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Doubly degenerate entanglement spectrum and nonzero string order in the spin-1/2 Heisenberg–Ising chain

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ABSTRACT

The ground-state properties and quantum phase transitions (QPTs) in spin-1/2 Heisenberg-Ising alternating chain has been investigated by the iTEBD algorithm. Four different ground-state phases, *i.e.*, a ferromagnetic phase (FM), an antiferromagnetic phase (AF), a stripe phase (SP), and a disordered phase were distinguished. The disordered phase, which has nonzero string orders and the doubly degenerate entanglement spectrum, was observed as Heisenberg coupling $J_H > 0.5$. The disordered phase in such a model is found to belong to the same topological phase as the Haldane state. In the disordered phase, every two nearest-neighbor spin-1/2 spins connected by the Ising coupling behave like an integer ($S=1$) spin. Furthermore, the QPTs from the disordered phase to the AF and SP phases belong to the Ising universality class with central charges $c=\bar{c}=1/2$.

1. Introduction

Some magnetic materials which exhibit quasi-one-dimensional characters can be well described by spin chains. However, it is interesting that there exists a fundamental difference between half-integer-spin chains and integer-spin chains. In detail, the half-integer antiferromagnetic Heisenberg chain has gapless excitations. In contrast, there exists a distinct energy gap between the first excited state and the ground state (Haldane phase) for integer-spin chain [1]. Since Haldane's prediction, the integer spin chains have been attracting much attention. The concept of the string order introduced firstly by den Nijs and Rommelse [2] and later by Tasaki [3] is found to be capable of clarifying the physical nature of the Haldane phase which possesses a hidden long-range "string" order accompanied by the breaking of a hidden "$Z_2 \times Z_2$" symmetry [4,5].

In order to elucidate the properties of the spin-1 Heisenberg chain, the spin-1/2 ferromagnetic–antiferromagnetic alternating chain was proposed and investigated explicitly by Hida [6,7]. The ferromagnetic coupling should be infinitely strong to force the spins interacting ferromagnetically to form a local triplet, this way resulting in a spin-1 chain. It is interesting that the string order is found to be finite not only in the Haldane-gap phase but also in the dimer phase. Therefore this order parameter must be useful to distinguish the static valence-bond-type disordered states from other disordered states. The string order parameter which was originally defined for the spin-1 Heisenberg chains [2] has been generalized to the spin-1/2 ferromagnetic–antiferromagnetic alternating chain. This ground state belongs to the same topological phase as the Haldane state, and interpolates those of the uniform spin-1/2 and spin-1 Heisenberg chains. Recently, the ground-state phases of a spin-1/2 ferromagnetic–antiferromagnetic alternating Heisenberg chain with ferromagnetic next-nearest-neighbor (NNN) interaction were investigated [8]. In addition to the Haldane phase and the ferromagnetic phase, a series of topologically distinct spin-gap phases with various magnitudes of edge spins were reported.

Theoretically, it is also interesting for us to reduce the Heisenberg couplings on even bonds to a classical (Ising) type. It means that the couplings on the odd bonds are Heisenberg type, but that on the even bonds are Ising type. Such a model is called the one-dimensional (1D) spin-1/2 Heisenberg–Ising alternating model. This model, which has been originally proposed by Lieb et al. [9] and re-examined subsequently by Yao et al. [10], represents a valuable example of rigorously solved quantum spin chain. The spin-1/2 Heisenberg–Ising alternating model is described by

$$\hat{H} = \sum_{i}^{N/2} [J_H \hat{S}_{2i-1} \cdot \hat{S}_{2i} + J_I S^z_{2i} S^z_{2i+1}], \tag{1}$$

where $\hat{S}$ is the spin-1/2 operator, and N is the length of the spin chain. J_H and J_I denote the Heisenberg and Ising couplings on the odd and even bonds, respectively. Based on fundamental quantum mechanical principles, the ground state as well as excited state of this model was obtained. This model with (J_H, $J_I > 0$) has been

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investigated previously, and a gap–gap QPT from the disordered dimer phase to the antiferromagnetic phase was determined exactly at $J_I/J_H=2$. It is well known that, when $J_I=0$, the ground state is composed of local dimers that are formed by spins on sites $2i-1$ and $2i$. In other words, the model reduces to the dimer model with pairwise interactions. In the limit of strong antiferromagnetic coupling $J_I\to+\infty$, it should have ideal Néel states (↑↓ or ↓↑) on sites $2i$ and $2i+1$. Subsequently, by Jordan-Wigner and Bogoliubov transformations, the anisotropic version of the antiferromagnetic spin-1/2 Heisenberg–Ising bond alternating chain was re-examined [10], and low-energy excitations with a gap when $J_I\neq 2$ were observed. The ground-state properties of such a model with Dzyaloshinskii–Moriya interaction were investigated recently [11], and an interesting nonanalytic behavior accompanied by a gapless excitation spectrum was observed whenever the condition $J_I/J_H=2$ is met. Recently, the ground-state behavior of the frustrated quantum spin-1/2 two-leg ladder with the Heisenberg intra-rung and Ising inter-rung interactions, which can be regarded as an extension of the spin-1/2 Heisenberg–Ising alternating model, was examined [12]. A ground-state phase diagram consisting of five ordered and one quantum paramagnetic (disordered) phase was obtained. The disordered phase was characterized through short-range spin correlations, which indicate a dominating character of the rung singlet-dimer state in this phase.

As mentioned above, these previous studies mainly focused on the behavior of the ground-state energy, the excitation spectrum, and the short- and long-range correlations. Many other interesting ground-state properties, such as entanglement spectrum and string orders, are still unclear. Especially, it is also an interesting issue whether the spin-1 behavior observed in the spin-1/2 ferromagnetic–antiferromagnetic alternating chain [6,8] exists in the spin-1/2 Heisenberg–Ising alternating chain. In this paper, we would like to reinvestigate the spin-1/2 Heisenberg–Ising alternating chain and analyze these issues. Based on the framework of the infinite matrix product state (iMPS) representation [13], the nonlocal string orders can be calculated directly by the iTEBD algorithm developed by Vidal [14]. As will be shown below, distinctive nonzero string orders and doubly degenerate entanglement spectrum will be observed in the disordered (Haldane) phase.

2. Methods and calculation details

For infinite 1D lattice systems, it has been shown [15,16] that any states of them fulfilling the area law can be efficiently described by matrix product state (MPS) [17,18]. Based on the framework of the infinite matrix product state (iMPS) representation, the ground-state wavefunction $|\psi_g\rangle$ can be obtained by the iTEBD method [14] by acting an imaginary time evolution operator $\exp(-\tau\hat{H})$ on an arbitrary initial state $|\psi_0\rangle$. As the τ is large enough, the resulting wavefunction $\exp(-\tau\hat{H})|\psi_0\rangle$ will converge to the ground state $|\psi_g\rangle$ of $\hat{H}$. In the practical iteration process, the operator $\exp(-\delta\tau\hat{H})$ with small enough $\delta\tau$ is expanded by a Suzuki–Trotter decomposition as a sequence of two-site gates $U^{[i,i+1]}$. We set $\delta\tau=10^{-1}$ first, and then diminish it down to $\delta\tau=10^{-8}$ gradually. In order to recover the evolved state in the iMPS representation, a singular value decomposition (SVD) is performed and the χ largest singular values are obtained. The χ denotes the cut-off bond dimension in the SVD process. The wavefunction of a 1D two-period quantum system can be generally described by

$$|\psi\rangle=\mathrm{Tr}\left[\prod_{i=1}^{N/2}\Gamma^a(m_{2i-1})\Lambda^a\Gamma^b(m_{2i})\Lambda^b\right]|\ldots,m_{2i-1},m_{2i},\ldots\rangle, \quad (2)$$

where m_i represents the local spin physical index, and N denotes the length of the spin chain. Γ^a and Γ^b are two 3-indexed tensors, and Λ^a and Λ^b are two χ by χ diagonal matrices on odd (even) bonds. To uncover possible four-period states, a four-period MPS should be introduced, hence four tensors (Γ^a, Γ^b, Γ^c, and Γ^d) and four diagonal matrices (Λ^a, Λ^b, Λ^c, and Λ^d) should be updated in every iTEBD iteration process. The details of the iTEBD algorithm can be found in references [14,19,20] and the references therein. With the ground-state wavefunction $|\psi_g\rangle$, the expected value of a physical operator $\hat{O}$ is obtained by $\langle\psi_g|\hat{O}|\psi_g\rangle$, which is simplified as $\langle\hat{O}\rangle$ in the following.

3. Numerical results

The case with ferromagnetic Ising interactions ($J_I=-1.0$) on even bonds (see Eq. (1)) is investigated in this section. The spontaneous magnetization ($M^z=(1/N)\sum_{i=1}^{N}M_i^z$) and stripe order parameter ($M^z_{stripe}=(1/N)|\sum_{i=1}^{N/2}(-1)^i(M^z_{2i}+M^z_{2i+1})|$) are calculated, and their curves versus varying Heisenberg coupling J_H are plotted in Fig. 1. The $M_i^z=\langle S_i^z\rangle$ denotes the local magnetization on the ith site. According to our calculation results, we find that there exists a fully polarized (ferromagnetic) phase with saturated magnetization $M^z=0.5$ in the region $J_H<0$. In the intermediate region $0<J_H<0.5$, the stripe order parameter M^z_{stripe} becomes nonzero, which represent the existence of the antiferromagnetic stripe phase (SP). The detailed local magnetization calculation shows that this stripe phase has a spin configuration "$\cdots+--+\cdots$". As $J_H>0.5$, the ground state has absolutely vanishing local magnetization on every site, therefore we call it a disordered phase.

Then, we calculate the long-range correlation function along z-axis $\langle\sigma_i^z\sigma_{i+L}^z\rangle$ ($L=1, 2, 3, \ldots$). It should be noted that the σ^α ($\alpha=x$, y, and z) denote spin-1/2 Pauli matrices, therefore the spin-1/2 operator $S^\alpha=\frac{1}{2}\sigma^\alpha$. The saturated ferromagnetic correlation ($\langle\sigma_i^z\sigma_{i+L}^z\rangle$ always equals 1) is obtained in the ferromagnetic phase (FM) region $J_H<0$. In the SP region, nonzero long-range correlation ($\langle\sigma_i^z\sigma_{i+L}^z\rangle\neq 0$) is found, and it has a periodic sign arrangement "$++--\cdots$", which is a typical antiferromagnetic stripe correlation. However, in the disordered phase, the correlations $\langle\sigma_i^z\sigma_{i+L}^z\rangle$ decay very quickly with increasing L, which means that no

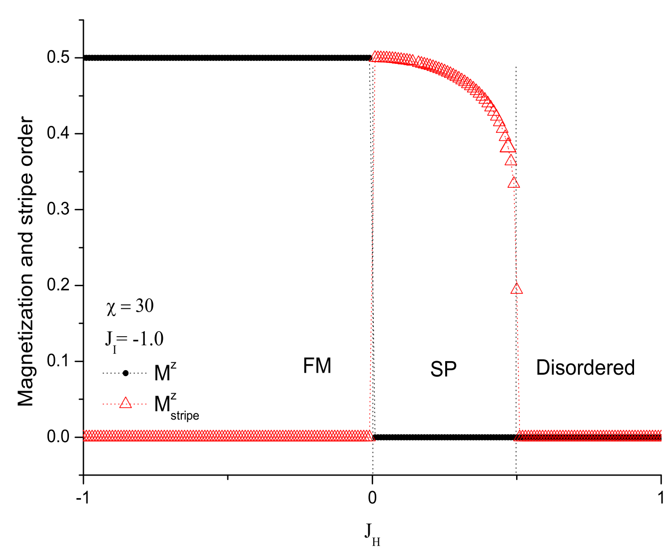

Fig. 1. Spontaneous magnetization $M^z=(1/N)\sum_{i=1}^{N}M_i^z$ and stripe order parameter $M^z_{stripe}=(1/N)|\sum_{i=1}^{N/2}(-1)^i(M^z_{2i}+M^z_{2i+1})|$ of the stripe configuration "$\cdots+--+\cdots$" versus varying Heisenberg coupling J_H. $M_i^z=\langle S_i^z\rangle$ denotes the local magnetization on the ith site. The FM denotes the ferromagnetic phase, and the SP represents the stripe phase.