Monte Carlo Study of a Mixed Spin-1 and Spin-3/2 Ising Ferromagnet

Y. Nakamura and J. W. Tucker

***Abstract*—The magnetic properties of a mixed spin-1 and spin-3/2 Ising ferromagnetic system on a cubic lattice are studied by Monte Carlo simulation. In particular the effect of a single-ion anisotropy on the phase diagram is investigated. Some qualitative features of the phase diagram obtained by a cluster variational treatment of the same system are confirmed.**

***Index Terms*—Mixed Ising system, Monte Carlo simulation, phase transition.**

I. Introduction

RECENTLY, the mixed spin-1 and spin-3/2 Ising system has been investigated with use of an effective field theory [1], [2], mean field theory [3] and a cluster variational method [4]. However, there are some disagreements among those theoretical studies as to the existence of tricritical points and other features. Furthermore, a great variety of topologies of the finite temperature phase diagram is predicted by the cluster variational method for the cubic lattice. As far as we know, no nonperturbative method, such as transfer-matrix, Monte Carlo simulation and so on, has been applied to the system. To help to resolve the differences among the results of theoretical studies, we have investigated the same model by Monte Carlo simulation. Although this mixed spin model has been studied primarily out of theoretical curiosity, it has been pointed out in [1] that knowledge of such models may assist in an understanding of some two- and three-dimensional bimetallic molecular ferrimagnets.

II. Model and Simulation

The model we studied is the mixed spin-1 and spin-3/2 Ising system on a cubic lattice described by the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} S_{iz}^A S_{jz}^B + D_A \sum_i (S_{iz}^A)^2 + D_B \sum_j (S_{jz}^B)^2 \quad (1)$$

where S_{iz}^A and S_{jz}^B are spin-1 and spin-3/2 on sublattices A and B, respectively. $J(>0)$ is the exchange interaction between nearest-neighbor pairs of spins and D_A and D_B are the single-ion anisotropies. The summation $\sum_{\langle ij \rangle}$ is performed for nearest-neighbor spin pairs and periodic boundary conditions are adopted. The system size is defined by L, the number of spins along each cubic axis.

We carried out a standard importance sampling method to simulate the system described by the Hamiltonian, (1). We initially chose $L = 20$ for the simulations. Configurations were generated by randomly sweeping through the lattice and making single-spin-flip attempts, which were accepted or rejected according to the Metropolis algorithm. Data were generated with 5×10^4 Monte Carlo steps per site after discarding the first 10^4 steps per site for equilibration. This number of Monte Carlo simulations was sufficient in this investigation since we were primarily concerned with comparing the qualitative (not quantiative) features of the phase diagram with those of the different theories. Since there were no significant differences in the results obtained when the lattice size was increased from $L = 20$ to 32, the initial choice of $L = 20$ was used in most of the computations in order to save computing time.

The total and sublatice magnetization and quadrupolar moments defined by

$$m_A = \langle M_A \rangle \qquad m_B = \langle M_B \rangle \qquad m = (m_A + m_B)/2$$
$$q_A = \langle Q_A \rangle \qquad q_B = \langle Q_B \rangle \qquad q = (q_A + q_B)/2$$

were all calculated. Here

$$M_A = \frac{\sum_i S_{iz}^A}{L^3/2} \qquad Q_A = \frac{\sum_i (S_{iz}^A)^2}{L^3/2}$$

with analogous expressions for M_B and Q_B, and the angular brackets denote an average over Monte Carlo configurations. In addition, the magnetic susceptibility

$$\chi = \beta L^3 \left\langle (M - \langle M \rangle)^2 \right\rangle$$

and the quadrupolar magnetic susceptibility

$$\chi_q = \beta L^3 \left\langle (Q - \langle Q \rangle)^2 \right\rangle$$

with $\beta = 1/(k_B T)$, were evaluated.

III. Results

To understand the results, knowledge of the phase diagram at zero temperature is instructive. Possible ground states in a (m_A, m_B, q_A, q_B) representation are: $O_1 \equiv (1, 3/2, 1, 9/4)$, $O_2 \equiv (1, 1/2, 1, 1/4)$, $D_1 \equiv (0, 0, 0, 9/4)$ and $D_2 \equiv (0, 0, 0, 1/4))$, and the phase diagram at zero temperature, in $(D_A/(zJ), D_B/(zJ))$ space, is shown in Fig. 1 where the phase boundary separating the O_1 and D_2

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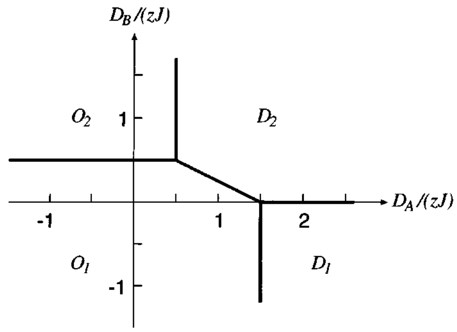

Fig. 1. Ground state phase diagram.

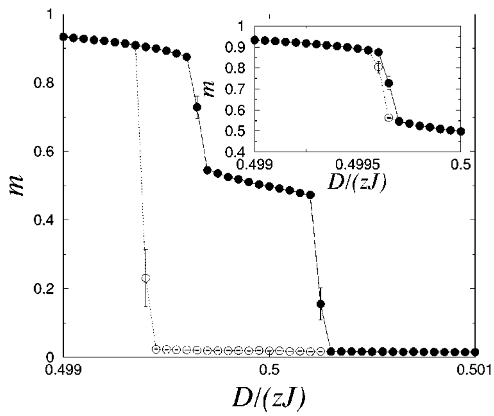

Fig. 2. The $D = D_A = D_B$ dependence of magnetization in the case of $k_BT/J = 0.2$. Solid lines with filled symbols obtained with increasing D and dotted lines with open symbols with D decreasing. In the inset we show the magnetization curve as D was cycled between 0.499 and 0.5.

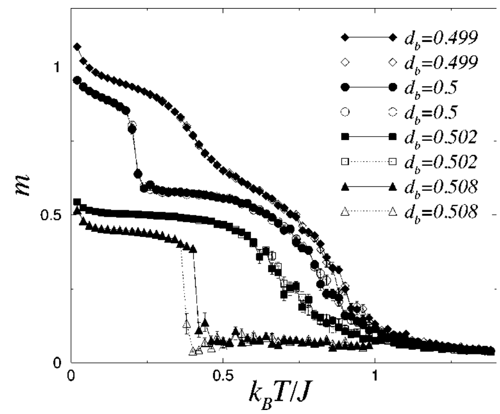

Fig. 3. Thermal variations of the magnetization for several $d_b \equiv D_B/(zJ)$ when $D_A/(zJ) = 0.499$. Solid lines with filled symbols obtained with increasing temperature and dotted lines with open symbols, as the temperature decreases.

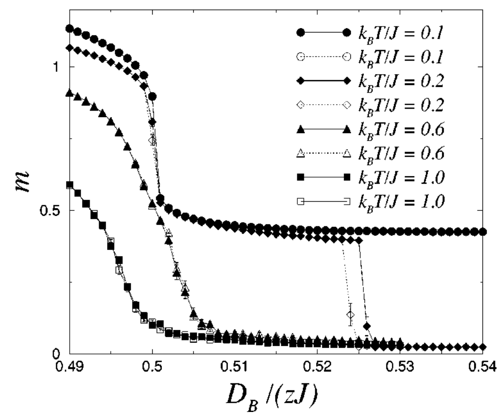

Fig. 4. Magnetization curves as a function of $D_B/(zJ)$ for selected temperatures in the case of $D_A/(zJ) = 0.499$. Solid (dotted) lines with filled (open) symbols indicate increasing (decreasing) cycling of $D_B/(zJ)$.

phases lies along the line $2D_A + 4D_B = 3zJ$. z is the lattice coordination number.

We consider first the case of equal anisotropy strengths ($D \equiv D_A = D_B$). Fig. 2 shows the magnetization curve in the case of $k_BT/J = 0.2$. It has a clear twofold hysteretic behavior as D is swept up and down, indicating the system exhibits two first-order transitions. The first-order transition at the larger D value is predicted in both [1] and [4], but the other, at smaller D was found only in [4].

Let us turn to the case of unequal anisotropy strengths. Fig. 3 shows the magnetization curves as a function of temperature for several values of $D_B/(zJ)$ in the case of $D_A/(zJ) = 0.499$. When $D_B/(zJ) = 0.5$, a large magnetization jump is observed near $k_BT/J = 0.25$, indicating a first-order transition. In addition, there is a second-order transition at higher temperature. As D_B is increased, this latter transition point is shifted to lower temperature and its nature is changed from second- to first-order. These qualitative features are in agreement with the phase diagram shown in [4, Fig. 8(b)], as can be seen by drawing lines of constant D_B to intersect the phase boundaries. The $D_B/(zJ)$ dependence of magnetization for several temperatures, for the same value of $D_A/(zJ)$ as in Fig. 3, are depicted in Fig. 4. When $k_BT/J = 0.1$, there is one first-order transition slightly above $D_B/(zJ) = 0.5$. When the temperature is increased there are two first-order transitions. As the temperature is further increased the first-order transitions disappear and only one second order transition exists. These results again support the results shown in [4, Fig. 8], as can be seen by drawing lines of constant temperature to intersect the phase boundaries.

Fig. 5 shows the magnetization, the magnetic susceptibility and the quadrupolar magnetic susceptibility as a function of the temperature for $D_A/(zJ) = 0.4965$ and $D_B/(zJ) = 0.501$. According to the theoretical results in [4] a first-order transition near $k_BT/J = 0.4$ and a second-order transition near $k_BT/J = 1.2$ are predicted. Unfortunately, we cannot confirm definitely the existence, or otherwise, of the first-order transition. As can be seen in Fig. 5, the magnetization curve shows neither a big discontinuity nor hysteresis near $k_BT/J = 0.4$. However, on the other hand, the quadrupolar magnetic susceptibility does have a relatively sharp peak indicating a first-order transition is possibly present [5]. We adopted this latter procedure for seeking the existence of a first-order transition, rather than the so-called Binder cumulant method [6], because it had already been used with success in [5], and did not require simulations over several lattice sizes.

In Fig. 6, it is seen that sublattice magnetization curves cross near $k_BT/J = 0.4$ for $D_A/(zJ) = 0.49$ and $D_B/(zJ) = 0.495$. Thus, if one were to consider the equivalent ferrimagnetic model ($J < 0$), a compensation point would occur. Such a phenomenon was predicted in [3] for the same set of $D_A/(zJ)$

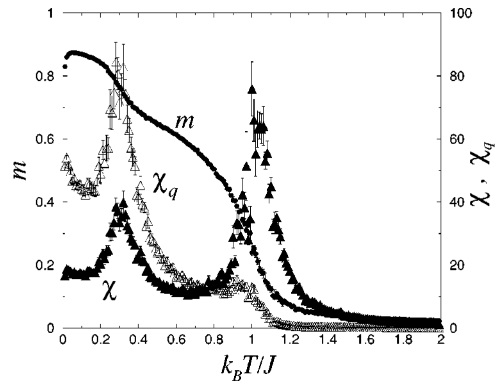

Fig. 5. Thermal variation of the magnetization, the magnetic susceptibility and the quadrupolar magnetic susceptibility. $D_A/(zJ) = 0.4965$, $D_B/(zJ) = 0.501$.

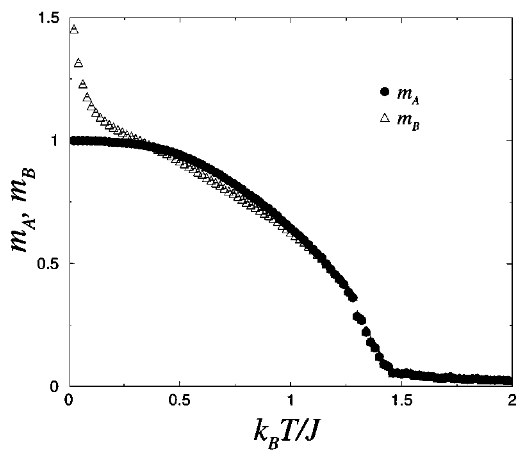

Fig. 6. Thermal variation of the sublattice magnetizations when $D_A/(zJ) = 0.49$, $D_B/(zJ) = 0.495$.

and $D_B/(zJ)$ values, although in that work a second compensation point was found at higher temperatures. However, the net magnetization between the compensation points was very small. Whether that is a real effect, or an artifact of the theoretical approximations remains unresolved. It is possible a second cross-over point does exist, but that is below the resolution of our current Monte Carlo simulations. Compensation points are also predicted in [4, Fig. 7], although they were not alluded to in that paper.

IV. Conclusion

We have applied Monte Carlo simulations to the study of a mixed spin-1 and spin-3/2 Ising ferromagnetic system on a cubic lattice, modeled by (1). In particular, we have examined the effect of single-ion anisotropy on the magnetic behavior. For the case of equal single-ion anisotropy strengths, we found two different ferromagnetic phases dependent on the value of $D/(zJ)$ in the low temperature region (Fig. 2). Those ordered phases are separated from each other and from the disordered phase by first-order transitions at low temperatures. This result is consistent with that in [4]. As was shown in Figs. 3 and 4, the behavior of magnetization strongly depends on the value of D_B in the case of $D_A/(zJ) = 0.499$. These results also reflect the findings of [4]. However, the first-order transition at a temperature close to $k_BT/J = 0.4$ which was predicted in [4] could not be confirmed conclusively. Finally, the fact that compensation points can exist in the ferrimagnetic spin 1–spin 3/2 system has been demonstrated by Monte Carlo simulation. Overall, the qualitative features of the results for the cubic lattice in [4] have been verified by the current Monte Carlo simulations. Simulations for the honeycomb and square lattice remain to be done. However, since the interesting features in the phase diagram of these lattices occur over an even smaller range of anisotropy strengths than in the cubic lattice, much longer simulations on lattice having a greater number of spins will be required to give results with any degree of certainty.

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