Solid State Communications 147 (2008) 494–497

Contents lists available at ScienceDirect

Solid State Communications

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

Magnetization plateaux in the antiferromagnetic Ising chain with single-ion anisotropy

Fabian Litaiff [a], J. Ricardo de Sousa [a,b,*], N.S. Branco [c]

[a] Departamento de Física, Universidade Federal do Amazonas, 3000 Japiim, 69077-000, Manaus-AM, Brazil

[b] Departamento de Física, ICEx, Universidade Federal de Minas Gerais, Av. Antônio Carlos 6627, CP 702, 30123-970, Belo Horizonte-MG, Brazil

[c] Departamento de Física, Universidade Federal de Santa Catarina, 88040-900, Florianópolis-SC, Brazil

ARTICLE INFO

Article history:
Received 10 June 2008
Accepted 26 June 2008 by A.H. MacDonald
Available online 4 July 2008

PACS:
75.10.Hk
75.10.FPg
75.40.Cx
75.50.Ee

Keywords:
A. Antiferromagnetic models
A. One-dimensional systems
D. Magnetic-field effects
D. Magnetization plateaux

ABSTRACT

Two one-dimensional spin-1 antiferromagnetic Ising models with a single-ion anisotropy under external magnetic field at low temperatures are exactly investigated by the transfer-matrix technique. The magnetization per spin (m) is obtained for the two types of models (denoted by model 1 and 2) as an explicit function of the magnetic field (H) and of the anisotropy parameter (D). Model 1 is an extension of the one recently treated by Ohanyan and Ananikian [V.R. Ohanyan, N.S. Ananikian, Phys. Lett. A 307 (2003) 76]: we have generalized their model to the spin-1 case and a single-ion anisotropy term have been included. In the limit of positive (or null) anisotropy ($D \geq 0$) and strong antiferromagnetic coupling ($\alpha = J_A/J_F \geq 3$) the $m \times H$ curves are qualitatively the same as for the spin $S = 1/2$ case, with the presence of only one plateau at $m/m_{sat} = 1/3$. On the other hand, for negative anisotropy ($D < 0$) we observe more plateaux ($m = 1/6$ and $2/3$), which depend on the values of D and α. The second model (model 2) is the same as the one recently studied by Chen et al. [X.Y. Chen, Q. Jiang, W.Z. Shen, C.G. Zhang, J. Mag. Mag. Mat. 262 (2003) 258] using Monte Carlo simulation; here, the model is treated within an exact transfer-matrix framework.

1. Introduction

For some one-dimensional (1D) antiferromagnets at low temperatures, a spin gap has been observed, which is induced by a finite magnetic field. Also a plateaux structure appears in the magnetization process. Experimentally, the magnetization plateaux were observed in high-field measurements of several magnetic materials such as the quasi one-dimensional compounds $SrCu_2O_3$ [1], Y_2BaNiO_5 [2], $Ni(C_2H_8N_2)_2NO_2ClO_4$ (abbreviated NENP) [3,4], and $Cu(NO_3)_2 2.5H_2O$ [5], the triangular antiferromagnets C_6Eu [6], $CsCuCl_3$ [7] and $RbFe(MoO_4)_2$ [8], and the quasi two-dimensional compound, with a Shastry–Sutherland lattice structure, $SrCu_2(BO_3)_2$ [9]. The mechanism for the appearance of these magnetization plateaux in quasi one-dimensional spin chains are *dimerization*, *frustration*, *single-ion anisotropy*, *periodic field* and so on.

From a general view point, Oshikawa et al. [10] concluded that the necessary condition for the magnetization plateaux in spin-S chains is $Q(S - m) =$ integer, where Q is the spatial periodicity of the magnetic ground state and m is the magnetization per site. For some range of the magnetic field H (i.e. $H_1 < H < H_2$), the system ceases responding to its increase and a plateau is formed in the magnetization versus the magnetic field curve. The values of m at which the plateaux appear are sensitive to small changes in the parameters of the model and are not only restricted to integer spin (Haldane conjecture [11]).

In the $S = 1/2$ antiferromagnetic Heisenberg model on a triangular lattice, a magnetization plateau was found at $m/m_{sat} = 1/3$ [6–8,12]. In an $S = 1/2$ trimerized Heisenberg model [13], the plateau appears at $m/m_{sat} = 1/6$. Recently, plateaux at $m/m_{sat} = 1/8$ and $1/4$ have been observed in the $SrCu_2(BO_3)_2$ [9], which has a Shastry–Sutherland lattice structure. However, *irrational* values have not been found, at least so far. Theoretically, various other models with spin $S = 1/2$ have been proposed to describe the magnetization plateaux. One of the first models was introduced by Hida [14], where a Heisenberg chain was considered, with antiferromagnetically coupled ferromagnetic trimers ($p = 3$). The three-dimerized Hamiltonian proposed by Hida to describe the $3CuCl_2.2$ dioxane compound is given by

$$\mathcal{H} = \mathcal{H}^{\text{trim}} + \mathcal{H}^{\text{int}} + \mathcal{H}^{\text{Zeeman}}, \tag{1}$$

with

$$\mathcal{H}^{\text{trim}} = -J_F \sum_i \left(\mathbf{S}_i \cdot \boldsymbol{\tau}_i + \boldsymbol{\tau}_i \cdot \boldsymbol{\sigma}_i\right), \tag{2}$$

* Corresponding author at: Departamento de Física, Universidade Federal do Amazonas, 3000 Japiim, 69077-000, Manaus-AM, Brazil.
E-mail address: jsousa@pq.cnpq.br (J.R. de Sousa).

0038-1098/$ – see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2008.06.037

$$\mathcal{H}^{\text{int}} = J_A \sum_i \boldsymbol{\sigma}_i \cdot \mathbf{S}_{i+1}, \tag{3}$$

and

$$\mathcal{H}^{\text{Zeeman}} = -\mu_B H \sum_i \left(S_i^z + \sigma_i^z + \tau_i^z\right), \tag{4}$$

where J_A and J_F are the antiferromagnetic and ferromagnetic interactions, respectively, $\mathbf{S}_i$, $\boldsymbol{\tau}_i$ and $\boldsymbol{\sigma}_i$ are the $S = 1/2$ spin operators at site i, μ_B is the Bohr magneton and H is the magnetic field. Using exact diagonalization of finite systems, Hida obtained, for J_F comparable to or smaller than J_A, a plateau at $m/m_{\text{sat}} = 1/3$. The plateau mechanism was considered to be a purely quantum phenomenon, where the concepts of magnetic quasiparticles and strong quantum fluctuations are regarded to be of major importance for understanding the process. On the other hand, Ohanyan and Ananikian [15] have recently studied the Hida model by using the transfer-matrix technique, replacing the spin operators ($\mathbf{S}_i$, $\boldsymbol{\tau}_i$ and $\boldsymbol{\sigma}_i$) by Ising variables (S_i^z, σ_i^z, τ_i^z). It was shown that, for this classical model and for $T = 0$ (ground state) and $J_A \geq 3J_F$ (strong antiferromagnetic coupling), a magnetization curve with plateau at $m/m_{\text{sat}} = 1/3$ is observed, indicating that the appearance of plateaux is not a quantum manifestation, but may be caused by the stability of spatially modulated spin structures.

Another model which presents magnetization plateaux is the one-dimensional spin-1 antiferromagnetic Heisenberg with single-ion anisotropy [16]. This model is described by the following Hamiltonian:

$$\mathcal{H} = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mu_B H \sum_i S_i^z + D \sum_i \left(S_i^z\right)^2, \tag{5}$$

where D is the single-ion anisotropy. For $D = 0$, the ground state is a singlet and the lowest excitation is a triplet (Haldane conjecture [11]); increasing D, the triplet splits into a higher-energy singlet and a lower-lying doublet, with the Haldane gap for $D = 0$, $\Delta(0)$, splitting into two gaps, as observed in neutron scattering of NENP [17]. The Haldane gap for general D, $\Delta(D)$, presents two different behaviors: for $D > D_c = J$, it increases with D, while for $D < D_c$ $\Delta(D)$ decreases as D increases.

Recently, spin $S \geq 1$ Ising antiferromagnetic chains with single-ion anisotropy have been studied by using classical Monte Carlo simulation [18] where the presence of $2S + 1$ plateaux for $D > 0$ was observed. Essentially, these classical models are obtained by replacing the spin operators ($\mathbf{S}_i$) by Ising variables (S_i^z) in Hamiltonian (5). From a theoretical point of view, the model studied by Chen, et al. [18] represents the 1D antiferromagnetic Blume–Capel model [19]; two different critical behaviors were observed, which depend on the anisotropy parameter D ($D < D_c$ and $D > D_c$, where $D_c = J$).

The purpose of this work is to obtain exact results for two classical models with spin $S = 1$ and in the presence of a single-ion anisotropy. In Section 2 the 1D models are presented and exactly solved by the transfer-matrix technique. The magnetization plateaux and ground-state phase diagrams are discussed in Section 3. Finally, the last section is devoted to conclusions.

2. Models and formalism

The transfer-matrix technique was proposed years ago by Kramers and Wannier [20,21], and it formed the basis for Onsager's solution [22] of the two-dimensional Ising model. In this section, we use this technique to obtain exact results for two one-dimensional models, in order to analyze the magnetization plateau mechanism.

2.1. Model 1: Three-dimerized chain

The first model we study is described by the following Hamiltonian (see Fig. 1):

$$\begin{aligned}\mathcal{H}_1 = &-J_F \sum_i \left(S_i^z \cdot \tau_i^z + \sigma_i^z \cdot \tau_i^z - \alpha \sigma_i^z \cdot S_{i+1}^z\right) \\ &- \mu_B H \sum_i \left(S_i^z + \tau_i^z + \sigma_i^z\right) \\ &- D \sum_i \left[\left(S_i^z\right)^2 + \left(\tau_i^z\right)^2 + \left(\sigma_i^z\right)^2\right],\end{aligned} \tag{6}$$

where $\alpha = J_A/J_F$ and the spin variables S_i^z, τ_i^z and σ_i^z can assume the values -1, 0, 1. The above Hamiltonian represents a nonuniform spin system in which ferromagnetic trimers composed of $S = 1$ spins (S_i^z, τ_i^z and σ_i^z) are coupled antiferromagnetically in one dimension, in the presence of a magnetic field (H) and single-ion anisotropy (D). In the limit $\alpha \to 0$ (strong intratrimer ferromagnetic interaction), the variables S_i^z, τ_i^z and σ_i^z form a single spin ξ_i with magnitude 3. Thus, the system can be approximated by a spin $S = 3$ antiferromagnetic Blume–Capel chain.

The transfer-matrix technique is based on the calculation of the eigenvalues $\{\lambda_i\}$, determined from the solution of the secular equation

$$\det(W_1 - \lambda I) = 0, \tag{7}$$

where I is the 3×3 identity matrix and W_1 the Wannier matrix, with the elements defined by

$$W_1(S, S') = \sum_{\sigma,\tau=0,\pm1} \exp[a(\tau)S + dS^2 + b(\sigma)S' + c(\tau, \sigma)], \tag{8}$$

with

$$a(\tau) = \beta J_F \tau + \beta \mu_B H, \tag{9}$$

$$b(\sigma) = -\alpha \beta J_F \sigma, \tag{10}$$

$$c(\tau, \sigma) = \beta J_F \sigma \tau + \beta \mu_B H(\tau + \sigma) + \beta D(\tau^2 + \sigma^2), \tag{11}$$

and

$$d = \beta D, \tag{12}$$

where $S, S' = 0, \pm 1$.

Using properties of the matrix trace, the partition function $Z = Tr(W^N)$ can be written as a sum of the Nth power of the eigenvalues $\{\lambda_i\}$ obtained from Eq. (7), i.e.,

$$Z = \sum_{i=1}^{3} \lambda_i^N. \tag{13}$$

In the thermodynamic limit ($N \to \infty$), the free energy, magnetization, magnetic susceptibility and specific heat (per atom) are expressed in terms of maximum eigenvalue $\lambda_{\max}$, respectively, as

$$f = \frac{-T}{3} \ln \lambda_{\max}, \tag{14}$$

$$m = \frac{T}{3\lambda_{\max}} \frac{\partial \lambda_{\max}}{\partial H}, \tag{15}$$

$$\chi = \frac{\partial m}{\partial H} = \frac{T}{3} \frac{\partial}{\partial H} \left(\frac{1}{\lambda_{\max}} \frac{\partial \lambda_{\max}}{\partial H}\right), \tag{16}$$

and

$$c = \frac{2T}{3\lambda_{\max}} \frac{\partial \lambda_{\max}}{\partial T} + \frac{T^2}{3} \frac{\partial}{\partial T} \left(\frac{1}{\lambda_{\max}} \frac{\partial \lambda_{\max}}{\partial T}\right), \tag{17}$$