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Scaling of the local quantum uncertainty at quantum phase transitions

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ABSTRACT

We investigate the local quantum uncertainty (LQU) between a block of L qubits and one single qubit in a composite system of n qubits driven through a quantum phase transition (QPT). A first-order QPT is analytically considered through a Hamiltonian implementation of the quantum search. In the case of second-order QPTs, we consider the transverse-field Ising chain via a numerical analysis through density matrix renormalization group. For both cases, we compute the LQU for finite-sizes as a function of L and of the coupling parameter, analyzing its pronounced behavior at the QPT.

1. Introduction

The interplay between quantum information theory and statistical mechanics has brought emerging connections between these research fields [1–3]. In particular, it has provided a deeper understanding about the role played by correlations in quantum phase transitions (QPTs). A seminal result in this direction is a link between the scaling of pairwise entanglement and QPTs in quantum spin chains [4,5]. This has been further developed by introducing a distinction between the characterization of first-order and continuous QPTs [6,7]. For a block analysis, entanglement entropy has been found to be related to the central charge of the Virasoro algebra associated with the conformal field theory behind the critical model [8–10]. More generally, it has been shown that quantum correlation measures such as provided by the quantum discord [11] are also able to identify quantum criticality [12,13]. Remarkably, pairwise quantum discord may exhibit a more robust characterization of QPTs than pairwise entanglement in certain cases. For instance, pairwise quantum discord between distant sites in a quantum chain may indicate a quantum critical point, while entanglement is absent already for very short distances [14,15]. In addition, for finite temperatures, pairwise quantum discord is able to reveal the QPT by non-analyticities in its derivatives, while the pronounced behavior in two-qubit entanglement disappears for even small temperatures [16].

In this work, we aim at investigating the behavior of the local quantum uncertainty (LQU) [17] at quantum criticality. The LQU has been introduced as a quantum discord-like measure, which is primarily related with the skew information [18,19]. In particular, it plays a role in the characterization of quantum metrology protocols [17,20]. The behavior of LQU between pairs of spins in a quantum spin chain has been recently considered [21,22]. Here, we generalize this previous analysis for systems of dimension 2×2 by considering the LQU for blocks of arbitrary dimension $D \times 2$ and also by discussing its finite-size behavior in both first-order and second-order QPTs. More specifically, we will evaluate the LQU between a block of L quantum bits (qubits) and one single qubit in a composite system of n qubits. For a first-order QPT, we will consider a Hamiltonian implementation of the quantum search, which is designed to find out a marked element in an unstructured search space of $N = 2^n$ elements. By analytical evaluation, we will show that the LQU exponentially saturates to a constant value at the critical point as we increase the block length L. This saturation is found to be enhanced by the system size n. On the other hand, at non-critical points, the LQU will be shown to vanish for large n. In the case of second-order QPTs, we consider the transverse-field Ising model with open boundary conditions. By implementing a numerical analysis via density matrix renormalization group (DMRG), we will show that the concavity of the LQU as a function of the block size L characterizes the QPT. For both first-order and second-order QPTs, we also consider the LQU as a function of the coupling parameter, showing that the LQU exhibits a pronounced behavior at the quantum critical point independently of the block sizes of L qubits. In particular, this pronounced behavior is sensitive to n, showing a scaling behavior as we increase the size of the system.

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2. Local quantum uncertainty

The uncertainty of an observable K in a quantum state ρ is usually quantified by the variance $V(\rho, K) = Tr\rho K^2 - (Tr\rho K)^2$. It may exhibit contributions from both quantum and classical sources. Quantum uncertainty comes from the noncommutativity between K and ρ, being quantified by the skew (not commuting) information [18,19]

$$I(\rho, K) = Tr\rho K^2 - Tr\rho^{1/2} K \rho^{1/2} K. \tag{1}$$

Indeed, suppose ρ and K commute. Then, ρ and K have a common basis of eigenstates $\{|k\rangle\}$, which means that the uncertainty of K in an individual eigenstate $|k\rangle$ vanishes. Hence, a nonvanishing uncertainty $V(\rho, K)$ is only possible if ρ is a classical mixing of $\{|k\rangle\}$. Therefore, the commutation of ρ and K implies that $V(\rho, K)$ has a classical origin.

The quantum uncertainty is intrinsically connected with the concept of quantum correlation. For example, let us consider a Bell state of two qubits, namely, $|\psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, where $\{|0\rangle, |1\rangle\}$ denotes the computational basis. This is an eigenstate of the global observable $\sigma_z \otimes \sigma_z$, so there is no uncertainty on the result of a measurement of such an observable. On the other hand, the measurement of local spin observables is intrinsically uncertain for the density operator $|\psi\rangle\langle\psi|$, since an entangled state cannot be an eigenstate of a local observable. In particular, the variance $V(\rho, K)$ for a local observable K will vanish if and only if the state is uncorrelated.

The concept of quantum uncertainty can be extended to mixed states. In this case, the skew information $I(\rho, K)$ vanishes if and only if ρ is not disturbed by the measurement of K. If K is a local observable, the states left invariant by local measurement are the states with zero quantum discord with respect to that local subsystem [23]. The quantum uncertainty on local observables is then intimately related to the notion of quantum discord and, as shown in Ref. [17], it can be used as a discord-like quantifier. We are now ready to define the local quantum uncertainty (LQU). Let $\rho = \rho_{AB}$ be the state of a bipartite system, and let K^Γ denote a local observable on B (K is represented by a Hermitian operator on B with nondegenerate spectrum Γ). The LQU as defined in [4], is given by

$$Q(\rho) = \min_{K^\Gamma} I(\rho, K^\Gamma). \tag{2}$$

Notice that Q is the minimum quantum uncertainty associated to a single measurement on subsystem B. If there is a K for which $Q = 0$ then there is no quantum correlation between the two parts of the state ρ. As proved in Ref. [17], the LQU satisfies all the good properties of a discord-like measure. An analytical expression for Q can be obtained if we consider a bipartite $D \times 2$ system. In this case

$$Q(\rho_{AB}) = 1 - \lambda_{max}(W_{AB}), \tag{3}$$

where λ_{max} is the maximum eigenvalue of the 3×3 symmetric matrix W whose elements are given by

$$(W_{AB})_{ij} = Tr[\rho_{AB}^{1/2}(I_A \otimes \sigma_{iB})\rho_{AB}^{1/2}(I_A \otimes \sigma_{jB})]. \tag{4}$$

In this work, we will consider a set of n qubits aligned in a chain, with the bipartition in subsystems A and B chosen as shown in Fig. 1.

3. LQU for the quantum search

The aim of the search problem is to find out a marked element in an unstructured list of N candidates. In a quantum setting, it is possible to solve the search problem with scaling $\sqrt{N}$, as proved by Grover [24]. Here, we consider a Hamiltonian implementation

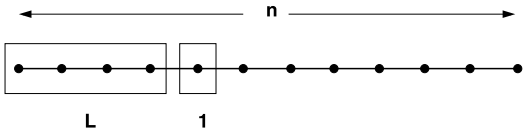

Fig. 1. Bipartition used to defined the subsystems A and B for the LQU evaluation. The size L of the block A is arbitrarily chosen and subsystem B is taken as one qubit.

through a quantum system composed of n qubits, whose Hilbert space has dimension $N = 2^n$. We denote the computational basis by the set $\{|i\rangle\}$ $(0 \le i \le N-1)$. Without loss of generality, we can assume an oracular model such that the marked element is the state $|0\rangle$. So the implementation of the quantum search can be achieved through the projective Hamiltonian

$$H(s) = (1-s)(\mathbb{1} - |\psi_0\rangle\langle\psi_0|) + s(\mathbb{1} - |0\rangle\langle 0|), \tag{5}$$

where $|\psi_0\rangle = (1/\sqrt{N})\sum_{i=0}^{N-1}|i\rangle$, and s denotes the normalized time $0 \le s \le 1$. By preparing the system in its ground state at time $t = 0$ and by considering an adiabatic dynamics, it evolves to the corresponding instantaneous ground state at later times. In particular, the system exhibits a first-order QPT at $s = 1/2$. The ground state energy in terms of the normalized time s reads

$$E(s) = \frac{1 - \sqrt{1 - 4s(1-s)\overline{N}}}{2}, \tag{6}$$

with $\overline{N} = 1 - 1/N$. For the ground state vector $|\psi(s)\rangle$, we obtain

$$|\psi(s)\rangle = \sqrt{a(s)}|0\rangle + \sqrt{c(s)}\sum_{i=1}^{N-1}|i\rangle, \tag{7}$$

where we have defined the quantities $a(s) = \frac{1}{1+(N-1)k_s^2}$, $c(s) = \frac{k_s^2}{1+(N-1)k_s^2}$, and $k_s = 1 - \frac{E(s)}{(1-s)N}$. Note that, in the thermodynamic limit $n \to \infty$, the structure of the Hamiltonian implies that the LQU can only be non-vanishing at the quantum critical point, even though its scaling is nontrivial at finite sizes. This can be observed from Eq. (5), where both $|0\rangle$ and $|\psi_0\rangle$ are product states that become orthogonal for $n \to \infty$. In this limit, the ground state is $|\psi_0\rangle$ for $0 \le s < 1/2$, with energy $E(s) = s$, while the ground state is $|0\rangle$ for $1/2 < s \le 1$, with energy $E(s) = 1 - s$. At $s = 1/2$ the ground state is degenerate. From Eq. (7), $|\psi(1/2)\rangle$ will be an equal superposition of $|0\rangle$ and $|\psi_0\rangle$ for $n \to \infty$. It then follows that $Q = 0$ everywhere except at $s = 1/2$.

In order to determine the scaling at finite size n, we consider the density matrix $\rho = |\psi(s)\rangle\langle\psi(s)|$ describing the system in the ground state, which can be written as

$$\rho(s) = \begin{bmatrix} a & b & b & \dots & b \\ b & c & c & \dots & c \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b & c & c & \dots & c \end{bmatrix}, \tag{8}$$

where $b = \sqrt{a(s)c(s)}$. As we trace out n' qubits of the system, the resulting partial density matrix $\rho'(s)$ will be given by

$$\rho'(s) = \begin{bmatrix} a' & b' & b' & \dots & b' \\ b' & c' & c' & \dots & c' \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b' & c' & c' & \dots & c' \end{bmatrix}, \tag{9}$$