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Phase diagram and tricritical behavior of the spin-1 Heisenberg model with Dzyaloshinskii–Moriya interactions

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Abstract

Using the two-spin cluster mean-field method, the spin-1 Heisenberg model with Dzyaloshinskii–Moriya (DM) interactions is studied for the simple cubic lattice. For the case of the DM vector coupling $\vec{D} = D\hat{z}$ (D is the DM interaction parameter and $\hat{z}$ is the unit vector of the z-axis direction), the phase diagram of this system and the thermal behavior of the magnetization are obtained, and it is found that the system exhibits the tricritical point. The critical behavior of the system may be interpreted as a result of a competition between the exchange interaction and the DM interaction.

Keywords: Spin-1 Heisenberg model; Dzyaloshinskii–Moriya interaction; Phase diagram; Tricritical point

1. Introduction

The critical properties of quantum magnetic systems have been subjects of intense research [1]. The spin-1 Heisenberg Hamiltonian deserves special attention since it provides a model for many magnetic materials. In recent years, there have been many interesting works dealing with the spin-1 Heisenberg model. For instance, Sólyom and Timonen transformed the spin-1 Heisenberg chain to the one-dimensional fermion gas and obtained phase diagrams of the fermion system [2], and Böhm et al. calculated the coefficients of the short-time expansion of the spin-pair correlations in one-dimensional spin model [3]. Besides, the ground-state properties of the spin-1 Heisenberg ferromagnet with an arbitrary crystal-field potential have been studied using the linked-cluster series expansion [4].

On the other hand, the Heisenberg model with anisotropy has been attracting much attention since various types of anisotropy have a profound influence on the properties of the systems. There are many different ways to introduce anisotropies in the Heisenberg model and an important type of anisotropic interaction is the Dzyaloshinskii–Moriya (DM) interaction [5,6], which is the antisymmetric spin coupling. The DM interaction plays an important role in describing certain class of insulators [7,8], in studying spin glasses [9–12] and also in explaining the electron paramagnetic resonance [13–15]. The Heisenberg models with DM interactions have

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been intensively studied over past years. Cordeiro et al. have obtained the phase diagram and critical exponents of a spin-$\frac{1}{2}$ Heisenberg model with DM interactions by using the renormalization group technique [16]. Subsequently, the phase diagram of this system was also obtained within a two-spin cluster version of mean-field technique [17], as well as within the framework of a new correlated effective-field theory [18]. In Refs. [17,18], the tricritical point (TCP) of this system was found, which had improperly been overlooked in all previous calculations. The tricritical behavior is a very important critical phenomenon, so there has been increasing interest in the study of the behavior [19–23]. In Ref. [20], it was observed that the TCP of antiferromagnetic La_2CuO_4 including the DM interaction was close to the Néel point. Recently, the effects of the DM interaction on the stability of the Néel phase and the energy gap for XXZ Heisenberg model have been studied using the linear spin-wave theory [24]. Pires has investigated the spin-$\frac{1}{2}$ alternating Heisenberg model with DM interactions in a fermion representation and calculated the ground state energy, the low-lying excitations and static nearest-neighbors correlation functions in the $T = 0$ limit [25]. In addition, by the density matrix renormalization group, the physical effects of the DM interaction in copper benzoate were found to produce a gap in the spin excitations [26].

In this paper, the effects of the DM interaction on properties of the spin-1 Heisenberg model are investigated systemically within the framework of the two-spin cluster mean-field method, and it is found that the system exhibits the TCP. The outline of the remainder of this paper is as follows. In Section 2, we give the formulation of this problem. Section 3 is the numerical results and discussions, and Section 4 is the conclusion.

2. Formulation

Let us describe the spin-1 Heisenberg model with DM interactions on the simple cubic lattice. The Hamiltonian is described as

$$H = -J\sum_{\langle i,j\rangle}[(1-\Delta)(S_i^xS_j^x + S_i^yS_j^y) + S_i^zS_j^z] - \sum_{\langle i,j\rangle}\vec{D}_{ij}\cdot(\vec{S}_i\times\vec{S}_j), \tag{1}$$

where the two sum terms are the ferromagnetic Heisenberg and DM interactions, respectively. The exchange coupling constant J is restricted to the nearest-neighbor pairs of spins. S_i^α ($\alpha = x, y, z$) are the components of the spin-1 operator at site i. $\Delta(\Delta \in [0,1])$ and $\vec{D}_{ij}$ are the exchange anisotropic parameter and the DM vector coupling, respectively. And the DM vector coupling is antisymmetric, i.e., $\vec{D}_{ij} = -\vec{D}_{ji}$.

For convenience, we shall take $\vec{D}_{ij} = D\hat{z}$, i.e., $\vec{D}_{ij}$ parallels to the z-axis direction which really is a special choice of the DM interaction term in Eq. (1). Thus, according to the two-spin cluster mean-field approximation, the two-spin cluster Hamiltonian H_{12}^{MFA} can be written as [17]

$$H_{12}^{\mathrm{MFA}} = -J[(1-\Delta)(S_1^xS_2^x + S_1^yS_2^y) + S_1^zS_2^z] - D(S_1^xS_2^y - S_1^yS_2^x) - J(q-1)m(S_1^z + S_2^z), \tag{2}$$

where q is the coordination number of the every site of the lattice and the magnetization m is the averaged magnetic moment along a fixed direction $\hat{z}$ related to the cluster with two spins (i.e., $m = \langle\frac{1}{2}(S_1^z + S_2^z)\rangle$). In the representation of the direct product of S_1^z and S_2^z, H_{12}^{MFA} can be written as the form of 9×9 matrix. We can get nine eigenvalues by diagonalizing the matrix of H_{12}^{MFA}. Thus, the partition function $Z = \mathrm{Tr}_{12}\exp(-\beta H_{12}^{\mathrm{MFA}})$ has the following expression:

$$\begin{aligned} Z(m,T) = &\left\{\sinh[2K(q-1)m] + \sinh\left[K\left((q-1)m + \sqrt{D_0^2 + (1-\Delta)^2}\right)\right]\right.\\ &\left. + \sinh\left[K\left((q-1)m - \sqrt{D_0^2+(1-\Delta)^2}\right)\right]\right\}\Big/\left\{\mathrm{e}^{-K} + 2\mathrm{e}^{K}\right.\\ &\times\cosh[2K(q-1)m] + 2\cosh\left[K\left((q-1)m - \sqrt{D_0^2+(1-\Delta)^2}\right)\right]\\ &+ 2\cosh\left[K\left((q-1)m + \sqrt{D_0^2+(1-\Delta)^2}\right)\right] + 2\mathrm{e}^{-K/2}\\ &\left.\times\cosh\left[\frac{K}{2}\sqrt{8(D_0^2+(1-\Delta)^2)+1}\right]\right\}, \end{aligned} \tag{3}$$