Physica A 453 (2016) 116–130

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Partition function zeros and magnetization plateaus of the spin-1 Ising–Heisenberg diamond chain

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HIGHLIGHTS

- We consider the spin-1 Ising–Heisenberg model on a diamond chain.
- Exact ground-state phase diagrams are derived.
- The existence of the magnetic and quadrupole moments plateaus is shown.
- Distributions of the Yang–Lee and Fisher zeros have been studied.

ARTICLE INFO

Article history:
Received 11 June 2015
Received in revised form 22 December 2015
Available online 17 February 2016

Keywords:
Ising–Heisenberg spin model
Magnetization plateau
Diamond chain
Yang–Lee zeros
Fisher zeros

ABSTRACT

We study the properties of the generalized spin-1 Ising–Heisenberg model on a diamond chain, which can be considered as a theoretical model for the homometallic magnetic complex $[Ni_3(C_4H_2O_4)_2-(\mu_3-OH)_2(H_2O)_4]_n\cdot(2H_2O)_n$. The model possesses a large variety of ground-state phases due to the presence of biquadratic and single-ion anisotropy parameters. Magnetization and quadrupole moment plateaus are observed at one- and two-thirds of the saturation value. The distributions of Yang–Lee and Fisher zeros are studied numerically for a variety of values of the model parameters. The usual value $\sigma=-\frac{1}{2}$ alongside an unusual value $\sigma=-\frac{2}{3}$ is determined for the Yang–Lee edge singularity exponents.

1. Introduction

Physical properties of low-dimensional quantum spin systems have attracted much attention over the last few decades. One class of such systems consists of exactly solvable Ising–Heisenberg models on a diamond chain, which are of current interest for a number of reasons [1–17]. These models can be solved exactly using different mathematical methods and they manifests a wide range of the interesting properties such as the appearance of intermediate plateaus in the magnetization curves, geometric spin frustration, multiple peak structure of the magnetic susceptibility and specific heat. Kikuchi et al. [18] have performed an elegant measurement on the real compound $Cu_3(CO_3)_2(OH)_2$, known as natural azurite, which may be represented as a distorted diamond chain. A considerable number of other studies have been devoted to the investigation of physical properties of natural azurite, both experimentally [19,20] and theoretically [1,9–17].

The synthesis and characterization of the metal–organic magnetic materials are amongst the most challenging topics in modern-day solid-state chemistry. It has been shown that atoms of homometallic magnetic complex $[Ni_3(C_4H_2O_4)_2-(\mu_3-OH)_2(H_2O)_4]_n\cdot(2H_2O)_n$ and molecular compound $[Ni_8(\mu_3-OH)_4(OMe)_2(O_3PR_1)_2(O_2C^tBu)_6(HO_2C^tBu)_8]$ also form

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http://dx.doi.org/10.1016/j.physa.2016.02.047
0378-4371/

a diamond chain or diamond clusters [21,22]. Magnetic-property measurements of compounds indicate the coexistence of both antiferromagnetic and ferromagnetic interactions between the magnetic centers, Ni ions with spin 1. It would be of great interest to investigate theoretically the magnetic properties of such compounds.

Partition function zeros are a powerful tool for the study of phase transitions. Yang and Lee [23] predicted in 1952 that the distribution of the partition function zeros of the system in the complex magnetic-field plane is closely connected with phase transitions. They showed that, in the thermodynamic limit, a phase transition takes place when the distribution of partition function zeros approaches the positive real axis. Furthermore, they demonstrated a circle theorem [24], which states that the partition function zeros of the ferromagnetic Ising model in an arbitrary nonzero external magnetic field are distributed on the unit circle in the complex-fugacity plane. The notion of Yang–Lee zeros was later extended to various physical systems [25–34] and recently has been experimentally observed in Ref. [35], by measuring quantum coherence of a probe spin coupled to an Ising-type spin bath.

Fisher [36] proposed to analyze the existence of phase transitions by studying the distribution of the partition function zeros in the complex temperature plane (Fisher zeros). It was shown that for the two-dimensional square-lattice, whose analytical solution is known since [37], partition function zeros lie on two circles in the complex temperature $v = \tanh(\beta J)$ plane. These circles pinch the real-v axis at $v = \pm(\sqrt{2}-1)$, where $v = \sqrt{2}-1$ ($v = 1-\sqrt{2}$) corresponds to the ferromagnetic (antiferromagnetic) transition point. Since then, Fisher zeros of the partition function have been studied for various physical systems such as spin models [38–41], proteins [42], polymers [43], and flexible polymers [44].

In the present paper we consider the generalized exactly solvable spin-1 Ising–Heisenberg model [7] (including the biquadratic XXZ-interaction term K, the single-ion anisotropy parameters for the Ising and Heisenberg spins and biquadratic Ising interaction term K_1) on a diamond chain. The exact solution of the model is given by means of the transfer-matrix method. The analysis of the ground-state phase diagrams at absolute zero temperature as well as low-temperature magnetic and quadrupole moments is presented. Moreover, the extension of the Yang–Lee circle theorem for the spin-1 Ising–Heisenberg model on the diamond chain is considered.

The rest of the paper is organized as follows. In the next section we define the model and give its exact solution by means of the transfer-matrix method. In Section 3 exact results for the ground-state phases are derived. In Section 4 we present the magnetic and quadrupole-moment properties of the spin-1 Ising–Heisenberg model on a diamond chain. Section 5 is devoted to the investigation of the partition function zeros in the complex magnetic-field plane. The behavior of the partition function zeros in the complex temperature plane is discussed in Section 6. Finally, in the last section summary of the work is given.

2. The model and its exact solution

We consider the spin-1 Ising–Heisenberg model on a diamond chain in the presence of an external magnetic field. The blocks of the diamond chain consist of two Heisenberg spins ($S_{a,i}$ and $S_{b,i}$) which interact with nearest-neighboring Ising spins (μ_i and μ_{i+1}) via an Ising-type interaction (see Fig. 1). The Hamiltonian of the system may be represented as a sum over block Hamiltonians, i.e. $\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}_i$, where

$$\begin{aligned}\mathcal{H}_i = {} & J(S^x_{a,i}S^x_{b,i} + S^y_{a,i}S^y_{b,i} + \Delta S^z_{a,i}S^z_{b,i}) + K(S^x_{a,i}S^x_{b,i} + S^y_{a,i}S^y_{b,i} + \Delta_1 S^z_{a,i}S^z_{b,i})^2 \\ & + J_1\left(S^z_{a,i} + S^z_{b,i}\right)\left(\mu^z_i + \mu^z_{i+1}\right) + D\left[(S^z_{a,i})^2 + (S^z_{b,i})^2\right] + D_1\frac{(\mu^z_i)^2 + (\mu^z_{i+1})^2}{2} \\ & + K_1\left[(S^z_{a,i}\mu^z_i)^2 + (S^z_{b,i}\mu^z_i)^2 + (S^z_{a,i}\mu^z_{i+1})^2 + (S^z_{b,i}\mu^z_{i+1})^2\right] - H_{\mathrm{H}}\left(S^z_{a,i} + S^z_{b,i}\right) - H_{\mathrm{I}}\frac{\mu^z_i + \mu^z_{i+1}}{2}. \end{aligned} \tag{1}$$

In this equation, $S^\alpha_{a,i}$, $S^\alpha_{b,i}$ ($\alpha = x, y, z$) and μ^z_i are the components of Heisenberg and Ising spin-1 operators, J is the bilinear XXZ Heisenberg interaction term, K is the biquadratic XXZ-interaction term parameter, Δ and Δ_1 are anisotropy parameters, J_1 is the interaction parameter between the nearest-neighboring Ising and Heisenberg spins, D (D_1) is the single-ion anisotropy parameter of Heisenberg (Ising) spins and the parameter K_1 is the analogue of a biquadratic Ising interaction term. The last two terms in the Hamiltonian (1) are contributions of a longitudinal external magnetic field interacting with the Heisenberg and Ising spins.

An important element for our calculation is the commutation relation between different block Hamiltonians: $[\mathcal{H}_i, \mathcal{H}_j] = 0$ for $i \neq j$, which will allow us to partially factorize the partition function of the model and represent it as a product of block partition functions

$$Z = \sum_{\mu_i}\prod_{i=1}^{N}\mathrm{Tr}_i e^{-\beta\mathcal{H}_i}, \tag{2}$$

where Tr_i means the trace over the states of Heisenberg spins of the ith block, $\beta = (k_B T)^{-1}$, k_B is Boltzmann's constant and T is the absolute temperature. Hereafter, for simplicity, the Boltzmann's constant is set to unity $k_B = 1$.