AC} = 0$ along with $\mathcal{C}^2_{AB} + \mathcal{C}^2_{AC} = \mathcal{C}^2_{A:BC}$ implies that three-qubit pure state is not genuinely multiparty entangled, and (ii) the relation (117) is strict unless $t_j = 0\ \forall j$ except one. The last equality comes from the fact that both EOF and QD reduce to the von Neumann entropy of the local density matrices [47, 714] for pure states. The discord monogamy score, therefore, is to the GHZ-class states as the entanglement witnesses [248, 251, 252] are to entangled states: $\delta_{\mathcal{D}} \geq 0$ implies that the state is from the GHZ class, while $\delta_{\mathcal{D}} < 0$ is inconclusive, provided the input is promised to be a three-qubit pure genuinely multipartite entangled state [716, 721].

B. Quantum channel discrimination

Another important aspect of the discord monogamy score is that it can distinguish between noisy channels [751]. Consider a game in which we are provided with a black box that is a quantum channel taking an arbitrary three-qubit state as an input, and which is promised to be a global noisy, or a local amplitude damping (ADC), or a local phase damping (PDC), or a local depolarizing channel (DPC) [3, 594]. The game is to find out what the channel is. The input states that have been used are the three-qubit gGHZ as well as the gW states, and the monogamy scores of QD ($\delta^{\rightarrow}_{\mathcal{D}}$) and negativity ($\delta_{\mathcal{N}}$) are considered as the distinguishing "order parameter". (See Appendix XV A 3 for a definition of negativity.) The Authors of Ref. [751] proposed a two-step protocol, for discriminating the global and local noises by using the gGHZ and gW states (see figure 15), where the choice of QC measure in the second step depends on the outcome of the first step. It works in the following way: Step 1: the gW state is taken as an input and after its passage through the unknown channel, $\delta^{\rightarrow}_{\mathcal{D}}$ is computed for the output. Step 2: According to the value of $\delta^{\rightarrow}_{\mathcal{D}}$ in Step 1, $\delta_{\mathcal{N}}$ or $\delta^{\rightarrow}_{\mathcal{D}}$ is calculated for the output state, when a gGHZ state (see Eq. (108)) with $0.65 \leq \sqrt{\alpha} \leq \frac{1}{\sqrt{2}}$ is sent through the same channel. If $\delta^{\rightarrow}_{\mathcal{D}} \geq 0$ in the first step, $\delta_{\mathcal{N}}$ is calculated in the next step, while for negative $\delta^{\rightarrow}_{\mathcal{D}}$, measurement of $\delta^{\rightarrow}_{\mathcal{D}}$ is performed again in the second step. If $\delta^{\rightarrow}_{\mathcal{D}} \geq 0$ in the first step together with $\delta_{\mathcal{N}} > 0$ in the second one, the channel is global, whereas $\delta_{\mathcal{N}} = 0$ implies that it is the DPC. On the other hand, if $\delta^{\rightarrow}_{\mathcal{D}} < 0$ in the first step, and if the value of $\delta^{\rightarrow}_{\mathcal{D}}$ lies within $[0.13, 0.3]$ in the second step, the channel can be identified as ADC, while if $\delta^{\rightarrow}_{\mathcal{D}} \in [0.019, 0.09]$ in the second step, the channel is the PDC. The accomplishment of the above protocol depends on two assumptions, namely (i) the strength of the noises should be "moderate" and (ii) the channels can be used twice.

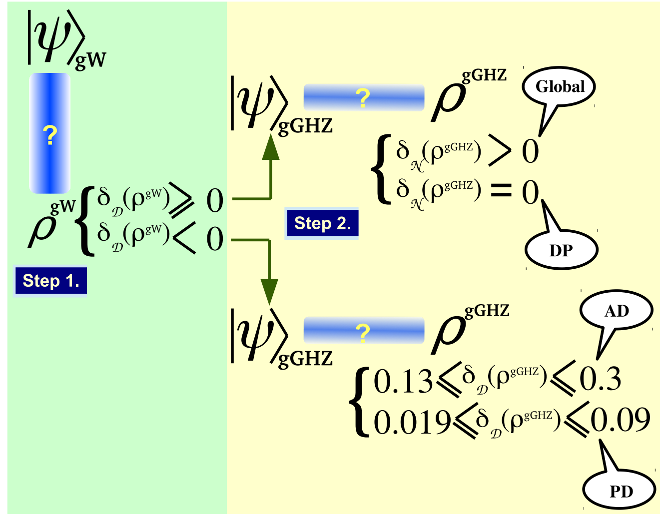

FIG. 15: Discrimination of quantum channels by using monogamy scores. The protocol is discussed in Sec. XI B by calculating $\delta^{\rightarrow}_{\mathcal{D}}$ (denoted in the figure as $\delta_{\mathcal{D}}$) and $\delta_{\mathcal{N}}$. The states $|gGHZ_3\rangle$ and $|gW_3\rangle$ are represented in the figure as $|\psi\rangle_{gGHZ}$ and $|\psi\rangle_{gW}$ respectively. The corresponding outputs are respectively denoted in the figure as ρ^{gGHZ} and ρ^{gW}. [Reprinted from Ref. [751] with permission. Copyright 2016 Elsevier.]

It was also observed that when the three-party states are sent through these noisy channels, $\delta^{\rightarrow}_{\mathcal{D}}$ is always monotonically decreasing with the increase of noise when gGHZ states are used as the input, while $\delta^{\rightarrow}_{\mathcal{D}}$ of the resulting states behave non-monotonically with noise parameters when the input states are gW states [751].

C. Connection with dense coding

In the bipartite domain, efficiency of quantum communication protocols, both classical information transfer via quantum states and quantum state transmission, are related to the QC content of the shared quantum state. It was found that the pattern of $\delta_{\mathcal{D}}$ can be used for understanding the capacity of dense coding (DC) involving multiple senders and multiple receivers. We will discuss three different DC protocols, namely, Case 1: multiple senders and a single receiver [752, 753], and Case 2: a single sender and many receivers [754].

The multiparty DC capacity (C_{multi}) [752, 753], of an N-party state $\rho_{12\ldots N}$, shared between $N-1$ senders and a single receiver, is given by

$$C_{multi}(\rho_{12\ldots N}) = \frac{1}{\log_2 d_{12\ldots N}} \max\{\log_2 d_1 d_2 \ldots d_{N-1}, \log_2 d_1 d_2 \ldots d_{N-1} + S(\rho_N) - S(\rho_{12\ldots N})\}, (119)$$

where $d_1, d_2, \ldots, d_{N-1}$ are dimensions of the systems in possession of the $N-1$ senders, and where the last party is taken to be the receiver, in possession of a system of dimension d_N. We set $d_{12\ldots N} = d_1 d_2 \ldots d_N$. Here, one may note that the amount of information that can be sent by using a "classical" protocol (i.e., without using a shared quantum state) is $\log_2 d_1 \ldots d_{N-1}$, and hence the positivity of the "coherent information" [3], $S(\rho_N) - S(\rho_{12\ldots N})$, guarantees the advantage of using the shared quantum state in classical information transmission, and is known as the DC advantage [755]. A connection between C_{multi} and $\delta_{\mathcal{D}}$ has been made for arbitrary pure states [756], by considering the receiver as a nodal observer, as given in the theorem below.

Theorem 10 [756]: *Among all multiparty pure states having equal amount of $\delta_{\mathcal{D}}$, C_{multi} is bounded below by that of the gGHZ state.*

Proof: For an arbitrary pure state $|\psi\rangle_{12\ldots N}$, the discord monogamy score is given by

$$\begin{aligned}\delta_{\mathcal{D}} &= \mathcal{D}_{12\ldots N-1:N} - \sum_i \mathcal{D}_{i:N} \\ &\leq \mathcal{D}_{12\ldots N-1:N} = S(\rho_N). \end{aligned} \tag{120}$$

Equating $\delta_{\mathcal{D}}$ for $|\psi\rangle_{12\ldots N}$ with $\delta_{\mathcal{D}}(|gGHZ_N\rangle)$, given in Eq. (111), one has

$$\begin{aligned} S(\rho_N) &\geq h(\alpha), \\ \text{which implies } C_{multi}(|\psi\rangle_{12\ldots N}) &\geq C_{multi}(|gGHZ_N\rangle). \end{aligned} \tag{121}$$

Hence the proof. ■

In other words, to send a fixed amount of classical information, in the scenario of Case 1, the gGHZ state requires the maximal multiparty QC, as quantified by $\delta_{\mathcal{D}}$, among all pure multipartite quantum states. This is prominently visible from figure 16(a). The DC capacity, given in Eq. (119), has been derived under the assumption that the encoded qubits are sent through the noiseless quantum channels to the receivers.

Let us now move to a scenario where the channels between the senders and the receivers are noisy. There are at least two different ways in which the noise can act. Firstly, it can affect the shared quantum state at the time of sharing the multipartite state. Secondly, noise can be present in the quantum channel by which the senders send their encoded part [757–760] to the receiver. The first case has already been incorporated in the capacity given in Eq. (119). The second case is not easy to handle, and a compact form of DC capacity for an arbitrary noisy channel is not known. However, for the covariant noisy channel[40], the capacity for DC can be obtained[41], in a useful form. Moreover, the capacity can be connected with $\delta_{\mathcal{D}}$, which establishes a relation between the noisy DC capacity of an arbitrary state with that of the gGHZ state, as has been obtained in the noiseless case in Theorem 10 (see figure 16(b)) [756].

Let us now consider a different classical information transmission protocol, viz. that corresponding to Case 2. Suppose that an N-party state $\rho_{12\ldots N}$ is shared between a single sender ("1") and $N-1$ receivers, and where the sender individually sends classical information to each receiver [754, 763]. In this case, the DC advantage (C_{adv}) [754] reads as

$$C_{adv}(\rho_{12\ldots N}) = \max\left[\{S(\rho_i) - S(\rho_{1i}) | i = 2, \ldots, N\}, 0\right]. \tag{123}$$

The connection between $\delta_{\mathcal{D}}$ and C_{adv} has also been analyzed. It was found that for three-qubit pure states, a complementary relation exists between the DC advantage and $\delta_{\mathcal{D}}$ [754]. Moreover, the equality of that relation is attained by an one-parameter family of states, given by $|\psi_\alpha\rangle = \frac{1}{\sqrt{2(1+\alpha^2)}}\big(|111\rangle + |000\rangle + \alpha(|101\rangle + |010\rangle)\big)$, with $\alpha \in [0, \frac{1}{2}]$, within the GHZ-class of states, and which has been called the "maximally-dense-coding-capable" states.

D. Discord monogamy score in cooperative phenomena

We now briefly discuss the behavior of QD monogamy score in cooperative quantum phenomena. Such many-body system include one-dimensional spin models and a biological model, mimicking the photosynthesis process.

1. *Many-body systems*

We have already discussed in Sec. VII about the effectiveness of QD as detector of different phases in many-body system. In this subsection, we will discuss whether QD monogamy score can also detect quantum critical points. The monogamy scores are the one of the few QC measures which quantify QC in a multiparty domain, that are relatively easy to compute. The monogamy score

[40] Covariant noise [758, 761], Λ^c, in a quantum channel is a completely positive trace preserving (CPTP) map which "commutes" with any one complete set of unitary operators $\{W_i\}$, defined on the same Hilbert space of operators which contains the state, that the channel will carry in the following sense:

$$\Lambda^c(W_i \rho W_i^\dagger) = W_i \Lambda^c(\rho) W_i^\dagger, \ \forall i,$$

where ρ is a quantum state passing through the quantum channel.

[41] The DC capacity [757–760] of a shared quantum state $\rho_{12\ldots N}$, under the covariant noise Λ^c between $N-1$ senders and a single receiver, where noise acts after the encoding, is given by

$$\begin{aligned} C^c_{multi}(\rho_{12\ldots N}) = \frac{1}{\log_2 d_{12\ldots N}} \max\{&\log_2 d_{12\ldots N-1}, \\ &\log_2 d_{12\ldots N-1} + S(\rho_N) - S(\tilde{\rho}_{12\ldots N})\}, \end{aligned}$$

where $\tilde{\rho}_{12\ldots N} = \Lambda^c\big((U^{\min}_{12\ldots N-1} \otimes \mathbb{I}_N)\rho_{12\ldots N}(U^{\min\,\dagger}_{12\ldots N-1} \otimes \mathbb{I}_N)\big)$, with $U^{\min}_{12\ldots N-1}$ being a unitary operator in the sender's subsystems. The unitary operator can be global or local depending on the type of encoding, and "min" in the superscript of $U^{\min}_{12\ldots N-1}$ indicates that the unitary operator minimizes the von Neumann entropy of $\tilde{\rho}_{12\ldots N}$.

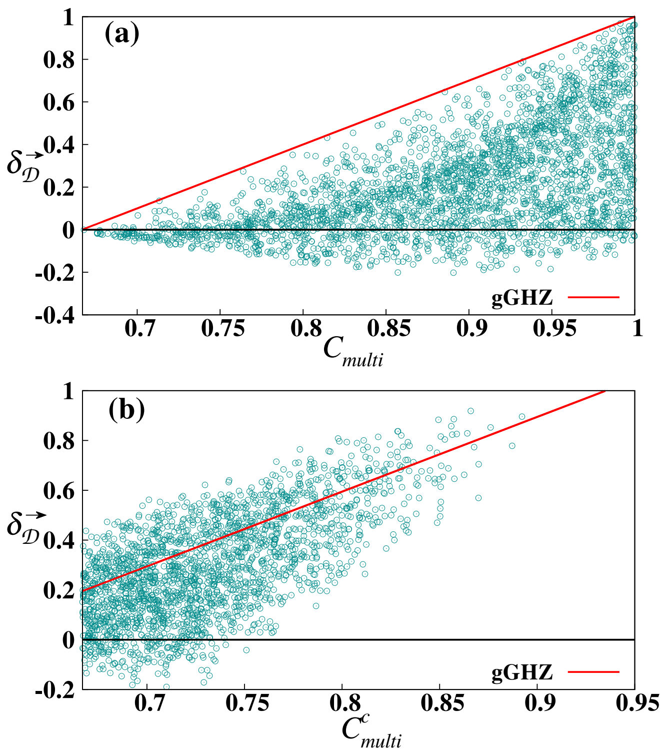

FIG. 16: Capacity of DC vs. the monogamy score of QD ($\delta_{\mathcal{D}}$). Blue dots represent Haar uniformly generated three-qubit pure states while the solid line is for the gGHZ state. The ordinates and the abscissae are respectively $\delta_{\mathcal{D}}$ and C_{multi}. In panel (a), the noiseless DC capacity of Case 1 is considered, and it is observed that all the points are bounded above by the gGHZ line, as shown in Theorem 10. On the other hand, panel (b) depicts noisy channels[a] between two senders and a receiver and it is observed in this case that all the points are moving leftward, with respect to their position in panel (a), as is expected due to the interaction of noise in the channels, and at the same time they cross the gGHZ line, thereby violating the constraint set in place in the noiseless case by Theorem 10. In both the cases, all the QDs are calculated by performing measurement on the nodal observer, which is the receiver. Both axes in both figures are measured in bits. [Adapted from Ref. [756] with permission. Copyright 2014 American Physical Society.]

[a]The covariant noise used in the depiction of the figure is the fully correlated Pauli noise [762], acting on the senders subsystem in the following way

$$\rho_{ABC} \to \Lambda^c(\rho_{ABC}) = \sum_i p_i(\sigma_A^i \otimes \sigma_B^i \otimes \mathbb{I}_2)\rho_{ABC}(\sigma_A^i \otimes \sigma_B^i \otimes \mathbb{I}_2), \tag{122}$$

with p_i being the probability or the noise parameters, $i \in \{0, x, y, z\}$ and $\sigma^0 = \mathbb{I}_2$. The noise parameters are taken to be $p_0 = p_3 = 0.485$ and $p_1 = p_2 = 0.015$.

of squared QD has been used to analyze the QPT at $\Delta = 1$ of the XXZ model (which is obtained by setting $\gamma = h = 0$ in the Hamiltonian in Eq. (69) [764]. In a triangular configuration, by varying J from positive to negative, the transverse Ising model ($\gamma = 1$ and $\Delta = 0$ in Eq. (69)) changes from a frustrated to a non-frustrated phase at $J = 0$. The ground state of this model has been simulated in the laboratory in an NMR system [765]. It was reported that the value of $\delta_{\mathcal{D}}$ is much higher in the non-frustrated regime than the frustrated one. Moreover, the transition point was accompanied with the vanishing of $\delta_{\mathcal{D}}$.

Another investigation of monogamy of QD has been carried out for strongly correlated electrons in the bond charge exended 1D Hubbard model [766]. The ground state of the model possesses three different phases. Varying the system parameters, it was shown that the discord monogamy score, which is always negative in this case, behaves differently, depending on the phases in which the system lies. For example, in one phase where off-diagonal long-range order is present, the ground state violates the monogamy relation maximally.

2. *Quantum biological systems*

Recent developments suggest that QC can play an important role in biological processes including the light harvesting protein complexes responsible for photosynthesis, avian magnetoreception, and tunnelling through enzyme-catalysed reactions [313–317, 767–769]. This, however, is still being debated. In the photosynthesis process, as modeled by the Fenna-Matthews-Olson (FMO) light-harvesting pigment-protein complexes [769], it was claimed that quantum coherence measures [770, 771], QD, and the Leggett-Garg inequality [772, 773] can help to understand the energy transfer mechanism [313, 774–778].

A recent study shows that the time-dynamics of discord monogamy scores between different sites of FMO complexes is useful for indicating the pathway of energy transfer from the pigment-protein antenna to the reaction center in the photosynthetic FMO complex [314]. The evolution was taken to be Markovian, represented by the Lindblad master equation with dissipative and dephasing effects. The initial state of the evolution is chosen to be an excited pure state at one of the sites closer to the antenna or an equal mixture of them. See figure 17 for a schematic diagram of the FMO complex.

E. Linking with Bell inequality violation

Monogamy of QD has also been connected to violation of Bell inequalities for multipartite pure states. For two-party system, all pure entangled states violate a Bell inequality [226, 227, 779–781]. This one-to-one correspondence is however missing in the case of multiparty pure states [782, 783] (cf. [784, 785]). For an arbitrary two-qubit state ρ_{AB}, which is possibly mixed, the maximal amount of violation of the Bell-CHSH [226, 779] inequal-

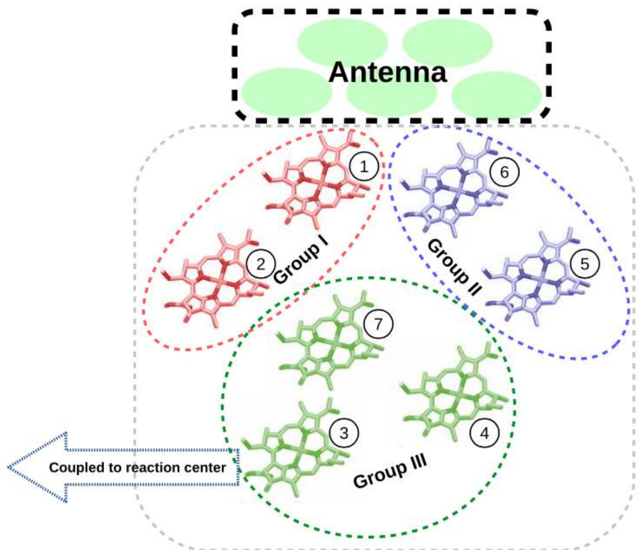

FIG. 17: Schematic structure of the FMO complex and the group classifications of different sites, as inferred from the dynamics of quantum correlations. [Reprinted from Ref. [314] with permission.]

ity is given by [786]

$$B^V_{AB} = B^V(\rho_{AB}) = \max\{2\sqrt{M(\rho_{AB})} - 2, 0\}, \quad (124)$$

where $M(\rho_{AB})$ is the sum of the two largest eigenvalues of the Hermitian matrix $T^T T$, with T being the classical correlation matrix T_{ij} (see Eq. (28)). Here the quantity B^V_{AB} is shifted, so that it is vanishing for Bell-inequality-satisfying states and non-vanishing otherwise.

For an N-party state $\rho_{12\ldots N}$, one may define a monogamy score for violation of Bell inequality (BVM) as

$$\delta_{B^V} = B^V(\rho_{1:\text{rest}}) - \sum_{i=2}^{N} B^V_{1:i}. \quad (125)$$

Let us begin by noting that for any N-qubit state, at most one reduced two-qubit state can violate the Bell-CHSH inequality [787]. Consider now a subset of N-qubit pure states, called "non-distributive" states, for which no two-qubit reduced state violates the Bell-CHSH inequality. It was shown in Ref. [788] that among all non-distributive N-qubit pure states having the same discord monogamy score, the BVM of a gGHZ state is the least. Restricting to the three-qubit case, but for all pure states, whether distributive or not, it was numerically found [788] that the lower bound was provided by the gGHZ state or the "special GHZ" state, depending on whether $\mathcal{D}^{\leftarrow}$ or $\mathcal{D}^{\rightarrow}$ is used to calculate the discord monogamy score. Here, the special GHZ state is given by $|sGHZ_N\rangle = \frac{1}{\sqrt{2}}\big(|00\ldots0\rangle_N + |11\rangle(\sqrt{\beta}|00\ldots0\rangle + \sqrt{1-\beta}|11\ldots1\rangle)_{N-2}\big)$. A numerically obtained complementarity relation between monogamy of Bell inequality violation and discord monogamy score was also reported in Ref. [789] (cf. [741]).

A connection between GQD and a maximum violation of CHSH inequality has also been established [287, 790]. For example, it was shown that in case of Bell-diagonal states for a given GQD, the violation of CHSH inequality [226] is bounded between $4\sqrt{\mathcal{D}_G}$ and $2\sqrt{1+2\mathcal{D}_G}$.

XII. MULTIPARTY MEASURES

It is natural to extend the notion of QC beyond entanglement to the multipartite regime, and this is the main aim in this section. Discord monogamy score, discussed in the preceeding section, is one approach to capture QC in multipartite states. Several other investigations have been carried out in search of multiparty QC beyond entanglement, including Refs. [117, 133, 647, 791–796].

A. Global quantum discord

Rulli and Sarandy [117] proposed a multipartite measure for QC, called global QD, by extending symmetric QD for bipartite systems (introduced in Sec. II A 3) to multipartite states.

Let us consider an N-party quantum state $\rho_{12\ldots N}$ on which a set of local measurements $\{\Pi^1_{j_1} \otimes \ldots \otimes \Pi^N_{j_N}\}$ has been performed. The global QD for $\rho_{12\ldots N}$ is then defined as

$$\mathcal{D}_{global}(\rho_{12\ldots N}) = \min_{\{\Pi_k\}} \{S(\rho_{12\ldots N}||\phi(\rho_{12\ldots N})) - \sum_{i=1}^{N} S(\rho_i||\phi_i(\rho_i))\}. \quad (126)$$

Here $\phi_i(\rho_i) = \sum_{j_i} \Pi^i_{j_i}\rho_i\Pi^i_{j_i}$ and $\phi(\rho_{12\ldots N}) = \sum_k \Pi_k\rho_{12\ldots N}\Pi_k$ with $\Pi_k = \Pi^1_{j_1} \otimes \ldots \otimes \Pi^N_{j_N}$, k being the indices $j_1 \ldots j_N$. By definition, the measure is symmetric with respect to exchange of subsystems, and it was shown that it is non-negative for an arbitrary multipartite state.

The optimization in the definition can be performed analytically for the tripartite mixed state given by

$$\rho_{ABC} = \frac{1-p}{8}\mathbb{I}_8 + p|GHZ_3\rangle\langle GHZ_3|, \quad (127)$$

where $0 \leq p \leq 1$ and $|GHZ_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)_{ABC}$. The expression of global QD for this state takes the form

$$\mathcal{D}_{global}(\rho_{ABC}) = -\frac{1}{4}(1+3p)\log_2(1+3p) + \frac{1}{8}(1-p)\log_2(1-p) + \frac{1}{8}(1+7p)\log_2(1+7p). \quad (128)$$

Note that $\mathcal{D}_{global} = 0$ for the maximally mixed state (with $p = 0$), while it is maximum for the GHZ state

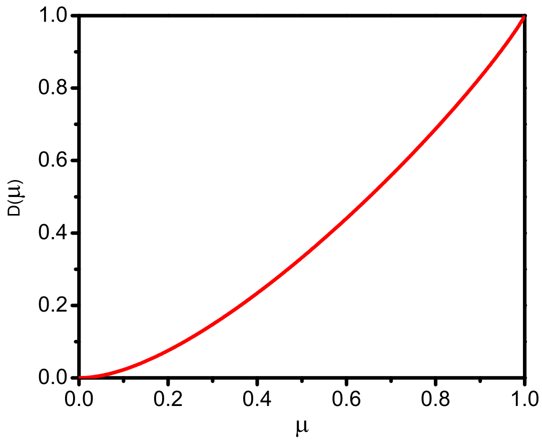

FIG. 18: Global QD for noisy GHZ states. Tripartite global QD for the GHZ state, admixed with white noise, is plotted as a function of the mixing parameter μ. In this plot, we have considered $\mu = p$ in the text. Note that global QD is a monotonic function of μ. Global QD is denoted as $D(\mu)$ in the figure while it is $\mathcal{D}_{global}$ in the text. All quantitites plotted are dimensionless. [Reprinted from Ref. [117] with permission. Copyright 2011 American Physical Society.]

($p = 1$) (see figure 18). The results can be generalized to the case of N-qubit GHZ states admixed with white noise. Comparing figures 2 and 18, we notice that the trends of QD for the Werner state are similar to that of the global QD for the GHZ state admixed with white noise.

Another class of N-qubit states, for which it is possible to analytically compute global QD, is given by

$$\rho_{12\ldots N} = \frac{1}{2^N}\left(\mathbb{I}_2^{\otimes N} + \sum_{i=1}^{3} c_i (\sigma^i)^{\otimes N}\right), \tag{129}$$

and the corresponding global QD is

$$\mathcal{D}_{global}(\rho_{12\ldots N}) = f(\rho_{12\ldots N}) - g(\rho_{12\ldots N}). \tag{130}$$

Here $f(\rho_{12\ldots N}) = -\frac{1+c}{2}\log_2\frac{1+c}{2} - \frac{1-c}{2}\log_2\frac{1-c}{2}$ with $c = \max\{|c_1|, |c_2|, |c_3|\}$. And $g(\rho_{12\ldots N}) = -\frac{1+d}{2}\log_2\frac{1+d}{2} - \frac{1-d}{2}\log_2\frac{1-d}{2}$ with $d = \sqrt{c_1^2 + c_2^2 + c_3^2}$ for odd values of N, while for even N, $g(\rho_{12\ldots N}) = -1 - \sum_{i=1}^{4}\lambda_i \log_2 \lambda_j$, where

$$\begin{aligned} \lambda_1 &= [1 + c_3 + c_1 + (-1)^{N/2} c_2]/4, \\ \lambda_2 &= [1 + c_3 - c_1 - (-1)^{N/2} c_2]/4, \\ \lambda_3 &= [1 - c_3 + c_1 - (-1)^{N/2} c_2]/4, \\ \lambda_4 &= [1 - c_3 - c_1 + (-1)^{N/2} c_2]/4. \end{aligned} \tag{131}$$

Here c_i's, $i = 1, 2, 3$ are real numbers constrained by $0 \le \sum_{i=1}^{3} c_i^2 \le 1$, when N is odd, or $0 \le \lambda_i \le 1$, $i = 1, 2, 3, 4$, when N is even.

Symmetric QD can be written in terms of mutual information as given in Eq. (17). Similarly, global QD can also equivalently be written as [120, 647]

$$\mathcal{D}_{global}(\rho_{12\ldots N}) = \min_{\phi}[I(\rho_{12\ldots N}) - I(\phi(\rho_{12\ldots N}))], \tag{132}$$

where the N-party mutual information is given by $I(\rho_{12\ldots N}) = \sum_{i=1}^{N} S(\rho_i) - S(\rho_{12\ldots N})$. Like symmetric QD, Eq. (132) can be used to interpret as the minimal loss of mutual information due to local measurements.

B. Quantum dissonance

In Secs. II A 3 and II B 1, we have seen that the relative entropy distance can be used to conceptualize measures of QC beyond entanglement in the bipartite case. Similar definitions are possible in the multipartite case. The options here are far more than in the bipartite case, partially due to the multitude of sets of states that can be identified as sets of "classically correlated" states.

An N-party quantum state will be called a product state if it is of the form

$$\Pi_{12\ldots N} = \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_N. \tag{133}$$

Clearly, the product state does not have any kind of correlation (classical or quantum). One may note that the set of product states are a subset of N-party c-c states $\chi_{12\ldots N} = \sum_{i_1 i_2 \ldots i_N} p_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle\langle i_1 i_2 \ldots i_N|$ with $\langle i_j | i'_j\rangle = \delta_{ii'}$ for $j = 1, 2, \ldots, N$. Compare with Eq. (23). The set of separable states $\sigma_{12\ldots N} = \sum_{i_1 i_2 \ldots i_N} p_{i_1 i_2 \ldots i_N} \rho_{i_1} \otimes \rho_{i_2} \otimes \ldots \otimes \rho_{i_N}$ (see Eq. (19) for the bipartite case) is a convex set and the sets of product as well as N-party c-c states are subsets of it. However, if a state cannot be written in the separable form, then it can be called a multiparty entangled state. The minimum relative entropy distance of an N-party state, $\rho_{12\ldots N}$, from the set of separable states, and from the set of N-party c-c states lead to two definitions of QC, and they are respectively a measure of relative entropy of entanglement and a measure of relative entropy-based discord.

Modi *et al.* [133] came up with another definition of nonclassical correlation, called "dissonance", in the following way. Suppose that for an arbitrary state $\rho_{12\ldots N}$, the relative entropy of entanglement, defined above, is attained for the separable state $\sigma_{\rho_{12\ldots N}}$. We now find the relative entropy-based quantum discord, as defined above, for $\sigma_{\rho_{12\ldots N}}$, and suppose that this minimum is attained at $\chi_{\sigma_{\rho_{12\ldots N}}}$. The last quantity is referred to as the dissonance of $\rho_{12\ldots N}$. Therefore the dissonance of $\rho_{12\ldots N}$ is given by

$$Q = \min_{\chi} S(\sigma_{\rho_{12\ldots N}} || \chi_{12\ldots N}), \tag{134}$$

where the minimization is over all N-party c-c states. It was shown in Ref. [133] that Q can be rewritten as

$$Q = \min_{|k'\rangle} S\left(\sum_{k'} |k'\rangle\langle k'|\sigma_{\rho_{12\ldots N}}|k'\rangle\langle k'|\right) - S(\sigma_{\rho_{12\ldots N}}), \tag{135}$$

where $\{|k'\rangle = |k_1 k_2 \ldots k_n\rangle\}$. On the other hand, the relative entropy-based QD of $\rho_{12\ldots N}$ is given by

$$\mathcal{D}_{rel} = \min_{|k'\rangle} S\left(\sum_{k'} |k'\rangle\langle k'|\rho_{12\ldots N}|k''\rangle\langle k'|\right) - S(\rho_{12\ldots N}). \tag{136}$$

Dissonance has been evaluated for certain classes of multipartite pure states [133]. For example, if one considers $|W_3\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$, the closest separable state for obtaining the relative entropy of entanglement is $\sigma_3 = \frac{8}{27}|000\rangle\langle 000| + \frac{12}{27}|W_3\rangle\langle W_3| + \frac{6}{27}|\bar{W}_3\rangle\langle\bar{W}_3| + \frac{1}{27}|111\rangle\langle 111|$, with $|\bar{W}_3\rangle = \frac{1}{\sqrt{3}}(|011\rangle + |101\rangle + |110\rangle)$ [797]. Now, χ_{σ_3} is obtained by dephasing σ in the x-basis, resulting in the dissonance of $|W_3\rangle$ to be approximately $Q = 0.94$. On the other hand, for the cluster states of 4 qubits [798, 799], given by $|C_4\rangle = |0+0+\rangle + |1+1+\rangle + |0-1-\rangle + |1-0-\rangle$, the closest separable state is $\sigma_4 = \frac{1}{4}\big(|0+0+\rangle\langle 0+0+| + |1+1+\rangle\langle 1+1+| + |0-1-\rangle\langle 0-1-| + |1-0-\rangle\langle 1-0-|\big)$, which is a four-party c-c state, leading to vanishing dissonance for $|C_4\rangle$. The possibility of using dissonance as resource in unambiguous quantum state discrimination was considered in Ref. [800].

XIII. MISCELLANEOUS

A set of disparate aspects of QD are collated in this section.

A. Quantum discord and Benford's law

Benford's law is an empirical law of distribution of the first significant digits of data obtained from natural sources or models and from mathematical sequences. The first significant digits of such data may intuitively be expected to be uniformly distributed. Benford's law proposes to rule out such intuition. By analyzing huge collections of data sets from different origins, Simon Newcomb in 1881 [801] and later, Frank Benford in 1938 [802], discovered that the relative frequency distribution of the the first significant digits, d, which can take values from 1 to 9, is given by $p_b(d) = \log_{10}(1 + 1/d)$.

To bypass certain trivialities, for any data set representing a quantity q, one defines the quantity $q_b = \frac{q - q_{\min}}{q_{\max} - q_{\min}}$, where $q_{\min}$ and $q_{\max}$ respectively denote the minimum and maximum values of q. Data sets ranging from biological phenomena to financial models in economy and astronomical data satisfy the law. However, there exists data sets which may violate Benford's law, and it turns out that the violation amount can be used to detect certain phenomena like the onset of earthquake [803], QPT [804], etc. The Benford violation parameter (BVP) can be defined as

$$v_{md} = \sum_{d=1}^{9} \left| \frac{p_0(d) - p_b(d)}{p_b(d)} \right|, \tag{137}$$

where $p_0(d)$ and $p_b(d)$ are respectively the observed relative frequency distribution and that predicted by Benford's law. The BVP can be seen as a distance between the two distributions. Other distance metrics such as the Bhattacharya metric [805] has also been considered [806, 807].

In Ref. [807], the first significant digit distributions for several entanglement as well as information-theoretic QC measures have been calculated using Haar-uniformly generated two-qubit states of varied ranks. It was observed that the distribution for QD is closer to the Benford prediction than for quantum WD. Moreover, it was also shown that for the transverse field XY model (Eq. (69) with $\Delta = 0$), one can detect the QPT by considering the leading digit distribution of $\mathcal{D}$ of the nearest-neighbor spin pairs of the zero-temperature state. Unlike entanglement measures, the observed frequency distribution, $p_0(d)$, for QD changes its pattern from a decreasing one (decreasing with respect to d) to an increasing one in the two phases, namely the antiferromagnetic and the paramagnetic phases. However, the BVP of $\mathcal{D}$ cannot detect the phase transition present in the XXZ model (Eq. (69) with $\gamma = 0$) and remains unchanged at the critical point.

B. Uncertainty relation

Uncertainty relations form one of the basic tenets of quantum mechanics. Entropic Uncertainty relations (EUR) [808, 809] were initially formulated by Deutsch [810] and latter improved by Massen and Uffink [811]. For an arbitrary pair of observables X and Y, the EUR reads

$$H(X) + H(Y) \geq -\log_2 c_{X,Y}. \tag{138}$$

Here $H(X)$ denotes the Shannon entropy of the probability distribution of the outcomes obtained by measuring the observable X on a quantum state ρ. Note that we have used the same notation to denote the Shannon entropy of a probability distribution corresponding to a classical random variable X in Sec. II A. $H(Y)$ represents the same for the observable Y on the same quantum state ρ. And $c_{X,Y} = \max_{i,j} |\langle x_i|y_j\rangle|^2$ with $\{|x_i\rangle\}$, $\{|y_i\rangle\}$ being the eigenbases of X and Y respectively. The right hand side of (138) gives a non-trivial lower bound when X and Y do not share any common eigenstate. This formulation of the uncertainty relation does not incorporate the possibility of the system being measured having a quantum memory. To overcome such disadvantage,

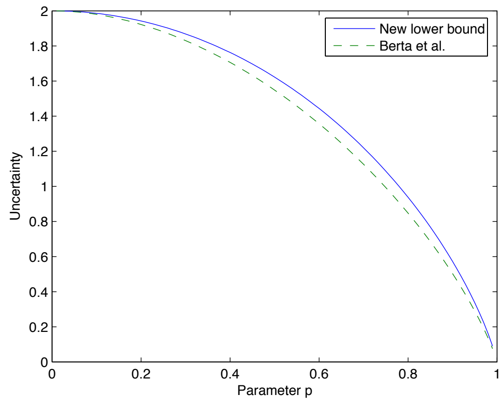

FIG. 19: Plot of the right-hand side of the EUR by Berta *et al.* [812] as mentioned in (139) (dashed green) and the right-hand side of the improved EUR derived by Pati *et al.* [813] as defined in (141) (solid blue line), as functions of the system parameter p, when the system-memory state is in a two-qubit Werner state $\rho_W(p)$. The horizontal axis is dimensionless, while the vertical one is in bits. [Reprinted from Ref. [813] with permission. Copyright 2012 American Physical Society.]

Berta *et al.* [812] provided a reformulation that incorporates a quantum memory. Consider a scenario in which the system A which performs the measurements and the memory B share a quantum state ρ_{AB}. The EUR in this case was proven to be of the form

$$S_{X|B} + S_{Y|B} \geq -\log_2 c_{X,Y} + \tilde{S}_{A|B}. \tag{139}$$

Here $\tilde{S}_{A|B} = S(\rho_{AB}) - S(\rho_B)$. $S_{X|B}$ and $S_{Y|B}$ are defined as follows. After measurement in the basis $\{|x_i\rangle\}$, post-measurement state is given by

$$\rho_{XB} = \sum_i p_i |x_i\rangle\langle x_i| \otimes \rho_B^i, \tag{140}$$

where $\rho_B^i = \frac{\mathrm{tr}_A(\langle x_i|\rho_{AB}|x_i\rangle)}{p_i}$, with $p_i = \mathrm{tr}_{AB}\langle x_i|\rho_{AB}|x_i\rangle$. Then $S_{X|B}$ is given by $S_{X|B} = S(\rho_{XB}) - S(\rho_B)$. $S_{Y|B}$ is similarly defined[42].

It was shown recently [813] that the lower bound obtained in (139) can be improved further. Precisely, it was shown that

$$\begin{aligned} S_{X|B} + S_{Y|B} \;\geq\; & -\log_2 c_{X,Y} + \tilde{S}_{A|B} \\ & + \max\{0, \mathcal{D}^{\rightarrow}(\rho_{AB}) - J_{B|A}\}. \end{aligned} \tag{141}$$

In particular, it has found that the sum of the LHS of (138), for the two-qubit Werner state (see Eq. (10)) coincides with the lower bound in (141), for $X = \sigma_x$ and $Y = \sigma_z$, clearly showing the improvement achieved in (141) over (139), as also depicted in figure 19. Comparative studies of trends of the above two EURs ((139) and (141)) for two-qubit states under different local decoherence models have been carried out [814]. The EUR in (141) turns out to be useful to obtain an upper bound of QD. For a two-qubit state ρ_{AB}, QD is bounded above by the von Neumann entropy of the measured subsystem (see Theorem 3 of Ref. [81]) i.e.,

$$\mathcal{D}^{\rightarrow}(\rho_{AB}) \leq S(\rho_A). \tag{142}$$

However, applying (141), one obtains a stronger upper bound of QD [815], as given by

$$\mathcal{D}^{\rightarrow}(\rho_{AB}) \leq \min\{S(\rho_A), I_{AB}, \Lambda_T\}, \tag{143}$$

where I_{AB} is the total correlation defined in Eq. (5) and Λ_T is given by $\Lambda_T = \frac{1}{2}(I_{AB} + S_{X|B} + S_{Y|B} + \log_2 c_{X,Y} - S_{A|B})$. Moreover, an observable-independent lower bound of the memory-assisted EUR, has recently been proposed [816], and is given by

$$S_{X|B} + S_{Y|B} \geq 2\, S_{A|B} + 2\, \mathcal{D}^{\rightarrow}(\rho_{AB}). \tag{144}$$

It turns out to be less tight than that obtained in (141), as can be illustrated by considering the Werner state and higher-dimensional isotropic states.

C. Complementarity between quantum discord and purity

A complementarity relation between purity and QC measures for multipartite states has recently been obtained [817]. The purity of a part of the system is shown to have connection with a quantum characteristic of that part with the remainder of the system. It was found to have potential connection with quantum cryptography [4]. Let us concentrate on a bipartite QC measure, $\mathcal{Q}'$ such that $\mathcal{Q}'(\rho_{AB:C}) \leq S(\rho_{AB})$, for a three-party quantum state ρ_{ABC}. The complementarity relation then reads

$$\mathcal{P}(\rho_{AB}) + \mathcal{Q}(\rho_{AB:C}) \leq 1, \text{ when} \log_2 d_1 d_2 \leq \log_2 d_3. \tag{145}$$

For $\log_2 d_1 d_2 > \log_2 d_3$, if we additionally assume $0 \leq \mathcal{Q}'(\rho_{AB:C}) \leq \log_2 d_3$, we get

$$\mathcal{P}(\rho_{AB}) + \mathcal{Q}(\rho_{AB:C}) \leq 2 - \frac{\log_2 d_3}{\log_2 d_1 d_2}. \tag{146}$$

Here $\mathcal{P}(\rho_{AB}) = \frac{\log_2 d_1 d_2 - S(\rho_{AB})}{\log_2 d_1 d_2}$ quantifies the normalized purity of the system in the AB part and $\mathcal{Q}(\rho_{AB:C}) = \frac{\mathcal{Q}'(\rho_{AB:C})}{\min\{\log_2 d_1 d_2, \log_2 d_3\}}$ represents the normalized QC measures of the system in the AB:C bipartition. Here $d_1 d_2$ and d_3 are the dimensions of the Hilbert spaces of AB and C respectively. Calculating QD for ρ_{ABC} in the $AB : C$ bipartition, and by measuring in the AB part, it follows that the QD is bounded by $S(\rho_{AB})$, and consequently

[42] The derivation of (139) also considers POVM measurement carried out by A.

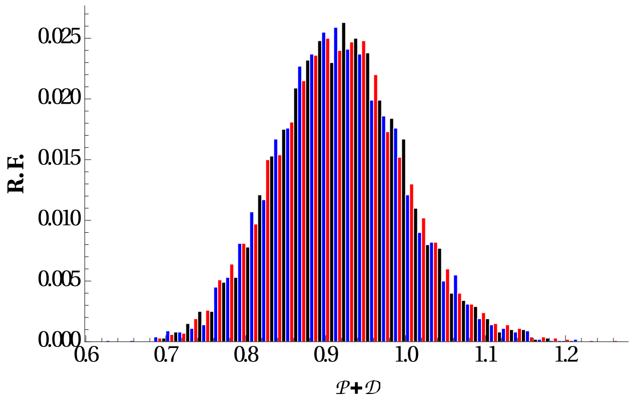

FIG. 20: The complementarity relation for three-qubit rank-2 states. The histogram exhibits the sum of the normalized purity $\mathcal{P}$ and normalized QD. See text for the definitions. The vertical axis represents the relative frequency (R.F.) of occurrence of a Haar uniformly generated rank-2 three-qubit state in the corresponding range of the sum of the two quantities on the horizontal axis. All quantities are dimensionless. [Adapted from Ref. [817] with permission. Copyright 2016 American Physical Society.]

the above relations are true for this variety of QD. When $d_1 = d_2 = d_3$, a dimension-independent complementarity bound can be obtained:

$$\mathcal{P}(\rho_{AB}) + \mathcal{Q}(\rho_{AB:C}) \leq \frac{3}{2}. \tag{147}$$

The complementary relation has also been numerically checked for measures not satisfying the entropy bound [817]. Figure 20 shows a histogram of the relative frequency distribution of the sum of the purity and QD for rank-2 three-qubit states.

XIV. CONCLUSION

Quantum discord, and measures resembling it, were first conceptualized about a decade and a half earlier. In the ensuing years, the concepts have been seen from a variety of approaches. The notions have also been criticized from several angles. One such is based on the fact that almost all two-party quantum states have a non-zero QD [66], the criticism being that if some quantity is present in almost all states, it cannot be useful for any task. One may however note that almost all pure states are coherent superpositions of a chosen basis of pure states. Such superpositions are known to be useful, for example, for security in quantum cryptography [4, 289, 292, 818].

Among the diverse topics that have been considered within the realm of QD and related measures, there are quite a few which have not been possible to cover within the limited span of this review.

Acknowledgments

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XV. APPENDIX: ENTANGLEMENT MEASURES

In this Appendix, we define certain bipartite and multipartite entanglement measures which we have used in different parts of this review. Bipartite QC measures can be classified into two broad categories. One contains those which are based on the entanglement-separability paradigm [2] and the other consists of those which are defined from an information-theoretic perspective. The latter was the main focus of this review.

A. Bipartite entanglement measures

Among bipartite entanglement measures, entanglement of formation (EOF) [57], concurrence [711], logarithmic negativity (LN) [516], and relative entropy of entanglement (RE) [130] are defined below.

1. *Entanglement of formation*

Entanglement of formation [57, 710–712] of an arbitrary bipartite quantum state ρ_{AB} is defined as the minimum number of singlet states required to prepare ρ_{AB} by LOCC. For a pure bipartite state $|\psi_{AB}\rangle$, EOF is defined as

$$\mathcal{E}(|\psi_{AB}\rangle) = S(\rho_A) \text{ or } S(\rho_B), \tag{148}$$

which is the minimal asymptotic rate at which singlets are required to create $|\psi_{AB}\rangle$ by LOCC [714]. For a mixed state ρ_{AB}, the EOF is defined by using the EOF of pure states and a convex roof extension, so that

$$\mathcal{E}(\rho_{AB}) = \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i S(\text{tr}_B|\psi_i\rangle\langle\psi_i|), \tag{149}$$

where the minimization is taken over all possible pure state decompositions of $\rho_{AB} = \sum_i p_i|\psi_i\rangle\langle\psi_i|$.

2. *Concurrence*

The EOF for an arbitrary mixed state, discussed in Eq. (149), is not easy to compute due to the minimization involved in the definition. For two-qubit systems, the minimization has been carried out [710–712], and is represented by

$$\mathcal{E}(\rho_{AB}) = h\left(\frac{1+\sqrt{1-\mathcal{C}^2}}{2}\right), \tag{150}$$

where $h(x)$ is given in Eq. (67). $\mathcal{C}$ is the "concurrence" defined as

$$\mathcal{C}(\rho_{AB}) = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}, \tag{151}$$

where $\{\lambda_i : i = 1, \ldots, 4\}$ are the eigenvalues of the non-Hermitian matrix $\rho_{AB}\tilde{\rho}_{AB}$ in descending order, with $\tilde{\rho}_{AB} = \sigma^y \otimes \sigma^y \rho^*_{AB} \sigma^y \otimes \sigma^y$ being the spin-flipped state. The complex conjugation of ρ_{AB} is in the computational basis. In case of a pure state $|\psi_{AB}\rangle$, we have $\mathcal{C} = 2\sqrt{\det\rho_A}$.

3. Negativity and logarithmic negativity

The negativity, $\mathcal{N}$, [247, 248, 258, 516, 819, 820] of a bipartite quantum state ρ_{AB} is based on the partial transposition criterion [247, 248]. The partial transposition of $\rho_{AB} = \sum_{i,j,\mu,\nu} p^{\mu\nu}_{ij} |ij\rangle\langle\mu\nu|$ with respect to subsystem A, denoted by $\rho^{T_A}_{AB}$, is defined as $\rho^{T_A}_{AB} = \sum_{i,j,\mu,\nu} p^{\mu\nu}_{ij} |\mu j\rangle\langle i\nu|$, and similarly with respect to B. A partial transposed state of a separable state $\rho_{AB} = \sum_i p_i \rho^i_A \otimes \rho^i_B$ is always positive semidefinite. The negativity of ρ_{AB} is then defined as

$$\mathcal{N}(\rho_{AB}) = \frac{||\rho^{T_A}_{AB}||_1 - 1}{2}, \tag{152}$$

where $||\rho||_1$ is the trace norm, defined as $||\rho||_1 = \mathrm{tr}(\sqrt{\rho^\dagger \rho})$. Therefore, the negativity is obtained by adding the moduli of all negative eigenvalues of the partial transposed state. On $\mathbb{C}^2 \otimes \mathbb{C}^2$, a non-zero negativity is a necessary and sufficient condition for entanglement.

Logarithmic negativity (LN) is then defined as

$$\mathcal{LN}(\rho_{AB}) = \log_2\left(1 + 2\mathcal{N}(\rho_{AB})\right) = \log_2 ||\rho_{AB}||_1. \tag{153}$$

It is interesting to note that $\mathcal{LN}$ is additive on tensor products of bipartite states, i.e. $\mathcal{LN}(\rho_{AB} \otimes \sigma_{AB}) = \mathcal{LN}(\rho_{AB}) + \mathcal{LN}(\sigma_{AB})$, while $\mathcal{N}$ is not.

4. Relative entropy of entanglement

Relative entropy of entanglement [130, 131, 821] of an arbitrary bipartite quantum state ρ_{AB} is the minimum relative entropy distance of ρ_{AB} from the set of separable state $\mathcal{S}$, and is given by

$$\mathcal{E}_R(\rho_{AB}) = \min_{\sigma_{AB} \in \mathcal{S}} S(\rho_{AB}||\sigma_{AB}), \tag{154}$$

where σ_{AB} is a bipartite separable state. It satisfies many of the properties required of entanglement measures, and reduces to local von Neumann entropy for pure bipartite states. The asymptotic relative entropy of entanglement is bounded below and above, respectively, by distillable entanglement and entanglement cost. See Ref. [822] in this regard. The definition of relative entropy of entanglement can be extended to the multiparty domain by considering the minimum distance from a suitable set of multipartite separable states [823].

B. Multiparty entanglement measures

Let us now move on to the multipartite scenario. We have already mentioned that multiparty entangled measures can be defined using the relative entropy distance.

Here we use another distance measure, and restrict to only pure states. Moreover, we try to identify a quantity to measure genuine multiparty entanglement. An N-party pure state $|\psi_N\rangle$ is said to be genuinely multiparty entangled if it is not a product across any bipartition of the N parties. The generalized geometric measure (GGM) of $|\psi_N\rangle$ is given by [743–745] (see also [746–748])

$$\mathcal{G}(|\psi_N\rangle) = 1 - \max_{|\chi\rangle} |\langle\chi|\psi_N\rangle|^2, \tag{155}$$

where the maximization is over all N-party pure states, $|\chi\rangle$, that are not genuinely multiparty entangled. It is a measure of genuine multiparty entanglement. The distance measure used here is known as the Fubini-Study metric [824]. Eq. (155) reduces to a simplified form, given by

$$\mathcal{G}(|\psi_N\rangle) = 1 - \max\{\lambda_{A:B} | A \cup B = \{1, 2, \ldots, N\}, A \cap B = \emptyset\}, \tag{156}$$

where $\lambda_{A:B}$ is the largest eigenvalue of the marginal density matrix ρ_A or ρ_B of $|\psi_N\rangle$. This makes it computable in any dimension and for an arbitrary number of parties. It can also be shown to be non-increasing under LOCC [743].

Multiparty entanglement measures can also originate from the concept of monogamy of bipartite QC measures. Examples include the tangle or the monogamy score of squared concurrence, $\delta_{\mathcal{C}^2}$ [403], and the squared negativity monogamy score, $\delta_{\mathcal{N}^2}$ [726].

XVI. APPENDIX: CLASSICAL CORRELATION DOES NOT INCREASE UNDER DISCARDING

We prove here that the quantity J is not increasing under discarding a subsystem. Precisely, for a tripartite state, ρ_{ABC}, we wish to show that J follows the relation given by

$$J_{A|BC} \geq J_{A|B}. \tag{157}$$

From the definition of J, given in Eq. (7), one has $J_{A|BC} = S(\rho_A) - S_{A|BC}$, with the conditional entropy $S_{A|BC} = \min_{\{\Pi_i^{BC}\}} \sum_i p_i S(\rho_{A|i})$, where $\rho_{A|i} = \mathrm{tr}_{BC}(\mathbb{I}^A \otimes \Pi_i^{BC} \rho_{ABC} \mathbb{I}^A \otimes \Pi_i^{BC})/p_i$, and $p_i = \mathrm{tr}(\mathbb{I}^A \otimes \Pi_i^{BC} \rho_{ABC} \mathbb{I}^A \otimes \Pi_i^{BC})$. The conditional entropy can also be written as [235]

$$S_{A|BC} = \min_{\{\Pi_i^{BC}\}} \left[S(\rho'_{ABC}) - S(\rho'_{BC})\right], \tag{158}$$

where $\rho'_{ABC} = \sum_i \mathbb{I}^A \otimes \Pi_i^{BC} \rho_{ABC} \mathbb{I}^A \otimes \Pi_i^{BC}$. From the strong subadditivity of von Neumann entropy [85], one gets

$$S(\rho'_{ABC}) - S(\rho'_{BC}) \le S(\rho'_{AB}) - S(\rho'_B), \tag{159}$$

where $\rho'_{AB} = \mathrm{tr}_C(\rho'_{ABC}) = \sum_k \mathbb{I}^A \otimes \Pi_k'^B \rho_{AB} \mathbb{I}^A \otimes \Pi_k'^{B\dagger}$, for some measurements $\{\Pi_k'^B\}$ derived from $\{\Pi_i^{BC}\}$. Suppose the optimization in $S_{A|B}$ is achieved for $\{\tilde{\Pi}_k^B\}$. As one can always have an extension of it in the higher-dimensional Hilbert space of BC, so from (159), one has

$$S_{A|B} = S(\rho''_{AB}) - S(\rho''_B) \ge S(\rho''_{ABC}) - S(\rho''_{BC}) \ge S_{A|BC}, \tag{160}$$

where $\rho''_{AB} = \sum_k \mathbb{I}^A \otimes \tilde{\Pi}_k^B \rho_{AB} \mathbb{I}^A \otimes \tilde{\Pi}_k^{B\dagger}$ and $\rho''_{ABC} = \sum_i \mathbb{I}^A \otimes \tilde{\Pi}_i^{BC} \rho_{ABC} \mathbb{I}^A \otimes \tilde{\Pi}_i^{BC\dagger}$, and where the equality and the last inequality in (160) were obtained from Eq. (158). Hence the result.

Acronyms

ADC Amplitude damping channel

AFM Antiferromagnetic

BB84 Bennett and Brassard quantum cryptography protocol in 1984

BD Bell-diagonal

BF Bit flip

BPF Bit-phase flip

BV Bell inequality violation

BVP Benford violation parameter

BVM Bell inequality violation monogamy score

B92 Bennett quantum cryptography scheme in 1992

CC Classical correlation

CHSH Clauser-Horne-Shimony-Holt inequality

CI Canonical initial

CLOCC Closed local operations and classical communication

CO Closed operation

CP Completely positive

CPTP Completely positive trace-preserving

CV Continuous variable

DC Dense coding

DE Distillable entanglement

DM Dzyaloshinskii-Moriya

DPC Depolarizing channel

DQC1	Deterministic quantum computation with single qubit
EOF	Entanglement of formation
EPR	Einstein-Podolsky-Rosen
EUR	Entanglement uncertainty relation
EW	Entanglement witness
E91	Ekert quantum cryptography protocol in 1991
FM	Ferromagnetic
FMO	Fenna-Matthews-Olson
GAD	Generalized amplitude damping
GGM	Generalized geometric measure
gGHZ	Generalized Greenberger-Horne-Zeilinger state
GHZ	Greenberger-Horne-Zeilinger state
GQD	Geometric quantum discord
gW	Generalized W state
JC	Jaynes-Cummings model
LB	Locally broadcastable
LOCC	Local operations and classical communication
LN	Logarithmic negativity
LU	Local unitary
MIN	Measurement-induced nonlocality
NMR	Nuclear magnetic resonance
NPPT	Non-positive partial transpose
PDC	Phase damping channel
PF	Phase flip
PM	Paramagnetic
POVM	Positive operator valued measurements
PPT	Positive partial transpose
PV	von Neumann projective measurement
QC	Quantum correlation
QD	Quantum discord
QDP	Quantum dynamical process
QIP	Quantum information processing
QKD	Quantum key distribution
QPT	Quantum phase transition
RE	Relative entropy of entanglement

RSP Remote state preparation

SCI Special canonical initial

SLOCC Stochastic local operation and classical communication

SPPT Strong positive partial transpose

SVD Singular value decomposition

UF Uniaxial field

WD Quantum work deficit

1D One-dimensional

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