Physics Letters A 372 (2008) 6531–6535

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Exact results of a mixed spin-1/2 and spin-1 Ising chain with both longitude and transverse single-ion anisotropies

Haina Wu [a], Guozhu Wei [a,b,*], Guangyu Yi [a]

[a] College of Sciences, Northeastern University, Shenyang 110004, China
[b] International Center for Material Physics, Academia Sinica, Shenyang 110015, China

ARTICLE INFO

Article history:
Received 22 July 2008
Received in revised form 31 August 2008
Accepted 3 September 2008
Available online 6 September 2008
Communicated by R. Wu

PACS:
75.10.Pq
02.30.Ik
75.10.Dg

Keywords:
Mixed spin Ising chain
Single-ion anisotropy
Exact result

ABSTRACT

The mixed spin-1/2 and spin-1 Ising chain with both longitude and transverse single-ion anisotropies D_z and D_x is solved exactly by means of a mapping to the spin-1/2 Ising chain with the alternating transverse fields and the Jordan–Wigner transformation. The analytical expressions of the quasi-particles' spectra Λ_k, 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 energy are obtained. The phase diagram of the ground state is also given. The results show that when $D_z \geqslant 0$ for any finite value of D_x, there is no quantum critical point and the ground state is always in a spin ordered phase disregard of the boundary condition in the present system.

1. Introduction

Quantum spin systems have been studied extensively in the last decades. One-dimensional spin models have been continuously attracting much attention in both theoretical and experimental condensed-matter physics since they are among the few exactly solvable quantum many-body systems. Heisenberg spin chain model and the anisotropic extensions of the Heisenberg exchange were exactly solved by the most powerful method Bethe ansatz [1–4]. Using fundamental quantum mechanical principles two spin models can be exactly solved, whose ground state and elementary excitations are obtained [5,6].

In last two decades, many quasi-one-dimensional mixed-spin materials [7–10] with each unit cell containing two spins of different spin value have been synthesized, such as $A\mathrm{Cu}(pba\mathrm{OH})(\mathrm{H_2O})_3 \cdot n\mathrm{H_2O}$ with $pba = 1,3$-proplyenebis(oxamato) and $A = \mathrm{Mn}$, Fe, Co, Mn, Zn and belong to the alternating or mixed spin chain family. A variety of the theoretical efforts have done for the spin systems mixed by different kinds of spins by means of different methods, many theoretical works dealt in two-dimension. But in one dimension, alternating spin-1/2 and spin-1 chain only solved by a variety of methods, such as DMRG methods, spin-wave theory [11,12], Monte Carlo simulations [13], mean-field theory [14], the Green's function approach [15] and so on. Previous studies undertaken within the mixed spin-1/2 and spin-1 chain have only considered some magnetic properties in the absence of external magnetic field or anisotropic single-ion field.

In this Letter we study a mixed spin-1/2 and spin-1 Ising chain with both longitude and transverse single-ion anisotropies. We show that this model can be solved exactly in principle by extending the analytical method used in solving the $S = 1/2$ quantum Ising chain [5]. The central idea of our exact diagonalization lies in the fact that the total Hilbert space of this mixed spin-1/2 and spin-1 Ising chain can be divided into a number of subspaces labeled by a conserved quantity, the number of holes. Here, a hole represents a local state with zero S_i^z of spin-1 at site i. This idea was motivated from the paper of Oitmaa and Brasch [16], where they mapped a ferromagnetic spin-1 Ising model with a transverse single-ion crystal-field term to the usual spin-1/2 transverse Ising model, and the other recent paper of Yang et al. [17], where they solve the spin-1 quantum Ising model with single-ion anisotropy by mapping it onto a series of segmented spin-1/2 transverse Ising chains, separated by the $S_i^z = 0$ states called holes. Our present study provides a further exactly solvable mixed spin-1/2 and spin-1 Ising system with both longitude and transverse single-ion anisotropies.

* Corresponding author at: College of Sciences, Northeastern University, Shenyang 110004, China.
E-mail address: guozhuwei02@sina.com (G. Wei).

0375-9601/$ – see front matter
doi:10.1016/j.physleta.2008.09.009

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 will be shown. In Section 3 the model is solved numerically and the phase diagrams are discussed. Finally, Section 4 is devoted to brief conclusion.

2. Model and method

2.1. The model Hamiltonian

Let us consider a mixed spin-1/2 and spin-1 Ising chain with both longitude and transverse single-ion anisotropies. To ensure exact tractability of the model system, we will further suppose that the odd sites are occupied by spin-1/2 atoms, and the even sites are occupied by the spin-1 atoms in the chain. The total Hamiltonian of the system reads:

$$H = -J\sum_{\langle i,j\rangle} s_i^z S_j^z - \sum_j \left[2D_x\left(S_j^x\right)^2 + D_z\left(S_j^z\right)^2\right], \tag{1}$$

where s_i^z and S_j^α $(\alpha = x, y, z)$ denote standard spatial components of the spin-1/2 and spin-1 operators, respectively. The first summation in Eq. (1) is carried out over nearest-neighboring spin pairs only, while the other two summations run over the sites of the chain. The last two terms D_z and D_x are the longitude and transverse single-ion anisotropies acting on the spin-1 atoms, respectively. J stands for the nearest-neighbor exchange interaction parameter.

At each even site of the chain, the eigenvalue m_j of S_j^z can take three values 0 and ± 1. Effectively, one can regard $m_j = \pm 1$ states as the two polarized spin states of a $S = 1/2$ spin operator and $m_j = 0$ state as a hole. It has been recently pointed out that the ferromagnetic $S = 1$ Ising lattices can be mapped onto the $S = 1/2$ Ising lattices provided the number of holes being a conserved quantity [16,17]. As did in Ref. [16], by introducing $\hat{N}_0 = \frac{L}{2} - \sum_j (S_j^z)^2$ for a periodic boundary chain with the total number of sites L which is even, we find that $[\hat{N}_0, H] = 0$. This means that the hole states with $m_j = 0$ are decoupled from the spin polarized states with $m_j = \pm 1$. So all the eigenstates of the model can be classified by the eigenvalue of $\hat{N}_0$, i.e., the total number of the local states $|0_j\rangle$ in the spin chain.

The holes in this system act like nonmagnetic impurities, they will separate the system into many independent segments of interacting $S = 1/2$ spins. In a system of p $(0 \leqslant p \leqslant L/2)$ holes, there are $p+1$ segments of non-hole systems at most. If these holes are located at $(x_1, \ldots, x_p)$ with $2p = x_p \leqslant L$, it is straightforward to show that Eq. (1) is exactly equivalent to the following Hamiltonian (setting $x_0 = 0$ and $x_{P+1} = L+1$),

$$H\{x_i, p\} = \sum_{n=1}^{p+1} h(l_n) + p(D_z - D_x) + E_0, \tag{2}$$

where the dynamic irrelevant constant $E_0 = -\frac{L}{2}(D_x + D_z)$ and

$$h(l_n) = -\frac{1}{2}J\sum_{j=x_{n-1}+1}^{x_n-2} \sigma_j^z\sigma_{j+1}^z - \sum_{j=x_{n-1}+1}^{x_n-2} D_j\sigma_j^x \tag{3}$$

is the Hamiltonian of the reduced subsystem which is equivalent to an $S = 1/2$ Ising chain of length $l_n = x_n - x_{n-1} - 3$ with the alternating transverse fields [18–20].

By denoting $|\psi(l_n)\rangle$ the eigenstate of the subsystem $h(l_n)$ with eigenvalue $\varepsilon(l_n)$, the generic eigenstate of $H(\{x_i, p\})$ is then given by $|\Psi_p(L)\rangle = \prod_{n=1}^{P} |\psi(l_n)\rangle \otimes |0_{x_n}\rangle$ with eigenvalue $E_p(L) = \sum_{n=1}^{p} \varepsilon(l_n) + p(D_z - D_x)$.

It is therefore of interest to discuss the Hamiltonian for each segment, which are essentially equivalent to the $S = 1/2$ quantum Ising systems with the alternating transverse fields.

2.2. Exact diagonalization of the system

It appears that the ground state of Eq. (1) always lies in the sector with $N_0 = 0$, i.e., with no sites in the $m_j = 0$ state when $D_z \geqslant 0$. Then, for the ground state, there are only two states per site and we can map the Hamiltonian to a spin-1/2 problem. The formal relations for the operator $\vec{S}_j$ of spin-1 are

$$S_j^z \to \sigma_j^z, \qquad S_j^+ S_j^+ \to 2\sigma_j^+, \qquad S_j^- S_j^- \to 2\sigma_j^-,$$
$$S_j^+ S_j^- \to 1 + \sigma_j^z, \qquad S_j^- S_j^+ \to 1 - \sigma_j^z,$$

where the σ_j are Pauli operators. Considering $s_i^z = \frac{1}{2}\sigma_i^z$, we map the Hamiltonian (1) to a spin-1/2 problem

$$h(L) = -\frac{1}{2}J\sum_{j=1}^{L-1}\sigma_j^z\sigma_{j+1}^z - \sum_{j=1}^{L/2} D_x\sigma_{2j}^x, \tag{4a}$$

where the constant $E_0 = -\frac{L}{2}(D_x + D_z)$ is omitted. Let $\Omega_{2j-1} = D_1 = 0$ and $\Omega_{2j} = D_x$ for $j = 1, 2, \ldots, L/2$, above Hamiltonian can be rewritten as follows

$$h(L) = -\frac{1}{2}J\sum_{j=1}^{L-1}\sigma_j^z\sigma_{j+1}^z - \sum_{j=1}^{L}\Omega_j\sigma_j^x, \tag{4b}$$

which is just a spin-1/2 Ising chain with the alternating transverse fields.

According the Ref. [18], the above Hamiltonian of the spin-1/2 Ising chain with the alternating transverse fields can be exactly diagonalized, the entire eigenvalue spectrum and eigenfunctions can be obtained by employing the Jordan–Wigner transformation of the spin operators to spinless fermions [5]: $\sigma_j^- = K_j c_j$, $\sigma_j^+ = c_j^+ K_j^{-1}$, where c_j and c_j^+ are the spinless Fermi operators satisfying the commutation relations: $\{c_i, c_j^+\} = \delta_{ij}$, $\{c_i^+, c_j^+\} = \{c_i, c_j\} = 0$; K_j are kink operators and are self-conjugate, $K_j^{-1} = K_j^+$, which are used to impose the bosonic commutation relation. They can be simply represented as $K_j = \exp[-\pi i\sum_{l=1}^{j-1} c_l^+ c_l]$. The Hamiltonian (4b) is rewritten as

$$H = \sum_{i,j=1}^{L}\left[c_i^+ A_{ij} c_j + \frac{1}{2}\left(c_i^+ B_{ij} c_j^+ - c_i B_{ij} c_j\right)\right] + \frac{L}{2}D_x, \tag{5}$$

where $A_{ij} = -2\Omega_i\delta_{ij} - \frac{1}{2}J\delta_{i+1,j} - \frac{1}{2}J\delta_{i-1,j} = A_{ji}$, $B_{ij} = -\frac{1}{2}J\delta_{i+1,j} + \frac{1}{2}J\delta_{i-1,j} = -B_{ji}$.

Up to this step, the none hole sector is mapped onto the spinless fermionic system where each terms in Eq. (5) are bilinear. We can diagonalize Hamiltonian (5) further by use of the Bogolubov transformation in the following form

$$\eta_k = \sum_{j=1}^{L}\left(g_{kj}c_j + h_{kj}c_j^+\right), \qquad \eta_k^+ = \sum_{j=1}^{L}\left(g_{kj}c_j^+ + h_{kj}c_j\right). \tag{6}$$

Here, k parameterizes the quasi-momentum of the quasi-particle, determined by boundary conditions. For the periodic boundary condition $k_n = \frac{2\pi n}{L}$, $n = -\frac{L}{2}, -\frac{L}{2}+1, \ldots, \frac{L}{2}-1$. η_k and η_k^+ are quasi-particle operators, satisfying the usual fermionic commutation relations $\{\eta_k, \eta_{k'}^+\} = \delta_{k,k'}$.

The real functions g_{kj} and h_{kj} are defined such that the Hamiltonian (5) is diagonal in terms of the quasi-particle operators

$$h(L) = \sum_k \Lambda_k\left(\eta_k^+\eta_k - \frac{1}{2}\right), \tag{7}$$

where the total number of the allowed values of k in the summation is L. This leads to the equation of motion $\{\eta_k, H\} - \Lambda_k\eta_k = 0$.