Ground-State Properties of the Spin-1/2 Heisenberg–Ising Bond Alternating Chain with Dzyaloshinskii–Moriya Interaction

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Ground-state energy is exactly calculated for the spin-1/2 Heisenberg–Ising bond alternating chain with the Dzyaloshinskii–Moriya interaction. Under certain condition, which relates a strength of the Ising, Heisenberg and Dzyaloshinskii–Moriya interactions, the ground-state energy exhibits an interesting nonanalytic behavior accompanied with a gapless excitation spectrum.

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1. Introduction

Quantum spin chains provide an excellent playground for theoretical studies of collective quantum phenomena as they may exhibit numerous exotic ground states and quantum critical points [1]. The spin-1/2 Heisenberg–Ising bond alternating chain, which has been originally invented by Lieb et al. [2] and recently re-examined by Yao et al. [3], represents a valuable example of rigorously solved quantum spin chain. The present work aims to provide a generalization of this simple but nontrivial quantum spin model by taking into account the antisymmetric Dzyaloshinskii–Moriya interaction.

2. Heisenberg–Ising chain

Let us consider a bond alternating chain of $2N$ spins 1/2 with nearest-neighbor antiferromagnetic interactions, which are alternatively of the Heisenberg and Ising type, respectively. The total Hamiltonian of the model under consideration is given by

$$
H = \sum_{n=1}^{N} \left[ J_\text{H}(s_{2n-1}^z s_{2n}^z + s_{2n-1}^y s_{2n}^y + \Delta s_{2n-1}^z s_{2n}^z) + D(s_{2n-1}^x s_{2n}^x - s_{2n-1}^y s_{2n}^y) + 2J_\text{I} s_{2n}^z s_{2n+1}^z \right],
$$

(1)

where the parameter $J_\text{H}(\Delta)$ denotes the XXZ Heisenberg interaction between $2n-1$ and $2n$ spins, $\Delta$ is an anisotropy in this interaction, and the parameter $D$ stands for the $z$ component of the antisymmetric Dzyaloshinskii–Moriya interaction present along the Heisenberg bonds. Furthermore, the term $2J_\text{I}$ denotes the Ising interaction between $2n$ and $2n+1$ spins and the periodic boundary condition $s_{2N+1}^\alpha \equiv s_1^\alpha (\alpha = x, y, z)$ is imposed for convenience.

First, let us eliminate from the Hamiltonian (1) the Dzyaloshinskii–Moriya term after performing a spin coordinate transformation. The spin rotation about the $z$-axis by the specific angle $\tan \phi = D/J_\text{H}$, which is performed at all even sites $2n$ ($n = 1, \ldots, N$),

$$
s_{2n}^x \rightarrow s_{2n}^x \cos \phi + s_{2n}^y \sin \phi,
$$

$$
s_{2n}^y \rightarrow -s_{2n}^x \sin \phi + s_{2n}^y \cos \phi,
$$

ensures a precise mapping equivalence between the Hamiltonian (1) and the Hamiltonian

$$
H = \sum_{n=1}^{N} \left[ \sqrt{J_\text{H}^2 + D^2} (s_{2n-1}^x s_{2n}^x + s_{2n-1}^y s_{2n}^y) + J_\text{H} \Delta s_{2n-1}^z s_{2n}^z + 2J_\text{I} s_{2n}^z s_{2n+1}^z \right].
$$

(2)

From here onward, one may closely follow the rigorous procedure developed in Refs. [2, 3]. According to this, the Hamiltonian (2) is rewritten in terms of raising and lowering operators in the subspace where the ground state is, and subsequently, the Jordan–Wigner transformation is applied to express the relevant spin Hamiltonian as a bilinear form of the Fermi operators. The Fourier and Bogolyubov transformations are finally employed to bring the Hamiltonian relevant for the ground-state properties into the diagonal form

$$
H = -\frac{N}{4} J_\text{H} \Delta + \sum_k A_k \left( \beta_k \beta_k - \frac{1}{2} \right),
$$

(3)

where
$$A_k = \sqrt{\left(\sqrt{J_H^2 + D^2} + J_I\right)^2 - 4\sqrt{J_H^2 + D^2}J_I \cos^2 \frac{k}{2}}. $$

From Eqs. (3) and (4) one easily finds the exact result for the ground-state energy of the antiferromagnetic spin-1/2 Heisenberg–Ising bond alternating chain (1) for $N \rightarrow \infty$:

$$\frac{E_0}{N} = -\frac{1}{4}J_H \Delta - \frac{\sqrt{J_H^2 + D^2} + J_I}{\pi} \text{E}(a), $$

where $\text{E}(a) = \int_0^\frac{\pi}{2} \text{d}\theta \sqrt{1 - a^2 \sin^2 \theta}$ is the complete elliptic integral of the second kind with the modulus $a$,

$$a^2 = \frac{4\sqrt{J_H^2 + D^2}J_I}{\sqrt{J_H^2 + D^2} + J_I} \geq 0. $$

Recall that the complete elliptic integral of the second kind is a nonanalytic function of its modulus for $a^2 = 1 - (a')^2 \approx 1$, i.e., $\text{E}(a) - 1 \approx \ln a'(a')^2$. The condition $a^2 = 1$ holds just if $J_I = \sqrt{J_H^2 + D^2}$ and hence, one may expect nonanalytic behavior of the ground-state energy (5) under this special constraint, which relates a strength of the Ising, Heisenberg and Dzyaloshinskii–Moriya interactions.

Before proceeding to a more detailed discussion of the most interesting results, it is worthy to mention that our exact results correctly reproduce (in an absence of the Dzyaloshinskii–Moriya term) the results previously reported by Lieb et al. [2] for the isotropic version and by Yao et al. [3] for the anisotropic version of the antiferromagnetic spin-1/2 Heisenberg–Ising bond alternating chain. For simplicity, our subsequent analysis will be restricted just to a particular case of the model with the isotropic Heisenberg interaction ($\Delta = 1$), which exhibits all general features notwithstanding this limitation.

3. Results and discussion

In Fig. 1 we depict the elementary excitation energy spectrum $A_k$ calculated from Eq. (4) for two different values of the ratio $J_I/J_H$ and several values of the Dzyaloshinskii–Moriya anisotropy $D/J_H$. Generally, the excitations are gapped with exception of the particular cases that satisfy the condition $J_I = \sqrt{J_H^2 + D^2}$. The gapless excitation spectrum might be consequently found just if $J_I/J_H = 1$, which means that the Ising interaction must be at least twice as large as the Heisenberg one. If $D/J_H = 0$ is assumed, the system has gapless excitation spectrum for $J_I/J_H = 1$ in accordance with the previously published results [2, 3]. Interestingly, the gapless excitation spectrum emerges at higher values of the ratio $J_I/J_H$ regardless of the exchange anisotropy $\Delta$ whenever the Dzyaloshinskii–Moriya anisotropy is raised from zero.

The three-dimensional plot of the ground-state energy (5) is depicted in Fig. 2 as a function of the ratio $J_I/J_H$ between the Ising and Heisenberg interaction, as well as a relative strength of the Dzyaloshinskii–Moriya anisotropy $D/J_H$. Referring to this plot, the ground-state energy monotonically decreases upon strengthening the ratio $J_I/J_H$ and/or the Dzyaloshinskii–Moriya term $D/J_H$. In accordance with this statement, the ground-state energy $E_0/NJ_H = -3/4$ of a system of the isolated Heisenberg dimers, which is achieved in the limit $J_I/J_H \rightarrow 0$ and $D/J_H \rightarrow 0$, represents an upper bound for the ground-state energy. Within the manifold $J_I = \sqrt{J_H^2 + D^2}$, the ground-state energy exhibits a rather striking nonanalytic behavior. Although this weak nonanalytic behavior cannot be seen from Fig. 2, it should manifest itself in higher derivatives of the ground-state energy.

4. Conclusions

In the present work, the ground-state properties of the spin-1/2 Heisenberg–Ising bond alternating chain with the Dzyaloshinskii–Moriya interaction have been investigated using a series of exact (rotation, Jordan–Wigner, Fourier, Bogolyubov) transformations. Exact results for the ground-state energy and elementary excitation spectrum have been examined in relation with a strength of the ratio between the Ising and Heisenberg interaction, as well as the Dzyaloshinskii–Moriya term. The most interesting finding to emerge from our study closely relates
to a remarkable nonanalytic behavior of the ground-state energy, which is accompanied with the gapless excitation spectrum whenever the condition $J_l = \sqrt{J_H^2 + D^2}$ is met.

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