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Ground-State Energy and Entropy for One-Dimensional Heisenberg Chain with Alternating D-Term

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Abstract

We study the ground-state information of one-dimensional Heisenberg chain with alternating D-term. Given the ground-state phase diagram, the ground-state energy and the entanglement entropy are obtained by tensor-net work algorithm. The phase transition points are shown in the entanglement entropy figure. The results are agreed with the phase diagram.

Keywords

Ground-State Energy, Entropy, One-Dimensional, Heisenberg Chain

1. Introduction

Recent improvements in experimental techniques [1] [2] [3] [4] have given access to the quantum mechanical simulation of the dynamics of isolated, interacting quantum many-body systems with a variety of platforms, such as cold atoms in optical lattices and ion traps [5] [6]. Among them, the Haldane ground state of the S = 1 anti-ferromagnetic Heisenberg chain with a gap to the first excited state and the ground-state [7] [8] [9] [10] has been extensively studied by many authors, which is known to have a gapless ground-state for half-integer spin. The gaped state is destroyed by various types of perturbations such as exchange anisotropy, bond alternation and single-ion-type anisotropy. On the other hand, understanding the collective behavior of quantum many-body systems has long presented a formidable challenge due to the exponential growth of Hilbert space dimension with system size N, however, the numerical algorithms are made great progress, such as the matrix product states [11] [12] [13] [14] [15] in one spatial dimension and the projected entanglement-pair states [16] [17] [18] in two and higher spatial dimensions, which is a variational algorithm to compute the ground-state wave-function for transitionally invariant quantum systems on an infinite-size lattice. In this paper, we obtained the approximation ground-state wave-function by the matrix product states, meanwhile, the ground-state energy and the entanglement entropy are also given.

This paper is organized as follows: in the second section, the model Hamiltonian and the ground-state phase diagram are presented. The matrix product state algorithm is simply introduced. The figure for ground-state energy and entanglement entropy for left and right section are shown. The final section is devoted to a summary and discussion.

2. The Hamiltonian and Ground-State Phase Diagram

The anti-ferromagnetic Heisenberg chain with alternating D-term for spin-1 [19] is given as the follow

$$H = \sum_{l=1}^{N} J S_l S_{l+1} + D + \sum_{l=1}^{N/2} S_{2l-1}^{z2} + D_- \sum_{l=1}^{N/2} S_{2l}^{z2}, \quad (J > 0) \tag{1}$$

where J is the exchange coupling, $D_+ = D_0 + \delta D$, $D_- = D_0 + \delta D$, and S is the spin-1 operator.

$$S^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & i & 0 \\ i & 0 & -i \\ 0 & -i & 0 \end{pmatrix}, \quad S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

The parameters D_0 and δD represent uniform and alternating components of uniaxial single-ion anisotropy, respectively. In what follows we set $J = 1$ to fix the energy scale. The ground-state phase diagram is given in Ref. [19], which consists of the Haldane phase, the Large-D phase, udud and u0d0 phases. The Gaussian transition occurred between the Haldane phase and the Large-D phase, which is gapful phase to gapful phase transition. From symmetry consideration, these transitions between the Haldane phase, u0d0 phase and udud phase are Ising type transitions. The ground-state phase diagram is shown in **Figure 1**. In this paper, we set the $D_0 = 2$, and δD as the control parameter.

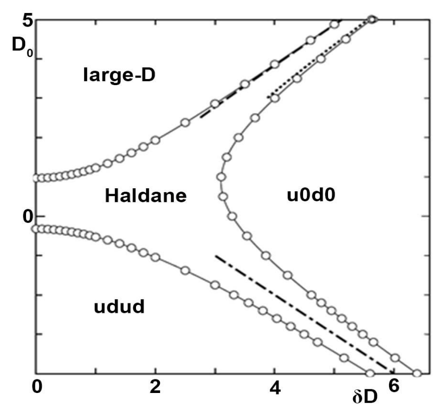

Figure 1. Ground state phase diagram of the Hamiltonian (1) [19]. The phases are separated with the symbols. The solid lines are the guide for eye. The broken and dotted lines represent the approximate phase boundary, respectively. The dash-dotted line is the line $\delta D = -D_0 + 2J$.

The conformal central charge is an important content in field theory, which gives the type of the phase transition in theory. With conformal central charge $c = 1$, the transition line between the Larged-D and Haldane is expected to be described by the conformal field theory. The phases u0d0 and udud are expected as gapless system.

3. The Matrix Product State Algorithm

The matrix product state algorithm is given in Ref [15], which exploits two facts, namely invariance under translations of the system and parallelizability of local updates in time-evolving block decimation algorithm. With time evolution for a quantum spin chain in the thermodynamic limit, the approximation ground-states are obtained. For a given wave-function

$$|\Psi_t\rangle = \exp(-iHt)|\Psi_0\rangle \tag{2}$$

the Schmidt decomposition of $|\Psi_t\rangle$ is written as

$$|\Psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha^{[r]} |\Phi_\alpha^{[\triangleleft r]}\rangle \otimes |\Phi_\alpha^{[r+1\triangleright]}\rangle \tag{3}$$

The Equation (3) can be rewritten as

$$|\Psi\rangle = \sum_{\alpha,\beta=1}^{\chi} \sum_{i=1}^{d} \lambda_\alpha^{[r]} \Gamma_{i\alpha\beta}^{[r+1]} \lambda_\beta^{[r+1]} |\Phi_\alpha^{[\triangleleft r]}\rangle |i^{[r]}\rangle |\Phi_\alpha^{[r+1\triangleright]}\rangle \tag{4}$$

where χ is the truncation dimension, d is the Hilbert space, λ is diagonal matrix, the Γ is three index tensor. By using the two-site Hamiltonian, which is expanded through a Suzuki-Trotter decomposition, the imaginary time evolution for the given wave-function is shown. The approximation ground-state wave-function is obtained until the approximation ground-state energy is lower enough.

4. Ground-State Energy and Entanglement Entropy

The simulation results of the approximation ground-state energy for Equation (1) are shown in **Figure 2** with truncation dimension $\chi = 8, 12, 16, 20$ in different label, respectively.

The approximation ground-state energies with different control parameter δD agree with each other.

During the numerical simulation, two phase transitions are obtained, which are shown in entanglement entropy. The figure for entanglement entropy of the left one and the right one are given in **Figure 3** and **Figure 4**. The parameters for the platform of the computer system are given as CPU: Intel(R) Core(TM) i5-64002.7 GHz; memory (RAM): 8.00 GB.

5. Summary

The anti-ferromagnetic Heisenberg chain with alternating D-term for spin-1 is investigated by using matrix product states. The approximation ground-state

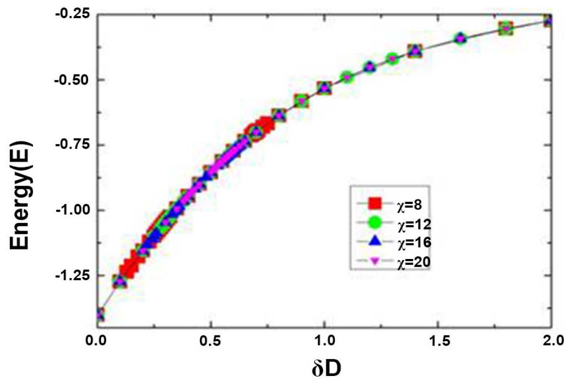

Figure 2. The approximation ground-state energy for the Hamiltonian (1). δD as the control parameter, the truncation dimensions are shown with $\chi = 8, 12, 16, 20$. The solid lines are the guide for eye.

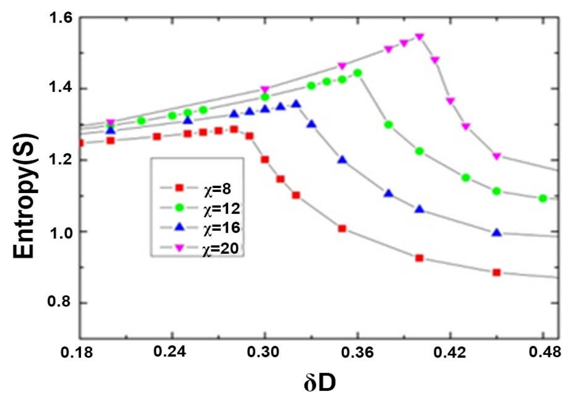

Figure 3. The entanglement entropy of the Hamiltonian (1) with truncation dimension χ = 8, 12, 16, 20, the transition points are δD = 0.287, 0.320, 0.361, 0.400. The solid lines are the guide for eye. The peak is bigger and bigger with larger and larger truncation dimension.

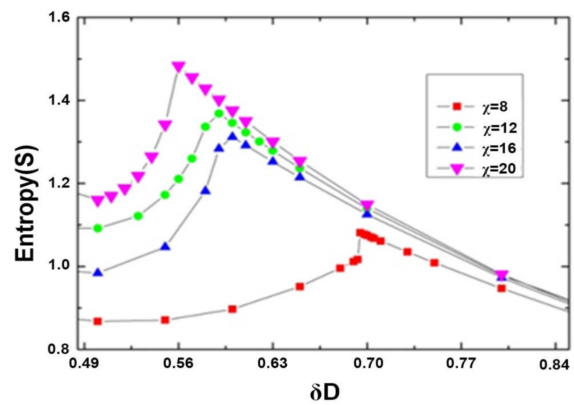

Figure 4. The entanglement entropy of the Hamiltonian (1) with truncation dimension χ = 8, 12, 16, 20, the transition points are δD = 0.695, 0601, 0.592, 0.561. The solid lines are the guide for eye. The peak is also bigger and bigger with larger and larger truncation dimension.

energy and the entanglement entropy are shown in this paper. We simply analyzed the results, however, as we have been unable to determine the local order parameter. This is the next direction of research. Besides, we will use alternative techniques beyond the MPS paradigm to yield the scaling behavior of physical observable, which may be more suitable.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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