Entanglement entropy and fidelity susceptibility in the one-dimensional spin-1 XXZ chains with alternating single-site anisotropy

Jie Ren\textsuperscript{1}, Guang-Hua Liu\textsuperscript{2} and Wen-Long You\textsuperscript{3}

\textsuperscript{1} Department of Physics and Jiangsu Laboratory of Advanced Functional Material, Changshu Institute of Technology, Changshu 215500, People’s Republic of China
\textsuperscript{2} Department of Physics, Tianjin Polytechnic University, Tianjin 300387, People’s Republic of China
\textsuperscript{3} College of Physics, Optoelectronics and Energy, Soochow University, Suzhou, Jiangsu 215006, People’s Republic of China

E-mail: jren01@163.com

Received 5 January 2015
Accepted for publication 2 February 2015
Published 23 February 2015

Abstract
We study the fidelity susceptibility in an antiferromagnetic spin-1 XXZ chain numerically. By using the density-matrix renormalization group method, the effects of the alternating single-site anisotropy $D$ on fidelity susceptibility are investigated. Its relation with the quantum phase transition is analyzed. It is found that the quantum phase transition from the Haldane spin liquid to periodic Néel spin solid can be well characterized by the fidelity. Finite size scaling of fidelity susceptibility shows a power-law divergence at criticality, which indicates the quantum phase transition is of second order. The results are confirmed by the second derivative of the ground-state energy. We also study the relationship between the entanglement entropy, the Schmidt gap and quantum phase transitions. Conclusions drawn from these quantum information observables agree well with each other.

Keywords: quantum phase transition, fidelity susceptibility, density-matrix renormalization group

(Some figures may appear in colour only in the online journal)

1. Introduction

In the last two decades, quantum phase transitions (QPTs) in quantum spin chains have attracted considerable interest both in experimental and theoretical research [1]. Among them, the spin $S = 1$ antiferromagnetic Heisenberg chain has been extensively studied by many authors [2–4], whose ground state is termed the Haldane phase. This phase has a peculiar nonlocal string order in which the spins with $|S_z = \pm 1\rangle$ are arranged antiferromagnetically if the sites with $|S_z = 0\rangle$ are skipped. As we know, the QPT has been traditionally described based on the behavior of expectation values of local operators and two-point correlators in accordance to the standard Ginzburg–Landau theory. Unlike the case of spontaneous symmetry breaking, the absence of the long-range order in the Haldane phase is accompanied by a hidden $Z_2 \times Z_2$ symmetry breaking. Furthermore, the Haldane state is gapped between a spin-singlet ground state and a spin-triplet excited state, indicating that the spin-$1$ Heisenberg model is sharply different from its spin-$1/2$ counterpart.

Experimentally, a few quasi-one-dimensional Haldane chain compounds have been investigated, such as $Y_2\text{BaNiO}_5$ [5], $\text{CsNiCl}_3$ [6–8], $\text{Dy}_2\text{BaNiO}_5$ [9], $\text{Nd}_2\text{BaNiO}_5$ [10, 11] were considered to realize $S = 1$ Haldane systems with a magnetic gap in the excitation spectra. However, an ideal one-dimensional (1D) spin-$1$ system is rare in real materials, usually followed by the interchain interactions and magnetic anisotropy, which may partially or completely suppress the
excitation gap and thus lead to an observation of long-range order in a quantum disordered magnet. The strength of single-ion anisotropy \( D \) was retrieved from inelastic neutron-scattering on quasi-one-dimensional spin-1 chain compound ANi\(_2\)V\(_2\)O\(_8\) (A = Pb and Sr) [12], electron spin resonance (ESR) study on PbNi\(_2\)V\(_2\)O\(_8\) [13], multifrequency ESR transmission spectroscopy on single crystals SrNi\(_2\)V\(_2\)O\(_8\) [14, 15]. With large single-site anisotropy \( D > 0 \), the Haldane ground state changes to the large-\( D \) single-ion anisotropy excitation gap and thus lead to an observation of long-range order. A concept from quantum information theory, i.e. the ground-state fidelity, can be applied to capture the occurrence of the QPTs. Taking a general Hamiltonian

\[
H = \sum_{i=1}^{N} J (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + (-1)^i D (S_i^z)^2,
\]

where \( S_i^{\alpha}(\alpha = x, y, z) \) are spin-1 operators on the \( i \)-th site and \( N \) is the length of the spin chain. The periodic boundary condition is considered and it is denoted that \( N + 1 = 1 \). The parameter \( J \) denotes the antiferromagnetic coupling and \( J = 1 \) is considered in the paper. The parameters \( \lambda \) and \( D \) are the anisotropic spin-spin interaction and single-site anisotropy, respectively.

2. Hamiltonian

The Hamiltonian of a 1D spin-1 XXZ chain with alternating single-site anisotropy is given by

\[
H = \sum_{i=1}^{N} J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda_i S_i^z S_{i+1}^z) + (-1)^i D_i (S_i^z)^2.
\]

3. Measurements and algorithm

A concept from quantum information theory, i.e. the ground-state fidelity, can be applied to capture the occurrence of the QPTs. Taking a general Hamiltonian \( H(D) = H_0 + DH_1 \) as an example, where \( H_0 \) is the main part, \( H_1 \) is the driving part and the quantum parameter \( D \) denotes its strength. If \( \rho(D) \) represents a density matrix of the system, the ground-state fidelity between \( \rho_0(D) \) and \( \rho_1(D + \delta D) \) can be defined as

\[
F(D, \delta D) = \text{Tr} [\sqrt{\rho_0^{1/2}(D) \rho_1(D + \delta D) \rho_0^{1/2}(D)}],
\]

where \( \delta D \) is a small deviation. For a pure state \( \rho_0 = |\psi_0\rangle \langle \psi_0| \), equation (2) can be rewritten as

\[
F(D, \delta D) = |\langle \psi_0(D) | \psi_0(D + \delta D) \rangle|,
\]

which represents the overlap of the wavefunctions at two adjacent quantum parameter points and \( F(D, \delta D) \) reaches its maximum value \( F_{\text{max}} = 1 \) at \( \delta D = 0 \). Expanding \( |\psi_0(D + \delta D)\rangle \) to the first order, we have

\[
|\psi_0(D + \delta D)\rangle = |\psi_0(D)\rangle + \delta D \sum_{n \neq 0} \frac{H_{n0} |\psi_n(D)\rangle}{E_0(D) - E_n(D)},
\]

where \( H_{n0} = \langle \psi_n(D) | H_1 | \psi_0(D) \rangle \) and the eigenstates \( |\psi_n(D)\rangle \) satisfy \( H(D) |\psi_n(D)\rangle = E_n |\psi_n(D)\rangle \). Therefore, the fidelity susceptibility removes the artificial variable \( \delta D \) [24, 26] and can be calculated by

\[
\chi_F(D) = \lim_{\delta D \to 0} \frac{-2\ln F(D, \delta D)}{\delta D^2},
\]

and then it yields

\[
\chi_F(D) = \sum_{n \neq 0} \frac{|\langle \psi_0(D) | H_1 | \psi_n(D) \rangle|^2}{[E_0(D) - E_n(D)]^2}.
\]

The divergence of \( \chi_F \) can directly locate the critical points. The related phase transition is exactly convincing [25, 26, 34].
The EE can be chosen as a measurement of the bipartite entanglement, which is defined as follows: assuming $|\text{g.s.}\rangle$ is the ground state of the target Hamiltonian, which can be divided into two subsystems $A$ and $B$. One convenient choice of subsystem $A$ is composed from the first site to the $L$th site and the subsystem $B$ is the rest of the system. The reduced density matrix of part $L$ can be obtained by taking the partial trace over system $N - L$, which is given by

$$\rho_A = \text{Tr}_B (|\text{g.s.}\rangle \langle \text{g.s.}|).$$

Then, the bipartite EE measures the entanglement between parts $A$ and $B$ as

$$S_L = -\text{Tr}(\rho_A \log_2 \rho_A).$$

In addition, as a local order parameter, the Schmidt gap can also be used to describe the QPTs [35]. It is defined as

$$G = g_1 - g_2,$$

where $g_1$ and $g_2$ are the first and the second largest eigenvalues of the reduced density matrix $\rho_A$ [equation (7)], respectively.

Thanks to the density-matrix renormalization-group (DMRG) [36–38] method, the ground state of the 1D system can be calculated with very high accuracy. We implement Matlab code to speed up the GPU for the finite-size DMRG with double precision. The maximum eigenstates kept are $m = 200$ during the procedure of basis truncation and the truncation error is smaller than $10^{-100}$. With such high performance calculation, we can precisely analyze the QPTs in terms of both the EE and the FS.

4. Numerical results

As a check, we plot the FS per site as a function of the single-site interaction for different system sizes with $\lambda = 1$. As shown in the figure 1, peaks in the ground-state FS are observed, which signal precursors of the phase transition from Haldane phase to the classical-like system. After reaching a local maximum, the variation of the EE becomes relatively small. When the $D$ increases further, the EE reaches another maximum and then decreases rapidly. Furthermore, the EE is insensitive to the system size, as a consequence of boundary law in 1D gapped Hamiltonian, while the maximum values of the EE grow with increasing $N$, which is a logarithmically divergent correction to the boundary law [41, 42]. The location of left peak in figure 4(a) moves to higher $D$ up to a particular value as the system size increases, while the location of right peak moves to lower $D$ up to a particular value as the system size grows. We fit the locations of maximums by the formula

$$D_c(N) \sim D_c + aN^{-b},$$

where $a$, $b$ are size-independent constants and $N$ is the system size. We obtain that $D_{c1} = 3.20$, $a_1 = 14.44$, $b_1 = 1.438$ and $D_{c2} = 4.760$, $a_2 = -14.45$, $b_2 = 1.506$; see figures 4(b) and (c).

We also investigate the Schmidt gap of the reduced density matrix after cutting a $N$-site chain into two half subsystems ($L = N/2$). The Schmidt gap labeled by $G$ is plotted as a function of $D$ for different system sizes in figure 5. It is seen that the Schmidt gap is large when the system is in the Néel phase. With increasing $D$, the Schmidt gap closes very rapidly when the system is in the Haldane phase, because $S = 1$.
Figure 2. (a) The fidelity susceptibility per site is plotted as a function of the single-site anisotropy $D$ for different system sizes with $\lambda = 2$. Inset: $\chi_F^\text{max}/N$ for various sizes $N$. The lines are fitting lines. (b) The second derivative of the ground-state energy density is plotted as a function of the single-site interaction for different system sizes with $\lambda = 2$.

Figure 3. The string order parameter $O_x$ is plotted as a function of the single-site anisotropy for different system sizes with $\lambda = 2$.

Haldane phase is a topological phase protected by specific global symmetry and is characterized by a double degeneracy of the entanglement spectrum [43]. When $D$ increases further, the Schmidt gap opens very rapidly again when system is in the periodic Néel phase.

In figure 6, we portray the $D-\lambda$ phase diagram of the Hamiltonian (1), which is detected via the EE, the Schmidt gap and the FS. When $D = 0$, the quantum transition from Haldane spin liquid to Néel spin solid is continuous and belongs to a second-order QPT at $\lambda = 1.18$ [3, 22]. The critical points between the periodic Néel phase and the Haldane phase decrease with $\lambda$ increases. The critical points between the Néel phase and the Haldane phase increase as $\lambda$ increases. Two critical lines will merge each other when $\lambda$ increases, where the Haldane phase disappears and the Néel-periodic Néel transition becomes first order at $D = 2\lambda$.

5. Discussion

In this paper, we have investigated the QPTs in the 1D spin-1 XXZ chains with alternating single-site anisotropy by analysing the bipartite entanglement, the Schmidt gap and the FS by using the DMRG technique. Their relation with QPTs is under discussion. It is important to note that the quantum phase transitions from the Néel ordering to Haldane spin liquid to periodic Néel spin solid can be well characterized by the FS. The finite-size scaling demonstrates that FS should diverge in the thermodynamic limit at the pseudo-critical point and...
the locations of extreme points approach a quantum critical point accordingly. It also shows a power-law divergence at criticality, which indicates the QPT is of second order and the critical exponent can be obtained. We compare the FS with the second derivative of the ground-state energy and find both of them exhibit similar peaks. The critical point can also be successfully detected by the EE and the Schmidt gap. To sum up, the quantum information observables are effective tools for detecting diverse QPTs in spin-1 models.

Acknowledgments

This work is supported by the National Natural Science Foundation of China (NSFC) under Grants No. 11104021, No. 11347008 and No. 11474211, as well as the Natural Science Foundation of Jiangsu Province of China under Grant No. BK20141190.

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