



Magnetic properties of the mixed spin- $\frac{3}{2}$ and spin- $\frac{1}{2}$ anisotropic Heisenberg model

A. Bobák*, Z. Fecková, M. Žukovič

Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovak Republic

ARTICLE INFO

Article history:

Received 7 September 2010

Received in revised form

22 October 2010

Available online 10 November 2010

Keywords:

Oguchi approximation

Mixed-spin Heisenberg model

Single-ion anisotropy

Magnetic properties

ABSTRACT

The effects of both an exchange anisotropy and a single-ion anisotropy on the phase diagram and magnetization curves of the ferromagnetic mixed spin- $\frac{3}{2}$ and spin- $\frac{1}{2}$ Heisenberg model are investigated by the use of an Oguchi approximation. Although the theory is developed for lattices with general coordination number z , we treat in detail numerically the model on the simple cubic lattice ($z=6$). In particular, some outstanding features are found in the ground-state behaviours of sublattice and total magnetizations. The origin and nature of the ordered phase in the quantum mixed-spin system at the low temperature region are also discussed.

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1. Introduction

In the past years there has been considerable interest in the theoretical study on the magnetic properties of two sublattice mixed Heisenberg spin systems because they have been proposed as possible models to describe a certain type of molecular-based magnetic materials studied experimentally (see, e.g. [1–3]). These materials are usually quasi-one- or two-dimensional and contain two different translational-metal magnetic ions of different spin values, which are alternatively distributed on the lattice. For these systems, the Hamiltonians involved are relatively simple and the low dimensionality often allows very accurate numerical treatments (see, e.g. [4] and references therein). Indeed, there have been many interesting works dealing with the mixed-spin quantum Heisenberg model without and with anisotropy in one- [5–14] and two-dimensional [15–21] systems.

Although the majority of studies have focused on the low-dimensional systems, the three-dimensional mixed-spin quantum Heisenberg model are not without interest. Indeed, there have been earlier theoretical studies which focused on the critical temperature dependence on the anisotropy of the spins by the use of the pair model approximation [22–25] and the Green function theory [26,27]. However, apart from indications of the second-order transition lines (including the tricritical points in Ref. [25]), these works do not provide any insight on the origin and nature of ordered phases in the quantum alternating spin system which can be induced by the single-ion anisotropy at the low temperature

region. On the other hand, in a recent paper [28], it has been already pointed out for the mixed spin-1 and spin- $\frac{1}{2}$ anisotropic Heisenberg model that the quantum fluctuations may induce new magnetic properties different from those of the classical mixed-spin Ising models. Therefore, it is interesting now to extend the previous study to a mixed-spin anisotropic Heisenberg model with half-odd-integer spins only to clarify whether or not the same theory predicts different qualitative features of the phase diagrams for the systems with different spin values. Namely, we focus our attention on the phase diagram topology of the mixed spin- $\frac{3}{2}$ and spin- $\frac{1}{2}$ anisotropic Heisenberg model by using of the Oguchi pair approximation [29,30], which was also applied to study the magnetic properties of the mixed-spin anisotropic Heisenberg model in Ref. [28].

2. Formulation

The Hamiltonian of the mixed spin- $\frac{1}{2}$ and spin- $\frac{3}{2}$ anisotropic Heisenberg model in a zero magnetic field is given by

$$\hat{H} = -J \sum_{\langle ij \rangle} [(1-\Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D \sum_{i \in A} (\hat{S}_{iA}^z)^2, \quad (1)$$

where J is the nearest-neighbour exchange interaction, Δ is the exchange anisotropy parameter, $\hat{S}_{iA}^\alpha$ and $\hat{S}_{jB}^\alpha$ ($\alpha = x, y, z$) are components of the spin $S_A = \frac{3}{2}$ and $S_B = \frac{1}{2}$ operators on sublattices A and B , respectively, and D is the single-ion anisotropy field strength acting on sublattice A . Here, we shall restrict ourselves to the case where the exchange interaction J is ferromagnetic (i.e. $J > 0$ and $0 \leq \Delta \leq 1$).

* Corresponding author. Fax: +421 55 6222124.
E-mail address: andrej.bobak@upjs.sk (A. Bobák).

Thus $\Delta = 0$ and 1 correspond to the isotropic Heisenberg and Ising models, respectively.

According to the Oguchi approximative procedure [29,30], the pair-spin Hamiltonian, associated to a two spin-cluster, obtained from Eq. (1) is given by

$$\hat{H}_{ij} = -J[(1-\Delta)(\hat{S}_{iA}^x \hat{S}_{jB}^x + \hat{S}_{iA}^y \hat{S}_{jB}^y) + \hat{S}_{iA}^z \hat{S}_{jB}^z] - D(\hat{S}_{iA}^z)^2 - (h_i \hat{S}_{iA}^z + h_j \hat{S}_{jB}^z), \quad (2)$$

with

$$h_i = J(z-1)m_B, \quad h_j = J(z-1)m_A, \quad (3)$$

where z is the number of nearest neighbouring spins and the sublattice magnetizations m_A and m_B are the thermal averages of $\hat{S}_{iA}^z$ and $\hat{S}_{jB}^z$, respectively, along a fixed z -axis direction in space, i.e., $m_A = \langle \hat{S}_{iA}^z \rangle$ and $m_B = \langle \hat{S}_{jB}^z \rangle$. Therefore, within this approach, the transverse magnetizations to the z -axis direction are equal to zero.

In the representation of the direct product of $\hat{S}_{iA}^z$ and $\hat{S}_{jB}^z$, the Hamiltonian (2) can be written in the form of 8×8 matrix. Then by solving the eigenvalue equation,

$$\hat{H}_{ij}|\psi_n\rangle = E_n|\psi_n\rangle \quad (n = 1, 2, \dots, 8) \quad (4)$$

we obtain the energy levels

$$\begin{aligned} E_1 &= H_{11}, \quad E_2 = \frac{1}{2}(H_{22} + H_{33} + \omega_{23}), \quad E_3 = \frac{1}{2}(H_{22} + H_{33} - \omega_{23}), \\ E_4 &= \frac{1}{2}(H_{44} + H_{55} + \omega_{45}), \quad E_5 = \frac{1}{2}(H_{44} + H_{55} - \omega_{45}), \\ E_6 &= \frac{1}{2}(H_{66} + H_{77} + \omega_{67}), \quad E_7 = \frac{1}{2}(H_{66} + H_{77} - \omega_{67}), \quad E_8 = H_{88}, \end{aligned} \quad (5)$$

where

$$H_{11} = -\frac{3}{4}J - \frac{9}{4}D - \frac{3}{2}h_i - \frac{1}{2}h_j, \quad H_{22} = \frac{3}{4}J - \frac{9}{4}D - \frac{3}{2}h_i + \frac{1}{2}h_j,$$

$$H_{33} = -\frac{1}{4}J - \frac{1}{4}D - \frac{1}{2}h_i - \frac{1}{2}h_j, \quad H_{44} = \frac{1}{4}J - \frac{1}{4}D - \frac{1}{2}h_i + \frac{1}{2}h_j,$$

$$H_{55} = \frac{1}{4}J - \frac{1}{4}D + \frac{1}{2}h_i - \frac{1}{2}h_j, \quad H_{66} = -\frac{1}{4}J - \frac{1}{4}D + \frac{1}{2}h_i + \frac{1}{2}h_j,$$

$$H_{77} = \frac{3}{4}J - \frac{9}{4}D + \frac{3}{2}h_i - \frac{1}{2}h_j, \quad H_{88} = -\frac{3}{4}J - \frac{9}{4}D + \frac{3}{2}h_i + \frac{1}{2}h_j,$$

$$H_{23} = H_{67} = -\frac{\sqrt{3}}{2}J(1-\Delta), \quad H_{45} = -J(1-\Delta), \quad (6)$$

with

$$\omega_{23} = \sqrt{(H_{22} - H_{33})^2 + 4H_{23}^2}, \quad (7)$$

$$\omega_{45} = \sqrt{(H_{44} - H_{55})^2 + 4H_{45}^2}, \quad (8)$$

$$\omega_{67} = \sqrt{(H_{66} - H_{77})^2 + 4H_{67}^2}, \quad (9)$$

and the corresponding eigenvectors are given by

$$\begin{aligned} |\psi_1\rangle &= |\varphi_1\rangle \equiv |\frac{3}{2}, +\frac{3}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_2\rangle &= a|\varphi_2\rangle + b|\varphi_3\rangle \equiv a|\frac{3}{2}, +\frac{3}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j + b|\frac{3}{2}, +\frac{1}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_3\rangle &= -b|\varphi_2\rangle + a|\varphi_3\rangle \equiv -b|\frac{3}{2}, +\frac{3}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j + a|\frac{3}{2}, +\frac{1}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_4\rangle &= c|\varphi_4\rangle + d|\varphi_5\rangle \equiv c|\frac{3}{2}, +\frac{1}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j + d|\frac{3}{2}, -\frac{1}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_5\rangle &= -d|\varphi_4\rangle + c|\varphi_5\rangle \equiv -d|\frac{3}{2}, +\frac{1}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j + c|\frac{3}{2}, -\frac{1}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_6\rangle &= e|\varphi_6\rangle + f|\varphi_7\rangle \equiv e|\frac{3}{2}, -\frac{1}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j + f|\frac{3}{2}, -\frac{3}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_7\rangle &= -f|\varphi_6\rangle + e|\varphi_7\rangle \equiv -f|\frac{3}{2}, -\frac{1}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j + e|\frac{3}{2}, -\frac{3}{2}\rangle_i |\frac{1}{2}, +\frac{1}{2}\rangle_j, \\ |\psi_8\rangle &= |\varphi_8\rangle \equiv |\frac{3}{2}, -\frac{3}{2}\rangle_i |\frac{1}{2}, -\frac{1}{2}\rangle_j, \end{aligned} \quad (10)$$

where

$$\begin{aligned} a &= \frac{1}{\sqrt{1 + \frac{1}{4H_{23}^2}(H_{22} - H_{33} - \omega_{23})^2}}, \\ b &= -\frac{\frac{1}{2H_{23}}(H_{22} - H_{33} - \omega_{23})}{\sqrt{1 + \frac{1}{4H_{23}^2}(H_{22} - H_{33} - \omega_{23})^2}}, \\ c &= \frac{1}{\sqrt{1 + \frac{1}{4H_{45}^2}(H_{44} - H_{55} - \omega_{45})^2}}, \\ d &= -\frac{\frac{1}{2H_{45}}(H_{44} - H_{55} - \omega_{45})}{\sqrt{1 + \frac{1}{4H_{45}^2}(H_{44} - H_{55} - \omega_{45})^2}}, \\ e &= \frac{1}{\sqrt{1 + \frac{1}{4H_{67}^2}(H_{66} - H_{77} - \omega_{67})^2}}, \\ f &= -\frac{\frac{1}{2H_{67}}(H_{66} - H_{77} - \omega_{67})}{\sqrt{1 + \frac{1}{4H_{67}^2}(H_{66} - H_{77} - \omega_{67})^2}}. \end{aligned} \quad (11)$$

For the Ising limit, i.e., $\Delta = 1$, we have $H_{23} = H_{45} = H_{67} = 0$ and $a = c = e = 1$, $b = d = f = 0$. In this case, the eigenvectors (10) reduce to

$$|\psi_k\rangle = |\varphi_k\rangle \quad (k = 1, 2, \dots, 8). \quad (12)$$

With the eigenvalues (5), the partition function $Z = \text{Tr}_{ij}[\exp(-\beta \hat{H}_{ij})]$ can be written as

$$\begin{aligned} Z &= \exp(-\beta H_{11}) + \exp(-\beta H_{88}) \\ &\quad + 2\exp\left[-\frac{\beta}{2}(H_{22} + H_{33})\right] \cosh\left(\frac{\beta \omega_{23}}{2}\right) \\ &\quad + 2\exp\left[-\frac{\beta}{2}(H_{44} + H_{55})\right] \cosh\left(\frac{\beta \omega_{45}}{2}\right) \\ &\quad + 2\exp\left[-\frac{\beta}{2}(H_{66} + H_{77})\right] \cosh\left(\frac{\beta \omega_{67}}{2}\right), \end{aligned} \quad (13)$$

where $\beta = 1/k_B T$. Then the sublattice magnetizations per site m_A and m_B in the Oguchi approximation are given by

$$\begin{aligned} m_A &= \frac{1}{Z} \frac{\partial Z}{\partial (\beta h_i)} = \frac{1}{Z} \left\{ \frac{3}{2} [\exp(-\beta H_{11}) - \exp(-\beta H_{88})] \right. \\ &\quad + \exp\left[-\frac{\beta}{2}(H_{22} + H_{33})\right] \left[2\cosh\left(\frac{\beta \omega_{23}}{2}\right) - \frac{H_{22} - H_{33}}{\omega_{23}} \sinh\left(\frac{\beta \omega_{23}}{2}\right) \right] \\ &\quad - \frac{H_{44} - H_{55}}{\omega_{45}} \exp\left[-\frac{\beta}{2}(H_{44} + H_{55})\right] \sinh\left(\frac{\beta \omega_{45}}{2}\right) \\ &\quad \left. - \exp\left[-\frac{\beta}{2}(H_{66} + H_{77})\right] \left[2\cosh\left(\frac{\beta \omega_{67}}{2}\right) + \frac{H_{66} - H_{77}}{\omega_{67}} \sinh\left(\frac{\beta \omega_{67}}{2}\right) \right] \right\} \end{aligned} \quad (14)$$

and

$$\begin{aligned} m_B &= \frac{1}{Z} \frac{\partial Z}{\partial (\beta h_j)} = \frac{1}{Z} \left\{ \frac{1}{2} [\exp(-\beta H_{11}) - \exp(-\beta H_{88})] \right. \\ &\quad + \frac{H_{22} - H_{33}}{\omega_{23}} \exp\left[-\frac{\beta}{2}(H_{22} + H_{33})\right] \sinh\left(\frac{\beta \omega_{23}}{2}\right) \end{aligned}$$

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