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Anisotropic Heisenberg model for the mixed spin-2 and spin-1/2 in the Oguchi approximation on the simple cubic lattice

Erhan Albayrak

Erciyes University, Department of Physics, 38039, Kayseri, Turkey

HIGHLIGHTS

- The mixed spin-2 and spin-1/2 Heisenberg model is studied on a simple cubic lattice.
- Oguchi approximation to examine the effects of exchange anisotropy and crystal field.
- The phase diagrams are obtained on various planes for given values of Δ and D/J.
- The model yields second and first-order phase transitions.
- The model also gives two compensation temperatures, they exhibit reentrant behavior.

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ABSTRACT

The mixed spin-2 and spin-1/2 Heisenberg model is studied on a simple cubic lattice by using the Oguchi approximation to examine the effects of exchange anisotropy and crystal field. The thermal variations of the order-parameters, i.e. magnetization and quadrupole moment, are investigated to obtain the possible phase diagrams of the model. The detailed phase diagrams are obtained on the $(D/J, k_BT/J)$ and $(\Delta, k_BT/J)$ planes for given values of Δ and D/J, respectively. In the phase diagrams all possible solutions are illustrated whether stable or not. The model yields second and first-order phase transitions, in addition to the tricritical and isolated critical points. The model also gives two compensation temperatures for given system parameters, therefore, they exhibit reentrant behavior. The low temperature behavior of the model is very complicated, therefore, the reliability of the Oguchi approximation should be investigated further.

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1. Introduction

After the detailed investigations of single spin type Ising models, the next logical step was to mixed them up with different spins in various structures. The studies of mixed-spin systems revealed an important property called as the compensation temperature which has many technological applications such as magnetic recording etc. In addition to this, the phase diagrams become much richer, therefore, they also got a lot of attention. In the Ising model the spins can only align along one axis which is usually chosen as the z-axis. When this limitation is lifted, i.e. giving spins the possibility of aligning in three-dimensional space may lead to much more complicated systems which are quantum mechanical in nature and they are studied in terms of the Heisenberg models. In this model, the spin operators do not commute with each other, therefore, there are certain types of uncertainties in the measurement of physical observables. Thus the exact solutions are

E-mail address: albayrak@erciyes.edu.tr.

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usually unavailable, therefore, it is always necessary to use some kind of approximations which may give some qualitative pictures but usually has many shortcomings. In this work, we wish to investigate the mixed spin-2 and spin-1/2 Heisenberg ferrimagnetic system on a simple cubic lattice in the Oguchi approximation (OA).

The Heisenberg model in the OA was considered for either single-spin or mixed-spin systems and interesting results were obtained. The thermodynamic properties of spin-1/2 anisotropic Heisenberg model with Dzyaloshinskii–Moriya interaction were studied [1]. The same spin system was also considered where the effects of the second-nearest-neighbor exchange interactions on the magnetization, internal energy, heat capacity, entropy and free energy were considered [2]. The effects of both exchange and single-ion anisotropies were investigated on the phase diagrams of the mixed spin-1 and spin-1/2 [3], including the compensation temperature studies [4] and including the investigation of magnetic susceptibility [5]. The similar properties was also considered in the ferromagnetic mixed spin-3/2 and spin-1/2 model [6]. In all these works only the simple cubic lattice structures were considered since Mermin–Wagner theorem states that continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$ [7]. Thus the OA does not give the results in agreement with the Mermin–Wagner theorem for the planar isotropic Heisenberg model, therefore, in this work we take $z = 6$, i.e. the number of nearest-neighbor spins, corresponding the simple cubic lattice in order not to violate the Mermin–Wagner theorem.

As far as in our knowledge, the mixed spin-2 and spin-1/2 system was mostly considered in the Ising models: The critical behaviors of some mixed ferrimagnetic systems were studied on a square lattice in which the two interpenetrating square sublattices had spins $\sigma(\pm 1/2)$ and $S(\pm 2, \pm 1, 0)$ and the exact ground state calculations were carried out and Monte Carlo (MC) simulations were performed to obtain the finite-temperature phase diagram of the model [8]. The thermal behaviors of the order-parameters and phase diagrams were studied in the Blume–Capel model for the nearest-neighbor interactions on the Bethe lattice by using the exact recursion equations for the coordination numbers $z = 3, 4, 5$ and 6 [9]. The magnetic properties of a ferromagnetic diamond chain were studied by effective-field theory (EFT) and MC simulation based on the Ising model [10]. The only work in terms of Heisenberg model investigated the compensation and critical behaviors on a square lattice theoretically by the two-time Green's function technique, which takes into account the quantum nature of Heisenberg spins [11]. It should be mentioned that in these works usually the effects of crystal field were considered, but for the three-dimensional case the spins may interact strongly in one direction than the others, thus, one can intend to add an exchange anisotropy term to study its effects on the phase diagrams too.

There are not many experimental works including mixed spin-2 and 1/2 system but we can at least give two experimental works such as: A polymer with a large density of cross-links and an alternating connectivity of radical modules with unequal spin quantum numbers (S), macrocyclic $S = 2$, and cross-linking $S = 1/2$ modules, were designed which permits large net S values for either ferromagnetic or antiferromagnetic exchange coupling between the modules [12]. The second one studies the specific heat data on two samples of $YBa_2Cu_3O_{7-\delta}$ with relatively low concentrations of paramagnetic centers and show the presence of both spin-2 and spin-1/2 moments [13].

In this work, the effects of exchange anisotropy and crystal field for the mixed spin-2 and spin-1/2 Heisenberg model on a simple cubic lattice are investigated by using the Oguchi approximation. The detailed phase diagrams are obtained on the $(D/J, k_BT/J)$ and $(\Delta, k_BT/J)$ planes for given values of Δ and D/J respectively by investigating the thermal variations of the order-parameters. It is found that the model gives second- and first-order phase transitions and some critical points in addition to compensation temperatures.

The rest of the work is set up as follows: The next section is dedicated to the formulation of Heisenberg model in the Oguchi approximation for the mixed spin-2 and 1/2 system. The third section comprises from the phase diagrams and some of the illustrations for thermal variations of the order-parameters in addition to some comparisons whenever possible. The last section is devoted to brief summary and conclusions.

2. Formulation

The usual Hamiltonian for the mixed spin-S_A and spin-S_B including exchange anisotropy parameter Δ may be given as

$$\hat{\mathcal{H}} = -J\sum_{\langle ij\rangle}[(1-\Delta)(\hat{S}^x_{iA}\hat{S}^x_{jB} + \hat{S}^y_{iA}\hat{S}^y_{jB}) + \hat{S}^z_{iA}\hat{S}^z_{jB}] - D\sum_{i\epsilon A}(\hat{S}^z_{iA})^2, \tag{1}$$

where S^δ_{iA} and S^δ_{jB} with $(\delta = x, y, z)$ are the components of spin-2 and spin-1/2 operators for the sublattices A and B, respectively. D is the crystal field acting only to the spin-2 sites, i.e. only on sublattice A, J is the nearest-neighbor (NN) bilinear exchange interaction parameter and the exchange anisotropy parameter only lies in the $0 \leq \Delta \leq 1$ range.

In the OA, the NN pair interactions between the spin components are treated exactly and the rest of interactions are replaced with the effective field terms as it is usually done in the mean-field approximations. Therefore, the effective Oguchi Hamiltonian for a pair of spins is given by

$$\hat{\mathcal{H}}_{ij} = -J[(1-\Delta)(\hat{S}^x_{iA}\hat{S}^x_{jB} + \hat{S}^y_{iA}\hat{S}^y_{jB}) + \hat{S}^z_{iA}\hat{S}^z_{jB}] - D(\hat{S}^z_{iA})^2 - h_i\hat{S}^z_{iA} - h_j\hat{S}^z_{jB} \tag{2}$$

where the mean-field terms are given as

$$\begin{aligned} h_i &= (z-1)JM_B \\ h_j &= (z-1)JM_A \end{aligned} \tag{3}$$

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