Anomalous behaviour of the magnetic susceptibility 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 magnetic susceptibility 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 magnetic susceptibility is determined numerically. Anomalous behaviour in the thermal variation of the magnetic susceptibility in the low-temperature region is found due to the applied negative single-ion anisotropy field strength. Also, the difference between the behaviours of the magnetic susceptibility of the Heisenberg and Ising models is discussed.

1. Introduction

Over recent years there has been considerable interest in the study of two sublattice mixed-spin Ising and quantum Heisenberg models. These 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. [1]). For instance, the phase diagrams of the mixed spin-1 and spin-$\frac{1}{2}$ anisotropic Heisenberg model with a single-ion anisotropy have been studied recently by using the Oguchi approximation (OA) [2,3] and two-site cluster approximation combined with the discretized path integral representation [4]. However, as far as we know, up to now no studies have been made concerning the magnetic susceptibility of the mixed-spin anisotropic Heisenberg model which is important physical quantity of magnetic materials and can be measured experimentally. Therefore, the purpose of this report is clarify the effects of both an exchange anisotropy and a single-ion anisotropy on the magnetic susceptibility of the mixed spin-1 and spin-$\frac{1}{2}$ system, using the same framework (OA) as that of the previous work [2]. Since anisotropy effect may play principal role in the system with spin value $S > \frac{1}{2}$, the influence of single-ion anisotropy strength on the magnetic susceptibility of the magnetic system is of prime importance. In particular, we find that, depending on the value of the single-ion anisotropy, the temperature dependence of the total magnetic susceptibility exhibits some outstanding features, such as the existence of broad (or sharp) maxima in the low-temperature region.
2. Theory

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

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

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 $\Delta$ is the exchange anisotropy parameter which can take values between 0 and 1. 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. By using the OA, we rewrite the Hamiltonian (1) as

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

with

\[
h_i = J(z - 1)m_B + h, \quad h_j = J(z - 1)m_A + h,
\]

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 $m_B = \langle \hat{S}_{jB}^z \rangle$. Taking the eigenvalues of the Hamiltonian (2), one can obtain the sublattice magnetizations per site $m_A$ and $m_B$ [2]. The total magnetization per site of the system is then defined by

\[
m = \frac{1}{2}(m_A + m_B).
\]

On the other hand, the sublattice magnetic susceptibility $\chi_\alpha (\alpha = A \text{ or } B)$ is defined by

\[
\chi_\alpha = \lim_{h \to 0} \frac{\partial m_\alpha}{\partial h}
\]

from which the total magnetic susceptibility per site is given by

\[
\chi = \lim_{h \to 0} \frac{\partial m}{\partial h} = \frac{1}{2}(\chi_A + \chi_B).
\]

It should be noted here that the total susceptibility represents the response of a whole mixed-spin ferromagnetic system on the infinitesimal external magnetic field which can be experimentally verified in contrast to its sublattice counterparts. However, the theoretical investigation of the thermal variation of sublattice susceptibilities will show us the origin of an anomalous behaviour of the total susceptibility in some cases.

3. Results and discussion

Let us study numerically the magnetic susceptibility of the mixed spin-1 and spin-$\frac{1}{2}$ system on the simple cubic lattice for $\Delta = 1$ and $\Delta = 0$ which corresponds to the Ising and the isotropic Heisenberg models, respectively. Before discussing the anomalous behaviour of the temperature dependence of the magnetic susceptibility for the negative single-ion anisotropy $D$, we notice
that for $D > 0$ the magnetic susceptibility exhibits normal behaviour with a divergence at the second-order transition temperature $T_c$ and the point of singularity shifts to a low temperature, upon decreasing the value of $D$, in agreement with the phase diagrams in [2]. However, for $D < 0$, the susceptibilities for both models exhibit, except the divergences at $T_c$, broad maxima at low temperatures which gradually become larger with the decrease of $D$. In particular, we have found that the low-temperature maximum is the largest, and simultaneously the susceptibility still exhibits singularity, for the value of $D$ corresponding to the position of a tricritical point $T_t$ of the model [2]. Such temperature dependencies of the magnetic susceptibilities are shown in figures 1 and 2 for the Ising and Heisenberg models, respectively. In these figures the dashed and solid lines represent the total and sublattice susceptibilities, respectively, while the dashed-dotted curve denotes the position of the singularity at $T_t$. We note that the susceptibilities in figures 1 and 2 diverge on both sides of $T_t$ with classical critical exponents $\gamma' = \gamma = 1$.

Indeed, it is seen from figure 1 that the total susceptibility for the Ising model with $D/J = -2.8102$ diverges at the tricritical temperature $k_B T_t/J = 1.2764$ and exhibits anomalous feature, namely a maximum in the low-temperature region. As seen from the figure, this anomalous result arises from the behaviour of the $\chi_A$ sublattice susceptibility. The physical scenario for the appearance of this anomaly is as follows. The $S_{iA}^z = \pm 1$ states on the sublattice $A$ are partially suppressed at the zero temperature for the negative value of $D$ and for $h = 0$. With the increase of the temperature these $S_{iA}^z = \pm 1$ states are gradually populated resulting, for $h \neq 0$, in a rather rapid increase of the $\chi_A$ sublattice susceptibility in the low-temperature region. The similar anomalous behaviour of the susceptibility in the low temperature region we can see also for the isotropic Heisenberg model in figure 2 with $D/J = -2.7116$ which diverges at the tricritical temperature $k_B T_t/J = 1.2152$. However, unlike Ising model, the susceptibility in figure 2 exhibits a finite jump (indicated by vertical dotted line) corresponding to the first-order transition between two different ordered phases which are separated, at low temperatures, by a first-order transition line terminating at an isolated critical point [2].

The temperature dependencies of the magnetic susceptibilities for the mixed-spin Ising and isotropic Heisenberg models exhibit another anomalous features for the negative value of $D$,
Figure 3. The total ($\chi$) and sublattice ($\chi_A, \chi_B$) susceptibilities vs temperature for the Ising model with $D/J = -2.97$. We observe that besides the finite jump of $\chi$ at the first-order transition point, the total susceptibility at low temperatures exhibits a sharp maximum. As seen from the figure, this variation again originates from the behaviour of the $\chi_A$ sublattice susceptibility. On the other hand, the susceptibility above the first-order transition point shows only a broad maximum and this anomalous result arises from the behaviour of both sublattice susceptibilities. In figure 4, we show the behaviour of $\chi$ for the isotropic Heisenberg model with $D/J = -2.76$. Now, the susceptibility exhibits two discontinuities: one due to the first-order transition at a higher temperature, and another at the lower temperature corresponding to the first-order transition between two ordered phases situated within the ferromagnetically ordered region (see [2]). However, the susceptibility for the Heisenberg model does not exhibit a broad maximum above the first-order transition at the high-temperature region.

Finally, we note that the total susceptibility for the Ising model again diverges for $D \leq -3.0$ at $T = 0$ K. Our numerical results indicate that the same behaviour should exhibit the total susceptibility of the Heisenberg model for $D/J \to -\infty$. However, it has not been possible to prove this result because of computational difficulties arising from overflow problems, that occur at low temperatures for a large negative value of $D$. Of course, it might be worth to test the main features of our effective-field results in a future by using quantum Monte Carlo calculation.

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