Journal of Magnetism and Magnetic Materials 324 (2012) 2429–2433

Contents lists available at SciVerse ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Critical behavior of an anisotropic Ising antiferromagnet in both external longitudinal and transverse fields

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ARTICLE INFO

Article history:
Received 4 November 2011
Received in revised form
8 February 2012
Available online 14 March 2012

Keywords:
Effective-field theory
Phase diagram
Ising model

ABSTRACT

In this paper we study the critical behavior of a two-sublattice Ising model on an anisotropic square lattice in both uniform longitudinal (H) and transverse (Ω) fields by using the effective-field theory. The model consists of ferromagnetic interaction J_x in the x direction and antiferromagnetic interaction J_y in the y direction in the presence of the H and Ω fields. We obtain the phase diagrams in the $H-T$ and $\Omega-T$ planes changing values of the Ω and H parameters, respectively for fixed value at $\lambda = J_x/J_y = 1$. At null temperature, the ground state phase diagram in the $\Omega-H$ plane for several values of λ parameter is analyzed. In the particular case of $\lambda = 1$ we compare our results with mean-field theory (MFT) and was not observed reentrant behavior around of the critical field $H_c/J_y = 2.0$ for $\Omega = 0$ by using EFT.

1. Introduction

The effect of transverse magnetic field on the low-dimensional spin systems has recently been attracted much interest from experimental and theoretical points of view. The observations [1] on the quasi-one-dimensional spin 1/2 antiferromagnet Cs_2CoCl_4 are a realization of the effect of a transverse field on the low-energy behavior of a quantum model. This shows a quantum phase transition from the spin-flop phase (ordered antiferromagnetically in the y direction) at the low magnetic field to a paramagnet phase for high field.

The pure transverse Ising model (TIM) has been used to describe a variety of physical systems, for example, strongly anisotropic materials in a transverse field [2] and in cooperative Jahn–Teller systems [3]. It was originally introduced by de Gennes [4] as a pseudospin model for hydrogen-bonded ferroelectric such as the KH_2PO_4 type [5,6]. From the theoretical point of view, the transverse Ising model (TIM) has been investigated by a variety of techniques such as renormalization group (RG) method [7], effective field theory (EFT) [8–10], cluster variation method (CVM) [11], mean field theory (MFT) [12], pair approximation (PA) [13] and Monte Carlo (MC) simulations [14]. In the previous works mentioned above, the authors focused attention on the critical behavior of the phase diagram, where has not been considering the antiferromagnetic system.

However, there are a few studies in the literature that include the longitudinal field as well as the transverse field interactions in the Ising antiferromagnet. Recently, a study of the effect of both the transverse field (Ω) and the longitudinal field (H) on the Ising antiferromagnet has shown that the TIM model presents a rich variety of critical phenomena. For example, Neto and de Sousa [15] have studied, by using EFT, the TIM antiferromagnet on two-dimensional lattices [honeycomb ($z=3$) and square ($z=4$)] and discussed the possible existence of a reentrant behavior obtained by MFT at which the phase transition changes from second-order in two critical temperatures around $H = H_c(\Omega = 0) = zJ$ critical value. By using the MFT technique, Geng and Wei [16,17] have investigated the influence of the mixed transverse and longitudinal fields on the phase diagrams of an Ising metamagnet. Similarly, Miao et al. [18] have studied this quantum model on a honeycomb lattice within the framework of the EFT with correlations. In these studies, the authors have reported the observation of reentrant and multicritical behavior on the system. The critical behavior of the TIM in one-dimensional has already been established by exact results [19]. The quantum TIM antiferromagnet is among the simplest conceivable classes of quantum models in statistical mechanics to study quantum phase transition [20,21]. From a theoretical point of view, ground-state phase diagram of metamagnetic systems have been studied [15,16,18] by using several methods.

In the present paper, we will investigate the phase transitions in the $H-T$ and $\Omega-T$ plane on the anisotropic Ising model in both

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0304-8853/$ - see front matter © 2012 Published by Elsevier B.V.
doi:10.1016/j.jmmm.2012.02.039

external longitudinal and transverse field by using the effective field theory (EFT) in finite cluster. Recently, this quantum model with a longitudinal magnetic field was treated numerically [22,23] and the ground state phase diagram in the $H-\Omega$ plane was studied for the one-dimensional transverse quantum spin-1/2 Heisenberg model. Also we extend the study of the TIM antiferromagnet in both external longitudinal and transverse fields on an anisotropic square lattice within the framework of the EFT approach in cluster with $N=1$ spin. The EFT included correlations through the use of the Van der Waerden identities and provided results which are much superior than the mean field theory (MFT). Our purpose is to investigate the ground state and finite temperature phase diagrams. The paper is organized as follows: in Section 2, we present the model and the relevant expressions in the EFT approach are derived; in Section 3, numerical results and discussions are given. Finally, the last section is devoted to conclusions.

2. Model and formalism

The model to be studied is the nearest-neighbor (nn) Ising antiferromagnetic in a mixed transverse and longitudinal field magnetic divided into two equivalent interpenetrating sublattices A and B, which is described by following Hamiltonian

$$\mathcal{H} = -J_x\sum_{i,\vec{\delta}_x}\sigma_i^z\sigma^z_{i+\vec{\delta}_x} + J_y\sum_{i,\vec{\delta}_y}\sigma_i^z\sigma^z_{i+\vec{\delta}_y} - H\sum_i\sigma_i^z - \Omega\sum_i\sigma_i^x, \quad (1)$$

where σ_i^μ are the $\mu(=x,y,z)$ components spin-1/2 Pauli operator at site i, $J_x(J_y)$ is the exchange coupling along the $x(y)$ axis, $\delta_x(\delta_y)$ denotes the nearest-neighbor vector along the $x(y)$ axis, H is the longitudinal magnetic field, Ω is the transverse magnetic field and $\lambda = J_x/J_y$ is the ratio between ferromagnetic and antiferromagnetic interactions. Since σ_i^x and σ_i^z do not commute, a nonzero field, Ω, transverse to the Ising direction, causes quantum tunneling between the spin-up and spin-down eigenstates of σ_i^z, hence causing quantum spin fluctuations. These fluctuations decrease the critical temperature T_c at which the spins develop long-range order. In the simplest scenario, where $J_x = -J_y = J > 0$, the ordered phase is ferromagnetic. At a critical field Ω_c, T_c vanishes, and a quantum phase transition between a long-range-ordered ferromagnetic phase and a quantum paramagnet state occur. To the best of our knowledge, the model (1) with transverse field has not yet been examined in the literature. The particular case of $\Omega = 0$ (classical model) has been recently studied by Neto et al. [24], thus, in this work we generalize it to include quantum effects.

The TIM is here generalized by considering competing ferromagnetic ($J_{ij} = J_x$) and antiferromagnetic ($J_{ij} = -J_y$) fixed couplings along the x- and y-axis, respectively. The ground-state of the model (1) is characterized by a parallel spin orientation in horizontal direction and an antiparallel spin orientation of a parallel spin orientation of nearest-neighbors in vertical direction and so it exhibits Néel order within the initial sublattices A and B (see Fig. 1), that is denoted by the superantiferromagnetic (SAF) state.

The model is exactly soluble for the $H = \Omega = 0$ limits, and the critical temperature is obtained by solving the following equation:

$$\sinh\left(\frac{2J_x}{k_BT_N}\right)\sinh\left(\frac{2J_y}{k_BT_N}\right) = 1, \quad (2)$$

in the particular case $J_x = J_y = J$ we have the known exact value $k_BT_N/J = 2/\ln(1+\sqrt{2})$.

In particular, at low fields and temperatures the model (1) presents a superantiferromagnetic (SAF) phase. For null transverse field, when longitudinal field's intensities increase the transition temperature decreases, where at $T=0$ (ground-state) a second-order transition occurs at $H_c = 2J_y$.

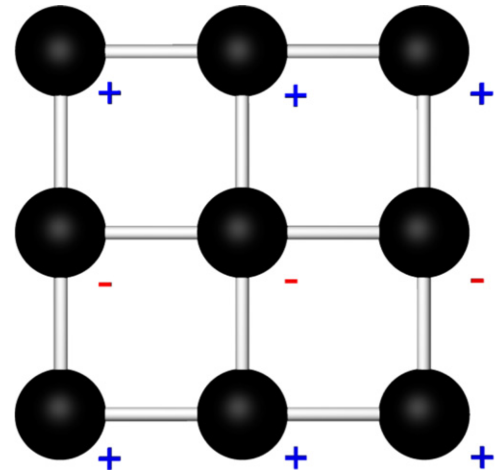

Fig. 1. Ground state of the quantum superantiferromagnetic Ising on an anisotropic square lattice described by the Hamiltonian in Eq. (1).

As a starting point, the averages of a general function involving spin operator components $O(n)$ are obtained by [25]

$$\langle \mathcal{O}(n)\rangle = \left\langle \frac{\mathrm{Tr}_{\{n\}} O(n)\exp(-\beta\mathcal{H})}{\mathrm{Tr}_{\{n\}}\exp(-\beta\mathcal{H})}\right\rangle, \quad (3)$$

where the partial trace $\mathrm{Tr}_{\{n\}}$ is taken over the set $\{n\}$ of spin variables (finite cluster) specified by the multispin Hamiltonian $H_{\{n\}}$ and $\langle\cdots\rangle$ indicates the usual canonical thermal average.

In order to treat the model (1) by the EFT approach, we consider a simple cluster on a lattice consisting of a central spin and z perimeter spins being the nearest-neighbors of the central one. The nearest-neighbor spins are substituted by an effective field produced by the outer spins, which can be determined by the condition that the thermal average of the central spin is equal to that of its nearest-neighbor ones. The Hamiltonian for this cluster is given by

$$\mathcal{H}_{1A} = \left(-J_x\sum_{\vec{\delta}_x}\sigma^z_{(i+\vec{\delta}_x)A} + J_y\sum_{\vec{\delta}_y}\sigma^z_{(i+\vec{\delta}_y)B} - H\right)\sigma^z_{1A} - \Omega\sigma^x_{1A}, \quad (4)$$

where A and B denote the sublattices.

Using the Hamiltonian (4) in the approximate Callen–Suzuki relation, Eq. (3), we obtain the average magnetizations in sublattice A, $m_A = \langle\sigma^z_{1A}\rangle$, that is given by

$$m_A = \left\langle \frac{H + a_{1A} - a_{1B}}{\sqrt{(H + a_{1A} - a_{1B})^2 + \Omega^2}}\tanh\left(\beta\sqrt{(H + a_{1A} - a_{1B})^2 + \Omega^2}\right)\right\rangle, \quad (5)$$

where $a_{1A} = J_x\sum_{\vec{\delta}_x}^z\sigma^z_{(1+\vec{\delta}_x)B}$ and $a_{1B} = J_y\sum_{\vec{\delta}_y}^z\sigma^z_{(1+\vec{\delta}_y)A}$.

Now using the identity $\exp(\alpha D_x + bD_y)F(x,y) = F(x+y+a+b)$ (where $D_\mu = \partial/\partial\mu$ is the differential operator) and the Van der Waerden relation for the two-state spin system, i.e., $\exp(a\sigma_i^z) = \cosh(a) + \sigma_i^z\sinh(a)$), Eq. (5) can be rewritten as

$$m_A = \left\langle \prod_{\vec{\delta}_x}^{2}(\alpha_x + \sigma^z_{(1+\vec{\delta}_x)A}\beta_x)\prod_{\vec{\delta}_y}^{2}(\alpha_y - \sigma^z_{(1+\vec{\delta}_y)B}\beta_y)\right\rangle F(x,y)\Bigg|_{x=y=0}, \quad (6)$$