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Critical properties of the mixed spin-1 and spin-$\frac{1}{2}$ anisotropic Heisenberg model in the Oguchi approximation

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ABSTRACT

The effects of both an exchange anisotropy and a single-ion anisotropy on the phase diagram of the mixed spin-1 and spin-$\frac{1}{2}$ Heisenberg model are investigated by the use of an Oguchi approximation. Particular emphasis is given to the simple cubic lattice with coordination number $z = 6$ for which the phase diagram and magnetizations are determined numerically. Besides second-order transitions, lines of first-order transitions terminating either at a tricritical point or an isolated critical point, are determined. The origin and nature of the new ordered phase in the quantum mixed-spin system at the low temperature region is also discussed.

1. Introduction

In the past years, much interest has been focused on the statistical mechanics of Ising and quantum Heisenberg spin systems with a single-ion uniaxial anisotropy field. However, the absence of an exact solution for such magnetic models makes a number of approximation methods rather useful: mean-field theory [1], Oguchi approximation (OA) [1,2], Bethe–Peierls–Weiss method [1,3], constant-coupling approximation [1,4], effective-field theory with correlations [5,6], series expansions [7], renormalization-group theory [8,9], Monte-Carlo simulations [10] etc. Several of these approximation schemes have been applied in the study of mixed-spin Ising systems which have less translational symmetry than their single-spin counterparts since they consist of two interpenetrating inequivalent sublattices. It is important to remark that the mixed-spin systems are studied not only out of purely theoretical interest but also because they have been proposed as possible models to describe a certain type of molecular-based magnetic materials studied experimentally (see, e.g. Refs. [11–14] and references therein).

Although the majority of studies have focused on mixed-spin Ising models, the mixed-spin quantum Heisenberg models are not without interest. Indeed, there have been many interesting works dealing with the mixed-spin quantum Heisenberg model in one- [15–20], two- [21–24], and three-dimensional [25–30] systems. In these works, the various magnetic properties of the quantum mixed-spin systems without and with anisotropy have been discussed. For instance, the critical properties of the mixed spin-1 and spin-$\frac{1}{2}$ anisotropic Heisenberg model including both the exchange anisotropy and the single-ion anisotropy have already been studied by the use of the OA in Refs. [25,30]. However, apart from indications of the second-order transition lines (including the tricritical points in Ref. [30]), these works do not provide any insight into the nature of possible first-order transition lines which can be induced by the single-ion anisotropy at the low temperature

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region. Moreover, when the temperature is low enough, the quantum fluctuation effects are remarkable and may induce new magnetic properties also in the mixed-spin quantum Heisenberg models different from those of the classical mixed-spin Ising models. Therefore, it may be worthwhile to calculate the correct free energy of the anisotropic Heisenberg ferromagnet with a mixed spin-1 and spin-$\frac{1}{2}$ by the use of the OA and to determine the complete phase diagram which has not been obtained yet. We note here that the similar approach, namely the Ising–Heisenberg two-atom cluster approximation [31,32] proposed for the description of the Heisenberg ferromagnet, although more accurate than the OA in the determination of second-order phase transitions, does not yield the expression for the free energy and hence fails in the investigations of complete phase diagrams, where first-order phase transitions can occur.

The Hamiltonian of the mixed spin-1 and spin-$\frac{1}{2}$ anisotropic Heisenberg model in the presence of a single-ion anisotropy field strength D and a magnetic field h applied along z axis is given by

$$\hat{\mathcal{H}} = -J\sum_{\langle i,j\rangle}[(1-\Delta)(\hat{S}_{iA}^x\hat{S}_{jB}^x + \hat{S}_{iA}^y\hat{S}_{jB}^y) + \hat{S}_{iA}^z\hat{S}_{jB}^z] - D\sum_{i\epsilon A}(\hat{S}_{iA}^z)^2 - h\left(\sum_{i\epsilon A}\hat{S}_{iA}^z + \sum_{j\epsilon B}\hat{S}_{jB}^z\right), \tag{1}$$

where $\hat{S}_{iA}^\alpha$ and $\hat{S}_{jB}^\alpha$ ($\alpha = x, y, z$) are components of the spin $S_A = 1$ and $S_B = \frac{1}{2}$ operators on sublattices A and B, respectively. The first summation is carried out only over nearest-neighbour pairs of spins on different sublattices, J is the nearest-neighbour exchange interaction being positive by convention and Δ is the exchange anisotropy parameter which is assumed to take values between 0 and 1. We note that the nearest neighbours of a spin on the A sublattice are only spins on the B sublattice and vice versa. The Hamiltonian (1) is of the interest because it has less translational symmetry than its single spin counterpart and for $\Delta = 0$ and $\Delta = 1$ corresponds to the isotropic Heisenberg and Ising models, respectively. However, owing to the requisite non-commutativity of operators in the Hamiltonian, deriving the eigenvalues of the Hamiltonian is very difficult. Thus the OA, in spite of its limitations, is an adequate starting point. Within this theoretical framework we determine numerically complete phase diagram of the system on a simple cubic lattice with coordination number $z = 6$. In particular, we find a new ordered phase at the low temperature region for $\Delta \neq 1$.

An outline of the remainder of this paper is as follows: A formulation of the problem within the OA is presented in Section 2. In Section 3, the effects of both the exchange anisotropy and single-ion anisotropy on a phase diagram of the system are numerically studied. In some special cases the temperature dependences of the magnetizations are also discussed. Finally, brief conclusions are presented in Section 4.

2. Formulation

In the OA, the interaction of a pair of nearest-neighbour spins, say $\hat{\mathbf{S}}_{iA}$ and $\hat{\mathbf{S}}_{jB}$, is treated exactly and the interactions of $\hat{\mathbf{S}}_{iA}$ and $\hat{\mathbf{S}}_{jB}$ with their remaining neighbouring spins are replaced by effective-field terms in exactly the same way as in the mean-field approximation. Starting from Eq. (1), the effective Oguchi Hamiltonian for a pair of spins is given by

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

with

$$h_i = J(z-1)m_B + h, \qquad h_j = J(z-1)m_A + h, \tag{3}$$

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 direction z in space, i.e., $m_A = \langle\hat{S}_{iA}^z\rangle$ and $m_B = \langle\hat{S}_{jB}^z\rangle$.

In the representation of the direct product of $\hat{S}_{iA}^z$ and $\hat{S}_{jB}^z$, the Hamiltonian (2) can be written as the form of 6×6 matrix. Then by solving the Schrödinger equation,

$$\hat{\mathcal{H}}_{ij}|\psi_n\rangle = E_n|\psi_n\rangle \quad (n = 1, 2, \ldots, 6), \tag{4}$$

we obtain the energy levels

$$\begin{aligned} &E_1 = a, \qquad E_2 = \frac{1}{2}(b+c) + \omega_1, \qquad E_3 = \frac{1}{2}(b+c) - \omega_1, \\ &E_4 = \frac{1}{2}(d-c) - \omega_2, \qquad E_5 = \frac{1}{2}(d-c) + \omega_2, \qquad E_6 = e, \end{aligned} \tag{5}$$

where

$$\begin{aligned} &a = -\frac{J}{2} - D - h_i - \frac{h_j}{2}, \qquad b = \frac{J}{2} - D - h_i + \frac{h_j}{2}, \qquad c = -\frac{h_j}{2}, \\ &d = \frac{J}{2} - D + h_i - \frac{h_j}{2}, \qquad e = -\frac{J}{2} - D + h_i + \frac{h_j}{2}, \qquad f = -\frac{J}{\sqrt{2}}(1-\Delta), \end{aligned} \tag{6}$$