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Rigorous studies on boundary effects of a dimerized $S=1$ Ising chain with single-ion anisotropy

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ABSTRACT

We investigate the influences of the boundary conditions on the ground state properties of a dimerized $S=1$ Ising chain with single-ion anisotropy, which are solved exactly by means of a mapping to the spin-1/2 Ising chain with the alternating transverse fields and the Jordan–Wigner transformation. We obtain the exact results of the minimal energy gap Δ_0 for exciting a fermion quasi-particle, the minimal energy gap Δ_h for exciting a hole and the ground state phase diagram under various boundary conditions. The results show that the boundary conditions do not change the quantum phase transition points of the system, but the minimal energy gaps in the cases of periodic and open boundary conditions are quantitatively different. When the dimerized transverse single-ion anisotropies parameter $D_1 > D_2$, the ground state is lied in the non-hole systems with arbitrary lattice sites. But if $D_1 < D_2$, holes will appear in the ground state of system with odd lattice sites.

1. Introduction

One-dimensional spin models have been continuously attracting much attention in both theoretical and experimental condensed-matter physics. On the one hand, those models are among the few exactly solvable quantum many-body systems [1–6]; on the other hand, deviations from the pure uniform crystalline system (e.g., disorder or regularly varying parameters) will heavily influence the properties of quantum spin systems [7–13], and some works showed that the system will exhibit a series of quantum phase transitions dependent on the dimerization strength of the crystal fields.

Besides the dimerization effects, the choice of boundary conditions might also severely affect the systems' properties [14–18]. In fact, due to the boundary edges, the open boundary condition (OBC) has a smaller number of joint points between the blocks than the periodic boundary condition (PBC) (one or two points, respectively), and the wave function loses the translational symmetry. Moreover, the analysis requires a set of results with accuracy as well as parameters. If either of the above is not fulfilled, one may no longer obtain a reliable result.

The motivation of the present work is to discuss how the boundary conditions and parity of lattice sites affect the ground state properties of a dimerized $S=1$ Ising chain with single-ion anisotropy. We examine how the critical behavior of quantum many-body states at finite system size is influenced by the boundary conditions. The ends of the chain and lattice sites L may be treated in four different but physically reasonable ways: (a) PBC with even L; (b) PBC with odd L: (c) OBC with even L; and (d) OBC with odd L. We show that (i) the ground state energy is almost the same in the above four cases; (ii) the minimal energy gap Δ_0 for exciting a fermion quasi-particle is the same in case of OBC regardless of the parity of lattice sites, but strongly depends on the magnitude of the dimerized transverse single-ion anisotropy; (iii) the minimal energy gap Δ_h for exciting a hole for even sites L system is always positive, but for odd L, when magnitude of the dimerized transverse single-ion anisotropy $D_1 > D_2$, Δ_h is positive but when $D_1 < D_2$, Δ_h is negative, which means that the system with odd L that have holes existed is more stable. As far as we know, no previous arguments, analytic calculations, or numerical studies predict the boundary effects of the dimerized spin-1 Ising chain under four boundary conditions.

The outline of this letter is as follows. In the next section, a detailed description of the model system is presented and then, exact diagonalization of the system under different boundary conditions will be shown. In Section 3 the model is solved numerically and the phase diagrams are discussed. Finally, Section 4 is devoted to one brief conclusion.

2. The lattice model Hamiltonian

We consider a dimerized spin-1 Ising model with both longitudinal and transverse single-ion anisotropies with period boundary conditions (PBC) and free boundary conditions (OBC). Let $\vec{S}_j$ be $S=1$ spin operators at the j-th site, satisfying the $SU(2)$ algebra

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$[S_i^a, S_j^b] = i\delta_{i,j}\varepsilon_{abc}S_i^c$, for $a,b,c = x,y,z$, and $(\overrightarrow{S}_j)^2 = S(S+1) = 2$. We also consider the single-ion effects associated with each lattice spins due to the crystal fields. So, the model Hamiltonian of a dimerized spin-1 Ising chain with both longitudinal and transverse single-ion anisotropies is described by

$$H = -\sum_j [J_j S_j^z S_{j+1}^z + 2D_j^x (S_j^x)^2 + D_j^z (S_j^z)^2]. \quad (1)$$

The model in the uniform case with $J_1 = J_2$, $D_1 = D_2$ was studied in Refs. [11,19,20]. When $D_1 = 0$ and $D_2 \neq 0$, it can be transformed to the model of a mixed spin-1/2 and spin-1 Ising chain [21,22].

2.1. Periodic boundary conditions

Let us first consider the periodic boundary conditions. On a chain with L sites the Hamiltonian is given by

$$H = -\sum_{j=1}^{L} [J_j S_j^z S_{j+1}^z + 2D_j^x (S_j^x)^2 + D_j^z (S_j^z)^2]. \quad (2)$$

The periodic boundary condition is imposed as usual: $S_{L+j}^a = S_j^a$. The dimerization is imposed on both the bond couplings and the anisotropy associated with the transverse crystal fields: $J_{2j-1} = J_1$, $J_{2j} = J_2$, $D_{2j-1}^x = D_1$, $D_{2j}^x = D_2$ and $D_{2j}^z = D_{2j-1}^z = D_z$ for $j = 1, 2, \ldots, L/2$ with even L, or $J_{2j-1} = J_1$, $D_{2j-1}^x = D_1$, where $j = 1, 2, \ldots, (L+1)/2$, and $J_{2j} = J_2$, $D_{2j}^x = D_2$, where $j = 1, 2, \ldots, (L-1)/2$ with odd L.

At each site of the chain, the eigenvalue m_j of S_j^z can take three values of 0 and ± 1. Effectively, one can regard $m_j = 0$ state as a hole and $m_j = \pm 1$ states as the two polarized spin states of a spin-1/2 spin operator. As done in Ref. [20], by introducing $\hat{N}_0 = L - \sum (S_j^z)^2$, one has $[\hat{N}_0, H] = 0$. This means that the hole states with $m_j^j = 0$ are decoupled from the spin polarized states with $m_j = \pm 1$, it is straight forward to show that Eq. (2) is exactly equivalent to the following Hamiltonian

$$H = -\sum_{j=1}^{L} J_j \sigma_j^z \sigma_{j+1}^z - \sum_{j=1}^{L} D_j \sigma_j^x + E_0, \quad (3)$$

where $E_0 = -\Sigma_{j=1}^{L} D_j - L \cdot D_z$, which, to within a constant, is just the spin-1/2 transverse Ising chain.

By the Jordan–Wigner transformation, the spin-1/2 Ising model is mapped onto the spinless Fermion system where each term in the Hamiltonian is of bilinear, namely,

$$H = \sum_{i,j} \left[c_i^\dagger A_{i,j} c_j + \frac{1}{2}(c_i^\dagger B_{i,j} c_j^\dagger + h.c.) \right] + \frac{1}{2} TrA, \quad (4)$$

where, $A_{ij} = -2D_i\delta_{i,j} - J_i\delta_{i+1,j} - J_{i-1}\delta_{i-1,j} = A_{ji}$, $B_{ij} = -J_i\delta_{i+1,j} + J_{i-1}\delta_{i-1,j} = B_{ji}$. According to Ref. [5], we introduce the quasi-particles, defined by $\eta_k = \sum_j (g_{k,j} + h_{k,j}) c_j/2 + (g_{k,j} - h_{k,j}) c_j^\dagger/2$, with a pair of real vectors $g_{k,j}$, $h_{k,j}$. The Hamiltonian is diagonalized as

$$H = \Sigma_k \Lambda_k (\eta_k^+ \eta_k - \frac{1}{2}) + E_0, \quad (5)$$

The eigenvalue Λ_k and the vectors $g_{k,j}, h_{k,j}$ satisfy the equations $[\eta_k, H]_+ = \Lambda_k \eta_k$, $\Sigma_i g_{k,i}((A-B)(A+B))_{i,j} = \Lambda_k^2 g_{k,j}$, $\Sigma_i h_{k,i}((A+B)(A-B))_{i,j} = \Lambda_k^2 h_{k,j}$. If we define $(\Phi_k)_j = g_{kj} + h_{kj}$ and $(\Psi_k)_j = g_{kj} - h_{kj}$, the eigenvalue Λ_k can be solved by

$$M_{ji}(\Phi_k)_i = \Lambda_k^2 (\Phi_k)_j, M_{ji}(\Psi_k)_i = \Lambda_k^2 (\Psi_k)_j, \quad (6)$$

with M being a symmetric matrix defined by $(A-B)(A+B)$, or $M_{ij} = (4D_iD_j + 4J_{i-1}J_{j-1})\delta_{ij} + 4D_iJ_{i-1}\delta_{i-1,j} + 4D_iJ_{j-1}\delta_{i,j-1} = M_{ji}$, or written explicitly for PBC,

$$M = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & \cdots & b_2 \\ b_1 & a_2 & b_2 & 0 & 0 & \cdots & \cdots \\ 0 & b_2 & a_1 & b_1 & 0 & \cdots & \cdots \\ 0 & 0 & b_1 & a_2 & b_2 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & b_2 & a_1 & b_1 \\ b_2 & \cdots & \cdots & \cdots & 0 & b_1 & a_2 \end{bmatrix}_{L\times L} \quad \text{for even } L \text{ or}$$

$$M = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & \cdots & b_2 \\ b_1 & a_2 & b_2 & 0 & 0 & \cdots & \cdots \\ 0 & b_2 & a_1 & b_1 & 0 & \cdots & \cdots \\ 0 & 0 & b_1 & a_2 & b_2 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & b_1 & a_2 & b_2 \\ b_1 & \cdots & \cdots & \cdots & 0 & b_2 & a_1 \end{bmatrix}_{L\times L} \quad \text{for odd } L, \quad (7)$$

where $a_1 = 4(D_1^2 + J_2^2)$, $a_2 = 4(D_2^2 + J_1^2)$, $b_1 = 4D_1J_1$, $b_2 = 4D_2J_2$.

Generally, its eigenvectors $g_{k,j}$ or $h_{k,j}$ take the following Ansatz: $[1 + (-1)^j\beta]\exp(ik)$, β being a parameter determined by the associated dimerization. For PBC $k_n = 2\pi n/L$, $n = -L/2, -L/2+1, \cdots, L/2-1$ for even L, and $n = -L-1/2, -L-1/2+1, \cdots, L-1/2-1$ for odd L. Thus, we can diagonalize Eq. (6) with this M matrix both analytically and numerically to obtain the quasi-particles' spectra.

In order to obtain the minimal hole excitation gap we also need to consider the case where is one hole in the spin chain. We simply assume that the hole, the $m_j = 0$ state at the $j = L$ site in the original chain, and use the same method to diagonalize this subsystem, the diagonal form Hamiltonian with one hole can be written as

$$H_1(L) = \sum_{\tilde{k}} \Lambda'_{\tilde{k}} (\eta_{\tilde{k}}^{+'} \eta'_{\tilde{k}} - \frac{1}{2}) + (D_z - D_L) + E_0. \quad (8)$$

Corresponding to Eq. (7) of matrix M of the none hole sector, the matrix M_h with one hole is written as

$$M_h = \begin{bmatrix} a_0 & b_1 & 0 & 0 & 0 & \cdots & 0 \\ b_1 & a_2 & b_2 & 0 & 0 & \cdots & \cdots \\ 0 & b_2 & a_1 & b_1 & 0 & \cdots & \cdots \\ 0 & 0 & b_1 & a_2 & b_2 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & b_1 & a_2 & b_2 \\ 0 & \cdots & \cdots & \cdots & 0 & b_2 & a_1 \end{bmatrix}_{(L-1)\times(L-1)} \quad \text{for even } L \text{ or}$$

$$M_h = \begin{bmatrix} a_0 & b_1 & 0 & 0 & 0 & \cdots & 0 \\ b_1 & a_2 & b_2 & 0 & 0 & \cdots & \cdots \\ 0 & b_2 & a_1 & b_1 & 0 & \cdots & \cdots \\ 0 & 0 & b_1 & a_2 & b_2 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & b_2 & a_1 & b_1 \\ 0 & \cdots & \cdots & \cdots & 0 & b_1 & a_2 \end{bmatrix}_{(L-1)\times(L-1)} \quad \text{for odd } L, \quad (9)$$

where $a_0 = 4D_1^2$.

2.2. Free boundary conditions

Let us now consider the dimerized spin-1 Ising model with free ends condition and with the Hamiltonian

$$H = -\sum_{j=1}^{L-1} J_j S_j^z S_{j+1}^z - \sum_{j=1}^{L} [2D_j^x (S_j^x)^2 + D_j^z (S_j^z)^2]. \quad (10)$$

The dimerization is imposed on both the bond couplings and the anisotropy associated with the transverse crystal fields: $J_{2j-1} = J_1$, $J_{2j} = J_2$, $D_{2j-1}^x = D_1$, $D_{2j}^x = D_2$ and $D_j^z = D_z$ for $j = 1, 2, \ldots, L/2$ when L is even and $J_{2j-1} = J_1$, $J_{2j} = J_2$, $j = 1, 2, \ldots, (L-1)/2$, $D_{2j-1}^x = D_1$, $j = 1, 2, \ldots, (L+1)/2$, $D_{2j}^x = D_2$, $j = 1, 2, \ldots, (L-1)/2$ when L is odd.

By using the Jordan–Wigner transformation (the same process in Section 2.1) the Hamiltonian of the system in the diagonal form can be written as

$$H = \sum_k \Lambda_k (\eta_k^+ \eta_k - \frac{1}{2}) - \sum_{j=1}^{L} (D_j^x + D_j^z). \quad (11)$$