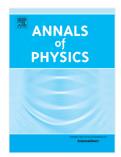
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## **ACCEPTED MANUSCRIPT**

### Global quantum discord in matrix product states and the application

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### Abstract

Global quantum discord (GQD) is a measure of quantum correlation for multi-site quantum states. In this paper, we propose an efficient procedure to calculate global quantum discord  $(G_n)$  for consecutive *n*site subsystems in infinite-size matrix product states (MPSs). We apply the method to study the scaling behavior of  $G_n$  in several one-dimensional infinite quantum spin chains, i.e., (1) a three-site interaction model whose ground state can be exactly expressed as MPSs, and (2) a spin- $\frac{1}{2}$  XXZ chain whose ground state is approximately expressed as MPSs with the help of infinite time-evolving block decimation (iTEBD) algorithm. In both models, as the increase of n,  $G_n$  shows an approximately linear growth. Unambiguous clue for the convergence of the incremental  $\Delta G_n = G_n - G_{n-1}$  is observed when n is large enough. Moreover, in non-critical (gapped) regions  $\Delta G_n$  converges very fast, while in critical (gapless) regions it converges relatively slow. The behaviors are explained in a model-independent physical picture with finite-range correlations. Based on these results, we propose to use "discord per site"  $(\frac{G_n}{n})$  to describe the global correlations in infinite-size spin chains. Moreover, we find that the global discord shows a size-independent maximum at the infinite-order quantum phase transition point of the XXZ model.

*Keywords:* Global quantum discord; Matrix product states; One-dimensional quantum spin chains; Quantum phase transition.

### 1. Introduction

Quantum entanglement in low-dimensional quantum systems has attracted much attention recently.[1–3] On the one hand, entanglement can be regarded as valuable resource to carry out quantum computation and information communication.[3] On the one hand, it can be used to characterize various quantum phase transitions (QPTs) in condensed matters.[4] The entanglement entropy  $E_n$ , which describes the quantum entanglement between an *n*-site subchain and its environment, has been studied in many one-dimensional quantum spin chains, and an interesting scaling behavior has been observed.[5, 6] For instance, in an exactly soluble spin-1/2 XY model, as the increase of n,  $E_n$  shows a logarithmic growth in the critical regions meanwhile achieves a finite saturation value in non-critical regions.[7] The result turns out to be a general conclusion in one-dimensional quantum spin chains, thus has greatly deepened our understanding of QPTs. Furthermore, the knowledge about the quantum entanglement in these quantum chains in turn promotes the improvements and developments of the density matrix renormalization group (DMRG) method.[8, 9]

Entanglement is not the only feature of quantum correlations. There are many other measures of quantum correlation, such as the quantum dissonance which measures the quantum correlation in un-entangled states, [10] and the quantum nonlocality which can be observed in Bell-type experiments [11, 12]. A useful review can be found in Ref. [10]. Among these measures of quantum correlation, there is an important measure which can capture all the quantumness of correlation in a two-site quantum state, namely, the quantum discord (QD). [13–18] QD has been investigated extensively in many quantum models, such as

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