Scaling behaviors of correlation measures in quantum spin systems

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We aim to study the scaling behaviors of important correlation measures including entanglement entropy and the newly proposed measure of purely quantum correlations, quantum discord (QD), which quantifies all nonclassical correlations including entanglement as a subset, in general quantum spin systems. In this work we emphasize on the latter measure (QD) and present the explicit derivation of the relations between QD and spin-correlation functions in Z_2-symmetric quantum spin lattice models, which are powerful tools for studying pairwise QD behaviors in these models, and analyze Heisenberg XXZ chain as an example, in the critical regime of which the QD is shown to decay polynomially at zero temperature, but with different critical exponent as of correlation functions. We also prove an area law for QD scaling in general noncritical quantum spin systems with local interactions, in contrast to the expected extensive behavior.

INTRODUCTION

Correlation, which can also be interpreted as the mutual information between systems, has always played an essential role in quite a few fields, especially information theory and many-body physics. In quantum many-body systems, the strikingly weird form of correlation – quantum entanglement, is also extremely important in studying remarkable phenomena such as quantum phase transitions [1], which are always the core topics in this field. Moreover, the scaling behaviors of entanglement exhibit quite anomalous properties, e.g., obeying an area law [2], which has been providing connections and insights into even the most fundamental aspects of physics. However, people found that nontrivial quantum correlation also exist in certain unentangled quantum systems, which stimulates people to study correlation measures beyond entanglement in quantum physics. Quantum discord (QD) is such a newly proposed quantity that quantifies the amount of all nonclassical correlations [3], including but not restricted to, entanglement, which has received wide attention in recent years. In this work we attempt to present some powerful tools in studying correlation measures, specifically QD, in a typical kind of quantum many-body system – quantum spin systems, and give a preliminary study of some interesting scaling behaviors of these correlations.

QUANTUM DISCORD (QD)

Quantum entanglement, as one of the most famous "spooky" features of the quantum physics, describes a unique form of correlations that can only show up in the quantum world. Naturally we may ask does entanglement describe all correlations that have no classical counterparts? The answer is not necessarily. People have found out that unentangled states in many cases may exhibit nonclassical physical behaviors [4]. So how do

we actually quantify the quantum and classical parts of correlations? This question has been of great interest of quantum information theory in recent years, and in 2001, Ollivier and Zurek proposed the concept of quantum discord (QD) [3], which aims at quantifying all nonclassical correlations.

Here we discuss two different physical perspectives to define and understand QD, and prove that they are equivalent. First for two classical distributions A and B, the amount of correlation between them is captured my the mutual information $I_{\text{cl}}(A : B) = H(A) + H(B) - H(AB)$ where $H(X) = -\sum_x p_x \log p_x$ denotes the famous Shannon entropy, where X is a classical variable with values x occuring with probability p_x. On the other hand, Bayes' rule allows us to define an equivalent form for the classical mutual information as $C_{\text{cl}}(A|B) = H(A) - H(A|B)$ with the conditional entropy $H(A|B) = \sum_b p_b H(A|b)$, which can be understood as the information of A that can be obtained via studying B. Note that for classical systems the mutual information yielded by these two definitions are exactly the same. For the case of quantum systems, we study subsystem B by making local measurements on it. Suppose we try all possible measurements formalized by POVMs or von Neumann projectors, as the quantum case counterpart of the second way of getting mutual information, we see

$$C_B(A : B) = S(A) - \min_{\{\Pi_B^k\}} \sum_k p_k S(A_k), \qquad (1)$$

where we run over all possible measurements denoted by $\{\Pi_B\}$ with outcome labeled by k, and A_k is the reduced state of subsystem S with k as the outcome of measurement on B, the density matrix of which reads $\rho_{A,k} = \text{tr}_B[(\mathbb{1}_A \otimes \Pi_B^k)\rho_{AB}]/p_k$ to preserve the trace constraint. As the measurement is locally done on party B, the mutual information we get in this way is purely classical, i.e., $C_B(A : B)$ quantifies the amount of classical mutual information. On the other hand the total mutual

information is obviously given by

$$I(A : B) = S(A) + S(B) - S(AB), \qquad (2)$$

where $S(X) = -\rho_X \log(\rho_X)$ denotes the von Neumann entropy of a quantum state X, and ρ_X is its density matrix. Therefore quite naturally, we have the following definition of QD:

Definition 1 (QD as non-classical correlation). QD, which quantifies the amount of purely quantum correlations, is the discrepancy of total mutual information and classical mutual information, i.e.,

$$D(A : B) = I(A : B) - C_B(A : B). \qquad (3)$$

We emphasize that classically $D(A : B)$ definitely goes to zero due to the equivalence of the classical counterparts of the two forms of mutual information, hence it does not have any classical analogs, i.e., quantifying only the 'quantumness' of correlations.

Alternatively, we can similarly define quantum conditional entropy as $S(A|B) \equiv S(AB) - S(B)$. For postmeasurement state it takes the form $S(A|\tilde{B}) \equiv \sum_k p_k S(A_k)$, where A_k is defined earlier. Therefore we can also understand the amount of quantum correlations as the minimum amount of mutual information that cannot be accessed via any kind of local measurements on a subsystem:

Definition 2 (QD as the minimum amount of mutual information that cannot be accessed via local measurements). QD is the minimal difference between the quantum conditional entropies of pre- and postmeasurement $S(A|\tilde{B})$ over all possible measurements. i.e.,

$$D(A : B) = \min_{\{\Pi_B^k\}} S(A|\tilde{B}) - S(A|B). \qquad (4)$$

Theorem 1. *The two definitions of QD are mathematically equivalent.*

Proof. We start from the mathematical form of QD in Definition 1:

$$\begin{aligned}
D(A : B) &= I(A : B) - C_B(A : B) \\
&= S(A) + S(B) - S(AB) - S(A) \\
&\quad + \min_{\{\Pi_B^k\}} \sum_k p_k S(A_k) \\
&= \min_{\{\Pi_B^k\}} \sum_k p_k S(A_k) + S(B) - S(AB) \\
&= \min_{\{\Pi_B^k\}} S(A|\tilde{B}) - S(A|B),
\end{aligned}$$

and arrived at Definition 2. $\qquad \square$

Interestingly, QD is generally a measure of correlation beyond entanglement for mixed quantum states, i.e., it can be non-zero even for some separable states. A very simple example is the following highly symmetric bipartite state:

$$\begin{aligned}
\rho_{AB} = \frac{1}{4}(&|+\rangle\langle+|_A \otimes |0\rangle\langle 0|_B + |-\rangle\langle-|_A \otimes |1\rangle\langle 1|_B \\
&+ |0\rangle\langle 0|_A \otimes |-\rangle\langle-|_B + |1\rangle\langle 1|_A \otimes |+\rangle\langle+|_B). \quad (5)
\end{aligned}$$

Using *Perez-Horodecki positive partial transpose (PPT) criterion* [5] we can easily see that this state is separable, i.e., unentangled. Numerically we can verify that for this two-qubit state $S(A_0) = S(A_1) = -\frac{1}{4}\log\frac{1}{4} - \frac{3}{4}\log\frac{3}{4} \approx 0.81$, and therefore $D(A : B) = \frac{3}{4}\log\frac{4}{3} \approx 0.31$, with the measurement basis $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ either on A or B, which is exactly the *Schmidt basis* (with which the density matrix is diagonal). Note that for pure states, QD trivially reduces to entanglement entropy $S(A) = S(B)$.

In the past few years, QD, as a very fruitful measure of quantum correlations beyond entanglement, has become a new hot topic in various fields related to quantum physics. We suggest one referring to a recent review paper [4] for more discussions.

Z_2-SYMMETRIC QUANTUM SPIN LATTICE MODELS

In this section we first present various powerful tools for analysing correlations between interacting pairs of spin-1/2 spins in quantum spin lattice models without introducing Z_2 symmetry breaking terms in the Hamiltonian, e.g., magnetic field. As the two-site reduced states are generally mixed, as we will see, studying QD in quantum many-body systems as the measure of non-classical correlations beyond entanglement may provide new physical insights. We systematically discuss the original calculations of pairwise QD in such models and the scaling behaviors of correlation measures via Heisenberg XXZ chain as a specific example.

Two-site reduced state

First we shall present some general properties of the reduced state of two sites in quantum spin models obeying Z_2 symmetry as preliminaries for further results.

In the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, the reduced density matrix of two sites i and j (tracing out other sites) in the Z_2-symmetric quantum spin models takes the form

$$\rho_{ij} = \begin{pmatrix} \varrho_{00} & 0 & 0 & \varrho_{03} \\ 0 & \varrho_{11} & \varrho_{12} & 0 \\ 0 & \varrho_{12}^* & \varrho_{22} & 0 \\ \varrho_{03}^* & 0 & 0 & \varrho_{33} \end{pmatrix}, \qquad (6)$$

with only the diagonal and anti-diagonal entries being non-zero, therefore bears the name of "X state", which is mixed in general, i.e., QD does not simply reduce to

forms of entanglement entropy. Here we only need to consider real X state, i.e., $\varrho_{12} = \varrho_{12}^*$ and $\varrho_{03} = \varrho_{03}^*$, because they can always be transformed into real numbers via local unitary transformations, which preserves physical quantities. Considering the trace constraint, we see that this density matrix actually has only five degrees of freedom. Thus we can non-redundantly define the five free parameters in terms of spin-correlation functions:

$$G_i^x = \langle \sigma_i^z \rangle = \mathrm{tr}(\sigma_i^z \rho_{ij}) = \varrho_{00} + \varrho_{11} - \varrho_{22} - \varrho_{33}, \quad (7)$$

$$G_j^x = \langle \sigma_j^z \rangle = \mathrm{tr}(\sigma_j^z \rho_{ij}) = \varrho_{00} - \varrho_{11} + \varrho_{22} - \varrho_{33}, \quad (8)$$

$$G_{ij}^{xx} = \langle \sigma_i^x \sigma_j^x \rangle = \mathrm{tr}[(\sigma_i^x \otimes \sigma_j^x)\rho_{ij}] = 2(\varrho_{12} + \varrho_{03}), \quad (9)$$

$$G_{ij}^{yy} = \langle \sigma_i^y \sigma_j^y \rangle = \mathrm{tr}[(\sigma_i^y \otimes \sigma_j^y)\rho_{ij}] = 2(\varrho_{12} - \varrho_{03}), \quad (10)$$

$$G_{ij}^{zz} = \langle \sigma_i^z \sigma_j^z \rangle = \mathrm{tr}[(\sigma_i^z \otimes \sigma_j^z)\rho_{ij}] = \varrho_{00} - \varrho_{11} - \varrho_{22} + \varrho_{33}, \quad (11)$$

with all of which ranging in [-1,1]. Here $G_l^z = \langle \sigma_l^z \rangle$ ($l = i, j$) and $G_{ij}^{\alpha\beta} = \langle \sigma_i^\alpha \sigma_j^\beta \rangle$ ($\alpha, \beta = x, y, z$) denote the magnetization density at site l and two-site spin-correlation function of sites i, j, respectively. This parametrization will be used in later discussions and the explicit QD calculation in the next subsection. More importantly, ρ_{ij} is naturally decomposed as

$$\rho_{ij} = \frac{1}{4}\left(\mathbb{1}_i \otimes \mathbb{1}_j + G_{ij}^{xx}\sigma_i^x \otimes \sigma_j^x + G_{ij}^{yy}\sigma_i^y \otimes \sigma_j^y + G_{ij}^{zz}\sigma_i^z \otimes \sigma_j^z + G_i^z\sigma_i^z \otimes \mathbb{1}_j + G_j^z\mathbb{1}_i \otimes \sigma_j^z\right). \quad (12)$$

This decomposition is very useful and will be referred to in later calculations.

In quantum spin models, the matrix elements of ρ_{ij} can be expressed in terms of spin-correlation functions [6] as follows:

$$\varrho_{00} = \tfrac{1}{4}(1 + G_i^z + G_j^z + G_{ij}^{zz}), \quad (13)$$

$$\varrho_{11} = \tfrac{1}{4}(1 + G_i^z - G_j^z - G_{ij}^{zz}), \quad (14)$$

$$\varrho_{22} = \tfrac{1}{4}(1 - G_i^z + G_j^z - G_{ij}^{zz}), \quad (15)$$

$$\varrho_{33} = \tfrac{1}{4}(1 - G_i^z - G_j^z + G_{ij}^{zz}), \quad (16)$$

$$\varrho_{12} = \varrho_{12}^* = \tfrac{1}{4}(G_{ij}^{xx} + G_{ij}^{yy}), \quad (17)$$

$$\varrho_{03} = \varrho_{03}^* = \tfrac{1}{4}(G_{ij}^{xx} - G_{ij}^{yy}). \quad (18)$$

For later calculations of the von Neumann entropy of this state, we work out the eigenvalues of ρ_{ij} here:

$$\lambda_1 = \tfrac{1}{4}(1 + G_{ij}^{xx} + G_{ij}^{yy} - G_{ij}^{zz}), \quad (19)$$

$$\lambda_2 = \tfrac{1}{4}(1 - G_{ij}^{xx} - G_{ij}^{yy} - G_{ij}^{zz}), \quad (20)$$

$$\lambda_3 = \tfrac{1}{4}(1 + G_{ij}^{zz} + \sqrt{4(G_i^z)^2 + (G_{ij}^{xx} - G_{ij}^{yy})^2}), \quad (21)$$

$$\lambda_4 = \tfrac{1}{4}(1 + G_{ij}^{zz} - \sqrt{4(G_i^z)^2 + (G_{ij}^{xx} - G_{ij}^{yy})^2}). \quad (22)$$

We note that the deriving analytical forms of QD, even for very simple cases, is extremely hard. Generally computing the exact value of QD has been proved to be NP-complete [7]. For X states we have some approximate results [8, 9], yet the accurate analytical formula is still unknown [10, 11]. However, we still have the following useful conclusions that can help us deal with states of general interest:

Lemma 2 (optimal measurement for real X states). *The local measurement on one subsystem (e.g., without loss of generality, B) that minimizes the quantum conditional entropy of postmeasurement bipartite X states $S(A|\tilde{B})$, i.e., gives the value of QD, is (i) σ_B^x, i.e., with respect to local projectors $\{|+\rangle\langle+|, |-\rangle\langle-|\}$ where $\{|+\rangle, |-\rangle\}$ form the eigenbasis of σ_B^x if*

$$\left|\sqrt{\varrho_{00}\varrho_{33}} - \sqrt{\varrho_{11}\varrho_{22}}\right| \le |\varrho_{12}| + |\varrho_{03}|, \quad (23)$$

or (ii) σ_B^z, i.e., with respect to local projectors $\{|0\rangle\langle0|, |1\rangle\langle1|\}$ where $\{|0\rangle, |1\rangle\}$ (computational basis) is the eigenbasis of σ_B^x if

$$(|\varrho_{12}| + |\varrho_{03}|)^2 \le (\varrho_{00} - \varrho_{11})(\varrho_{33} - \varrho_{22}). \quad (24)$$

The basic idea for the proof is to parametrize the general two-qubit POVM $\{E_B^k\}$ as $\{\mu^k(1 + \vec{n}^k\vec{\sigma}_B)\}_{k=1}^{K\le4}$, where $\sum_k \mu^k = 1$, $(\vec{n}^k)^2 = 1$, and $\sum_k \mu^k\vec{n}^k = 0$, or similarly parametrize the von Neumann measurement (as will be shown in the next subsection), and the value of $S(A|\tilde{B})$ (denoted as $S_B(\tilde{\rho}_{AB})$ in some literatures) turns out to be a concave function whose minimum is located on the boundary. Some details for proving case (1) are presented in [10]. Note that we shall assume $|G_{ij}^{xx}| \ge |G_{ij}^{yy}|$ (expressions in terms of matrix elements shown by Eq. (9) and (10)) without loss of generality since we can always switch the signs of the involved entries via a local unitary transformation, in which case (i) and (ii) have covered most possibilities, and in addition, even if we adopt σ_B^x or σ_B^z as the optimal measurement for all X states there is shown to be only a very small error for very few cases numerically. Using σ_B^x or σ_B^z as the optimal measurement suffices for our analysis here.

Pairwise QD

Here we present the calculations of two-site QD in Z_2-symmetric quantum spin lattices in terms of pairwise correlation functions. As the scaling laws of these correlation functions in a number of spin models have already been widely studied, the results in these subsections can serve as powerful tools to analyse the scaling behaviors of QD and generic correlation measures.

Projector parametrization method

Generally calculating QD involves extremization over all possible measurements formulated by POVMs (parametrization shown in the previous subsection) or von Neumann projective measurements. For the two-qubit case, we can parametrize the local projectors that accomplish the measurement on subsystem B as $\{V|0\rangle\langle 0|V^\dagger, V|1\rangle\langle 1|V^\dagger\}$ where

$$V = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{-i\phi} \\ \sin\frac{\theta}{2}e^{i\phi} & -\cos\frac{\theta}{2} \end{pmatrix}, \qquad (25)$$

and $\theta \in [0, \pi], \phi \in [0, 2\pi)$, i.e., $V \in U(2)$ [6]. Note that the mathematical form for calculating QD used in [6] is given by the discrepancy between total and purely classical mutual information, which we already know to be equivalent to the form we will consider according to Theorem 1.

Explicit calculation with optimal measurements

Here we adopt the difference of quantum conditional entropy between pre- and postmeasurement states as the mathematical form of QD and use the conclusions of optimal measurements to explicitly calculate pairwise QD.

First from the eigenvalues given in Eq. (19)–(22), we can easily obtain the von Neumann entropy of the total state $S(ij)$. Taking advantage of the decomposition Eq. (12), we simply trace out subsystem i and arrive at the reduced density matrix

$$\rho_j = \frac{1}{2}(\mathbb{1}_j + \nu\sigma_j^x) = \frac{1}{2}(\mathbb{1}_j + G_i^z\sigma_j^x), \qquad (26)$$

with eigenvalues $(1 \pm G_i^z)/2$, hence the subsystem von Neumann entropy is

$$S(j) = -\frac{1+G_i^z}{2}\log\frac{1+G_i^z}{2} - \frac{1-G_i^z}{2}\log\frac{1-G_i^z}{2}. \qquad (27)$$

So, the quantum conditional entropy of the original two-site state is given as

$$S(i|j) \equiv S(ij) - S(j) = -\sum_{\alpha=1}^4 \lambda_\alpha \log\lambda_\alpha + \frac{1+G_i^z}{2}\log(1+G_i^z) + \frac{1-G_i^z}{2}\log(1-G_i^z) - 1, \qquad (28)$$

with $\{\lambda_\alpha\}$ given in Eq. (19)–(22).

Next, according to Lemma 2 and the immediate discussions, there are two classes of postmeasurement states obtained by corresponding optimal measurement bases (i) $\{|+\rangle\langle+|, |-\rangle\langle-|\}$ or (ii) $\{|0\rangle\langle0|, |1\rangle\langle1|\}$. Now we compute the quantum conditional entropies of these two classes, and hence QDs, separately.

Class (i): $\{|+\rangle\langle+|, |-\rangle\langle-|\}$ *as the optimal measurement basis.* For ρ_{ij} in this class, the local measurement operation on the original bipartite density matrix is $(\mathbb{1}_i \otimes |\pm\rangle\langle\pm|_j)$, with two possible outcomes, whose corresponding postmeasurement density matrices are given by

$$\rho_{i\tilde{j},+} = (\mathbb{1}_i \otimes |+\rangle\langle+|_j)\rho_{ij}$$
$$= \frac{1}{4}\Big[\mathbb{1}_i \otimes |+\rangle\langle+|_j + G_{ij}^{xx}\sigma_i^x \otimes |+\rangle\langle+|_j + \frac{i}{2}G_{ij}^{yy}\sigma_i^y \otimes \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}_j + \frac{1}{2}G_{ij}^{zz}\sigma_i^z \otimes \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}_j$$
$$+ G_i^z\sigma_i^z \otimes |+\rangle\langle+|_j + \frac{1}{2}G_j^z\mathbb{1}_i \otimes \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}_j\Big], \qquad (29)$$

$$\rho_{i\tilde{j},-} = (\mathbb{1}_i \otimes |-\rangle\langle-|_j)\rho_{ij}$$
$$= \frac{1}{4}\Big[\mathbb{1}_i \otimes |-\rangle\langle-|_j - G_{ij}^{xx}\sigma_i^x \otimes |-\rangle\langle-|_j + \frac{i}{2}G_{ij}^{yy}\sigma_i^y \otimes \begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix}_j + \frac{1}{2}G_{ij}^{zz}\sigma_i^z \otimes \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}_j$$
$$+ G_i^z\sigma_i^z \otimes |-\rangle\langle-|_j + \frac{1}{2}G_j^z\mathbb{1}_i \otimes \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}_j\Big], \qquad (30)$$

respectively, with equal probabilities $p_1 = p_2 = 1/2$. Hence the reduced density matrices after tracing out j read

$$\rho_{i,+} = 2\mathrm{tr}_j\rho_{i\tilde{j},-} = \frac{1}{2}(\mathbb{1} + G_{ij}^{xx}\sigma^x + G_i^z\sigma^z), \quad (31)$$

$$\rho_{i,-} = 2\mathrm{tr}_j\rho_{i\tilde{j},+} = \frac{1}{2}(\mathbb{1} - G_{ij}^{xx}\sigma^x + G_i^z\sigma^z), \quad (32)$$

whose spectra are the same:

$$\lambda_{+,\pm} = \lambda_{-,\pm} = \frac{1 \pm \sqrt{(G_{ij}^{xx})^2 + (G_i^z)^2}}{2}. \quad (33)$$

The prefactors 2 come from probabilities on the denominators. So we obtain the quantum conditional entropy of the postmeasurement (optimal) state as

$$S(i|\tilde{j}) = -\lambda_{+,+}\log\lambda_{+,+} - \lambda_{+,-}\log\lambda_{+,-}, \quad (34)$$

which finally gives us the value of QD (for the first class we present the full expression in terms of eigenvalues):

$$D(i:j) = -\lambda_{+,+}\log\lambda_{+,+} - \lambda_{+,-}\log\lambda_{+,-} + \sum_{\alpha=1}^{4}\lambda_\alpha\log\lambda_\alpha - \frac{1+G_i^z}{2}\log(1+G_i^z) - \frac{1-G_i^z}{2}\log(1-G_i^z) + 1. \quad (35)$$

Class (ii): $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ *as the optimal measurement basis.* As the calculation procedures are similar with (i), we only give important results here. The postmeasurement density matrices are

$$\rho_{i\tilde{j},0} = \frac{1}{4}\Big[\mathbb{1}_i \otimes |0\rangle\langle 0|_j + G_{ij}^{xx}\sigma_i^x \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_j + G_{ij}^{yy}\sigma_i^y \otimes \begin{pmatrix} 0 & -i \\ 0 & 0 \end{pmatrix}_j + (G_{ij}^{zz} + G_i^z)\sigma_i^z \otimes |0\rangle\langle 0|_j + G_j^z\mathbb{1}_i \otimes |0\rangle\langle 0|_j\Big], (36)$$

$$\rho_{i\tilde{j},1} = \frac{1}{4}\Big[\mathbb{1}_i \otimes |1\rangle\langle 1|_j + G_{ij}^{xx}\sigma_i^x \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_j + G_{ij}^{yy}\sigma_i^y \otimes \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix}_j + (-G_{ij}^{zz} + G_i^z)\sigma_i^z \otimes |1\rangle\langle 1|_j + G_j^z\mathbb{1}_i \otimes |1\rangle\langle 1|_j\Big] (37)$$

and the corresponding reduced density matrices for i are

$$\rho_{i,0} = \frac{1}{2}[(1 + G_j^z)\mathbb{1} + (G_{ij}^{zz} + G_i^z)\sigma^z], \quad (38)$$

$$\rho_{i,1} = \frac{1}{2}[(1 - G_j^z)\mathbb{1} + (-G_{ij}^{zz} + G_i^z)\sigma^z], \quad (39)$$

which are already diagonal in matrix form, but notice that the eigenvalues corresponding to the two measurement outcomes are no longer the same. We omit boring technical steps here, and finally we will obtain

$$D(i:j) = -\sum_{\substack{\{k=0,1\} \\ \{l=+,-\}}} \lambda_{k,l}\log\lambda_{k,l} - S(i|j) \quad (40)$$

for this class, where $S(i|j)$ is given by Eq. (28), and

$$\lambda_{0,\pm} = \frac{1}{2}(1 + G_j^z \pm G_{ij}^{zz} \pm G_i^z), \quad (41)$$

$$\lambda_{1,\pm} = \frac{1}{2}(1 - G_j^z \mp G_{ij}^{zz} \pm G_i^z). \quad (42)$$

With all these results involving correlation functions and QD at hand, we are now well equipped to analyze their behaviors in spin models obeying Z_2 symmetry, including XXZ model, XY model and the transverse field Ising model etc. in one dimension.

An example: Heisenberg XXZ chain

In this subsection we shall preliminarily illustrate the two-site scaling behaviors of correlation measures via explicitly working out a specific example: the 1D spin-1/2 anisotropic Heisenberg XXZ spin model, whose Hamiltonian reads

$$H_{XXZ}(\Delta) = \sum_i(\sigma_i^x\sigma_{i+i}^x + \sigma_i^y\sigma_{i+i}^y + \Delta\sigma_i^z\sigma_{i+i}^z), \quad (43)$$

where the anisotropy parameter Δ controls the quantum phases. Note that this model can be solved by the Bethe ansatz [12]. For $\Delta > 1$, the system is in the antiferromagnetic Néel phase which breaks the lattice translation symmetry, and for $\Delta < -1$, the ferromagnetic Ising phase, which breaks the spin reflection symmetry. Both of the above phases are gapped and have two-fold degenerate groung states. $\Delta \to +\infty$ and $\Delta \to -\infty$ are respectively the antiferromagnetic and classical Ising limit. The model is in the critical XY phase (i.e., gapless) when $\Delta \in (-1, 1]$, which is known to be described by a $c = 1$ conformal field theory (CFT), as the correlation length diverges and the system becomes scale invariant [2].

Note that the XXZ chain exhibits $U(1)$ invariance [6], namely, $[H, \bigotimes_i \sigma_i^z] = 0$, which is even a stronger constraint over the elements of the density matrix than the Z_2 symmetry, i.e., the two-site reduced state is an X state and ϱ_{03} also vanishes, hence we are safe to use previous results.

Volumetric scaling of entanglement entropy

Quantum entanglement in many-body systems, especially of ground states, are extremely important in studying the behavior of the systems, e.g., quantum phase transitions [1]. For a total pure bipartite quantum state, the entanglement entropy corresponding to a certain partition is uniquely defined, which is very useful for indicating quantum criticality. The volumetric entanglement entropy scaling in different regimes of the XXZ model is discussed in [12, 13]. We briefly mention that in the 1D critical regimes (in this model, $\Delta \in (-1, 1]$), CFT yields that the (subsystem) entanglement entropy scales as

$$S_A(l) = \frac{c + \bar{c}}{6} \log l + k, \qquad (44)$$

where k is a model-dependent constant and $c, \bar{c}$ are holomorphic and antiholomorphic central charges respectively [14], indicating different universality classes.

Two-site scaling of QD

We are interested in the two-site QD scaling in the critical phase where $\Delta \in (-1, 1)$ at zero temperature as the pairwise correlation in gapped phases is naturally expected to decay exponentially. In this gapless regime, using our notations, the pairwise spin-correlation functions scales as [15]

$$G_{ij}^{xx} = G_{ij}^{yy} \sim |i - j|^{-\theta} \qquad (45)$$

$$G_{ij}^{zz} \sim |i - j|^{-2} + e^{2ik_F|i-j|}|i - j|^{-\theta^{-1}} \qquad (46)$$

with critical exponent given by

$$\theta = \frac{1}{2} - \frac{\arcsin(-\Delta)}{\pi} \in (0, 1), \qquad (47)$$

and $e^{2ik_F|i-j|}$ a phase factor. Here the leading order term in G_{ij}^{zz} seems to be uncertain, but it is always at higher order than G_{ij}^{xx}, G_{ij}^{yy}.

After plugging these spin-correlation functions into the parametrization Eq. (7)–(11), we will discover that Eq. (23) is satisfied, hence the two-site reduced state that we are studying falls into class (i) and the expression of QD is given by Eq. (35). Up to leading order, QD scales as

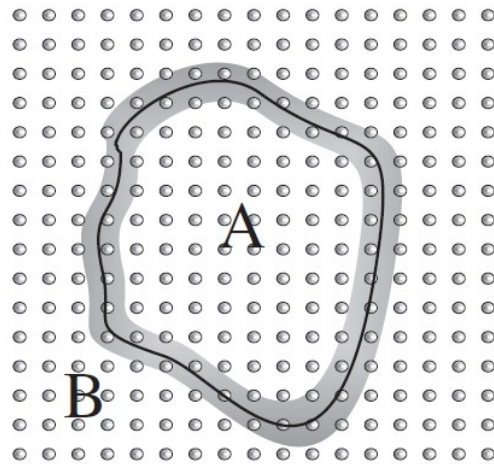$$D(i : j) \sim (G_{ij}^{xx})^2 \sim |i - j|^{-2\theta}, \qquad (48)$$

FIG. 1. (Adapted from [16]) Intuitively speaking, under locally interacting Hamiltonians, the correlation length is finite so that sites in A and B that are separated by a distance further than the correlation length (the shaded stripe) should not contribute to the mutual information or correlation measures between A and B, hence bounded by the number of sites at the boundary and therefore scales as the boundary area.

hence we conclude that in the critical XY phase at zero temperature, QD decays polynomially, which resembles the behavior of spin-correlation function, but with different critical exponents.

AREA LAWS FOR GENERAL SPIN SYSTEMS

Typically, the interactions in quantum maby-body systems are local, as inherited by the decay of correlation measures. Quite interestingly, the feature of locality is also reflected by the anomalous scaling behavior of ground state entanglement entropy, which grows linearly with respect to the boundary area of the subregion instead of the volume, which is in contrast with the expected extensive behavior. This kind of scaling behaviors are generally said to obey an "area law" [2]. The general mathematical statement if a physical quantity Φ of region A obeys

$$\Phi(A) = O(|\partial A|), \qquad (49)$$

where ∂A denotes the boundary area of A, we say that the area law is satisfied. The intuitive picture here is shown in Fig. 1. In locally interacting systems, the correlation length is finite so that sites in A and B that are separated by a distance further than the correlation length (the shaded stripe) should not contribute to the mutual information or correlation measures between A and B, hence bounded by the number of sites at the boundary and therefore scales as the boundary area.

In this section we briefly discuss the area laws for entanglement entropy and total mutual information for gen-

eral spin systems, and in turn present the area law for QD in locally interacting non-critical spin systems.

Entanglement entropy

The area laws of entanglement entropy in various contexts have been widely studied [2]. For quantum many-body systems on lattice (the entire system) W where A is a subregion and $B = W \setminus A$ its complement, $S(A) = O(|\partial A|)$ implies that the area law is satisfied in the system. We emphasize that, in fact, it is truly unusual for a quantum state to satisfy an area law [2] as it has been shown that the typical entropy of a subsystem is nearly maximal [17], indicating that it should scale as the volume instead of boundary area. For the purpose in this section it suffices to know that surprisingly for general ground states of quantum spin systems in gapped, i.e., non-critical phases the area law is obeyed. In 1D, the area law statement was first made rigorous by Hastings [18]. This is also another clue showing us the unique physical significance of ground states. Notable violations take place at quantum criticalities, models with Fermi surfaces etc., and the non-trivial topological order will result in a negative term in the ground state entanglement entropy, namely *topological entanglement entropy*.

It is worth mentioning that the area laws for entanglement entropy has deep connections [19, 20] with the famous area dependence of the Bekenstein-Hawking black hole entropy [21, 22], which suggests that the entropy of a black hole is proportional to its horizon area A:

$$S_{\mathrm{BH}} = \frac{kA}{4l_{\mathrm{P}}^2} = \frac{kc^3 A}{4G\hbar}, \tag{50}$$

where $l_{\mathrm{P}} = \sqrt{G\hbar/c^3}$ is the Planck length, as they share similar scaling behaviors. Actually these discoveries of black hole entropy scaling laws were the driving force for several studies of entanglement entropy scaling in quantum fields later on [23, 24].

Total mutual information

As has been mentioned in the introduction of QD, the total (quantum and classical) mutual information for a bipartite quantum state AB is defined as $I(A : B) = S(A) + S(B) - S(AB)$ where $S(\cdot)$ denotes the von Neumann entropy. Thermal states of the form $\rho_{AB} = e^{-\beta H}/\mathrm{tr}e^{-\beta H}$ with inverse temperature β minimizes the free energy $F(\rho) = \mathrm{tr}(H\rho) - S(\rho)/\beta$, and $F(\rho_{AB}) \leq F(\rho_A \otimes \rho_B)$. Therefore we obtain [16]

Lemma 3 (area law for total mutual information)**.** *We denote the total Hamiltonian as $H = H_A + H_B + H_\partial$ where H_∂ collects interactions crossing the boundary. The total*

mutual information is bounded by a first order function of H_∂, i.e.,

$$I(A : B) \leq \beta\mathrm{tr}[H_\partial(\rho_A \otimes \rho_B - \rho_{AB})], \tag{51}$$

hence satisfying the form of an area law.

More specifically if we only consider two-site interactions, we will have

$$I(A : B) \leq 2\beta|\partial A| \max_{i,j \in \partial A} ||h_{ij}||, \tag{52}$$

where $||h_{ij}||$ is the eigenvalue of the two-site interaction between i and j (across the boundary).

QD

For the same kind of quantum systems, we prove the following scaling theorem for QD:

Theorem 4 (area law for QD)**.** *For general quantum spin systems in non-critical regime with local interactions, the QD of subgraph A scales as the boundary area.*

Proof. As introduced, we denote the entire spin system as W and $B = W \setminus A$. From Definition 1 of QD, we have $D(A : B) = I(A : B) - C_B(A : B)$ with classical mutual information $C_B(A : B) \geq 0$, hence

$$D(A : B) \leq I(A : B). \tag{53}$$

According to Lemma 3, $I(A : B) \sim \partial A$ and $S(A)\partial A$, hence $D(A : B) \sim \partial A$. Intuitively QD is upper and lower bounded by two correlation measures that both satisfy the area law in our cases, therefore it naturally obeys area law either.

Specifically for two-site interactions [25], using Eq. (53) the relation in Lemma 3, we immediately see that $D(A : B) \leq I(A : B) \leq 2\beta|\partial A| \max_{i,j \in \partial A} ||h_{ij}||$. Given that $D(A : B) \geq S(A)$ we conclude that $D(A : B) \sim \partial A$, i.e., scales with the boundary area. $\square$

Further insight

In fact all sorts of correlations are fundamentally measures of some forms of mutual information. As indicated by the holographic principle, on the fundamental level the information of a region should depend on its surface area instead of volume. Therefore the studies on scaling behaviors of correlation measures are extremely fruitful.

Furthermore, the fundamental reason (e.g., possibly, the locality of interactions) for these area-dependent scaling laws of correlations measures, is still subject to debate. We suggest that the obedience of area law of various correlation measures implies the locality of corresponding interactions, and, as has been discussed, vice

versa, hence it may be considered as an indicator and physical definition for generically *local* interactions, and a necessary condition for a good correlation measure given that the interactions are local.

SUMMARY AND OUTLOOK

In this work we explicitly derived the relations between QD and spin-correlation functions in Z_2-symmetric quantum spin lattice models, and analyzed the scaling behaviors of entanglement entropy and QD in Heisenberg XXZ chain as an example. We see that in the critical phase QD decays polynomially at zero temperature, but with different critical exponent as of correlation functions. We also introduced the anomalous area laws for ground state entanglement entropy and total mutual information, which has been of extensive interest for years, and proved that in general noncritical quantum spin systems with local interactions QD also satisfies the area law. As we have mentioned in the last section, the studies on scaling behaviors of correlation measures are of great significance due to its connection with the holographic principle and black hole physics etc., hence may provide some unique insights into fundamentals of physics.

In the past few years, QD has become the most popular measure of quantum correlations beyond entanglement, and we believe this quantity shall provide significant insight and implications of the nature of quantum correlations and even quantum physics. However we cannot say it has been well understood yet. For instance we can only give reliable results or methods of calculating QD for very limited quantum systems. Recently we showed that energy cannot flow between systems with zero QD, and the energy flux is proportional to the diagonal QD define with respect to Schmidt basis. Concerning the scaling behaviors in quantum many-body systems, we still have lots of further questions, for instance

- What does the different critical exponents of correlation measures tell us?

- Will QD exhibit very different scaling behaviors compared to entanglement entropy for certain Hamiltonians? How do we construct them?

- Does the violation of area law of QD provide new physics?

- Will the scaling behaviors of QD reveal new kind of quantum orders, like topological entanglement entropy does?

- ...

As we see, these topics are quite new and many questions are waiting to be answered. We believe new insights may emerge at this interface between quantum information theory and many-body statistical physics.

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