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LETTER TO THE EDITOR

The ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system

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Abstract. The phase diagram and magnetization curves of a ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system are examined by the use of the effective-field theory with correlations. Some outstanding features are found in the temperature dependences of total and sublattice magnetizations.

Ferrimagnetism has been intensively investigated in the past both experimentally and theoretically. Ferrimagnets have several sublattices with a finite resultant moment. However, they normally take complicated magnetic structures [1]. Because of the complexity of the structures, very little work has been done in trying to apply more advanced theories to ferrimagnetism beyond the standard mean-field theory. From a theoretical point of view, on the other hand, the mixed-spin Ising system consisting of spin-$\frac{1}{2}$ and spin-S ($S > \frac{1}{2}$) has been introduced as a simple model showing ferrimagnetic behaviour. The Hamiltonian of the ferrimagnetic mixed-spin system is given by

$$H = J\sum_{ij} \mu_i^z S_j^z - D\sum_j \left(S_j^z\right)^2 \tag{1}$$

where S_j^z takes the $(2S + 1)$ values allowed for a spin S, μ_i^z can be $+\frac{1}{2}$ or $-\frac{1}{2}$, D is the crystal-field constant and the first summation is carried out only over nearest-neighbour pairs of spins.

This model has been extensively studied for the case $S = 1$, since the existence of tricritical behaviour is predicted in the system with a coordination number z larger than $z = 3$ [2]. An important point in studying this model is that the exact solution for the transition temperature can be obtained analytically when the structure of the system is chosen to be a honeycomb lattice ($z = 3$) [3]. As far as we know, however, no studies have been made of the magnetization curves of a ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ ($S = \frac{3}{2}$) Ising system, although the critical phenomena of the system with $D = 0.0$ in the BCC structure have been examined by the use of the high-temperature series-expansion method [4]. In this work, we shall discuss via the new effective-field theory with correlations [5] the magnetic properties (phase diagram and magnetizations) of the ferrimagnetic mixed-spin Ising system. The temperature dependence of the magnetization may exhibit some outstanding features different from the case $S = 1$ [6].

Within the formulation of the effective-field theory, the sublattice magnetizations σ and m of the system are given by

$$\sigma = \langle \mu_i^z \rangle = [A(J\nabla) - B(J\nabla)m + C(J\nabla)q - D(J\nabla)r]^z f(x)|_{x=0} \tag{2}$$

$$m = \langle S_j^z \rangle = [\cosh(J\nabla/2) - 2\sigma \sinh(J\nabla/2)]^z F(x)|_{x=0} \tag{3}$$

where $\nabla = \partial/\partial x$ is a differential operator and the parameters q and r are defined as

$$q = \left\langle (S_j^z)^2 \right\rangle \qquad r = \left\langle (S_j^z)^3 \right\rangle . \tag{4}$$

The functions $f(x)$ and $F(x)$ are defined by

$$f(x) = \tfrac{1}{2} \tanh(\beta x/2) \tag{5}$$

$$F(x) = \frac{1}{2} \frac{3 \sinh(3\beta x/2) + \exp(-2D\beta) \sinh(\beta x/2)}{\cosh(3\beta x/2) + \exp(-2D\beta) \cosh(\beta x/2)} \tag{6}$$

where $\beta = 1/k_B T$. The total magnetization M of the system is then

$$M = (N/2)(m + \sigma) \tag{7}$$

where N is the number of magnetic atoms.

Here, in order to derive the sublattice magnetizations, we have used the exact Ising spin identities as well as the exact van der Waerden identities for spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$. For treating the multispin correlation functions, the decoupling approximation has then been introduced:

$$\langle \mu_i^z S_j^z \dots S_l^z \rangle \simeq \langle \mu_i^z \rangle \langle S_j^z \rangle \dots \langle S_l^z \rangle \tag{8}$$

for $i \neq j \neq \dots \neq l$. As discussed in [5], the statistical accuracy of (8) corresponds to the Zernike approximation [7] of the spin-$\frac{1}{2}$ Ising model for the special case of $D/J = -\infty$. By the use of the exact van der Waerden identity for $S = \frac{3}{2}$, the coefficients A, B, C, D in (2) are given by

$$\begin{aligned} A(J\nabla) &= \tfrac{1}{8}[9\cosh(J\nabla/2) - \cosh(3J\nabla/2)] \\ B(J\nabla) &= \tfrac{1}{12}[27\sinh(J\nabla/2) - \sinh(3J\nabla/2)] \\ C(J\nabla) &= \tfrac{1}{2}[\cosh(3J\nabla/2) - \cosh(J\nabla/2)] \\ D(J\nabla) &= \tfrac{1}{3}[\sinh(3J\nabla/2) - 3\sinh(J\nabla/2)]. \end{aligned} \tag{9}$$

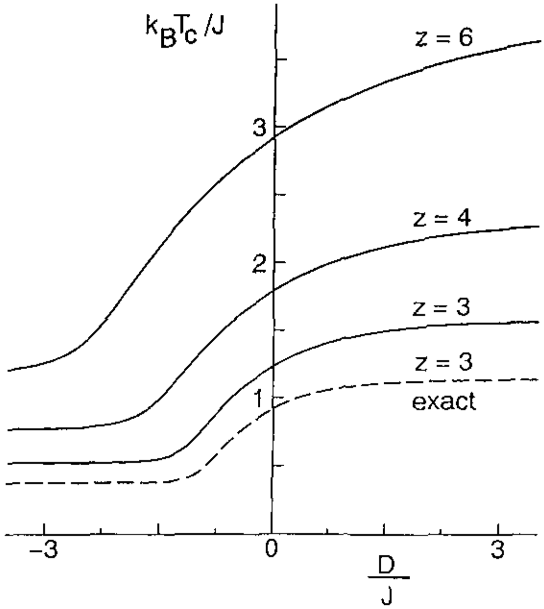

Figure 1. The transition temperature of the mixed-spin Ising system consisting of spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ is plotted as a function of D/J, when the coordination number z is changed. The dashed line expresses the exact solution of the system on a honeycomb lattice ($z = 3$).

The parameters q and r defined by (4) can also be derived in the same way as m and they have the same forms as (3) except that the function $F(x)$ in (3) is replaced by the following functions

$$G(x) = \tfrac{1}{4}\frac{9\cosh(3\beta x/2) + \exp(-2D\beta)\cosh(\beta x/2)}{\cosh(3\beta x/2) + \exp(-2D\beta)\cosh(\beta x/2)} \qquad \text{for } q \tag{10}$$

$$H(x) = \tfrac{1}{8}\frac{27\sinh(3\beta x/2) + \exp(-2D\beta)\sinh(\beta x/2)}{\cosh(3\beta x/2) + \exp(-2D\beta)\cosh(\beta x/2)} \qquad \text{for } r. \tag{11}$$

Now, the transition temperature T_c can easily be determined by requiring that the sublattice magnetizations m, σ and the parameter r tend to zero continuously as the temperature approaches a critical temperature, since in the present system there is no tricritical behaviour [5]. Then, the parameter q at $T = T_c$ is given by putting $\sigma = 0$ into the equation. The results (or phase diagram) are shown in figure 1 as a function of D/J. In the figure, the exact solution (dashed line) for the honeycomb lattice [3] is also depicted for comparison. Thus, it indicates that our formulation gives reasonable results. In particular, notice that the horizontal part (or $D/J \to -\infty$) of the curve labelled $z = 6$ reproduces both analytically and numerically the result of the Zernike approximation, namely

$$4k_BT/J = 5.073 \tag{12}$$

superior to the standard mean-field result ($4k_BT/J = 6$).

The main aim of this work is to investigate the temperature dependences of the magnetizations m, σ and M in the ferrimagnetic mixed-spin system. In figure 2, these quantities are examined by selecting $z = 3$ (that is, the honeycomb lattice) and changing the value of D.

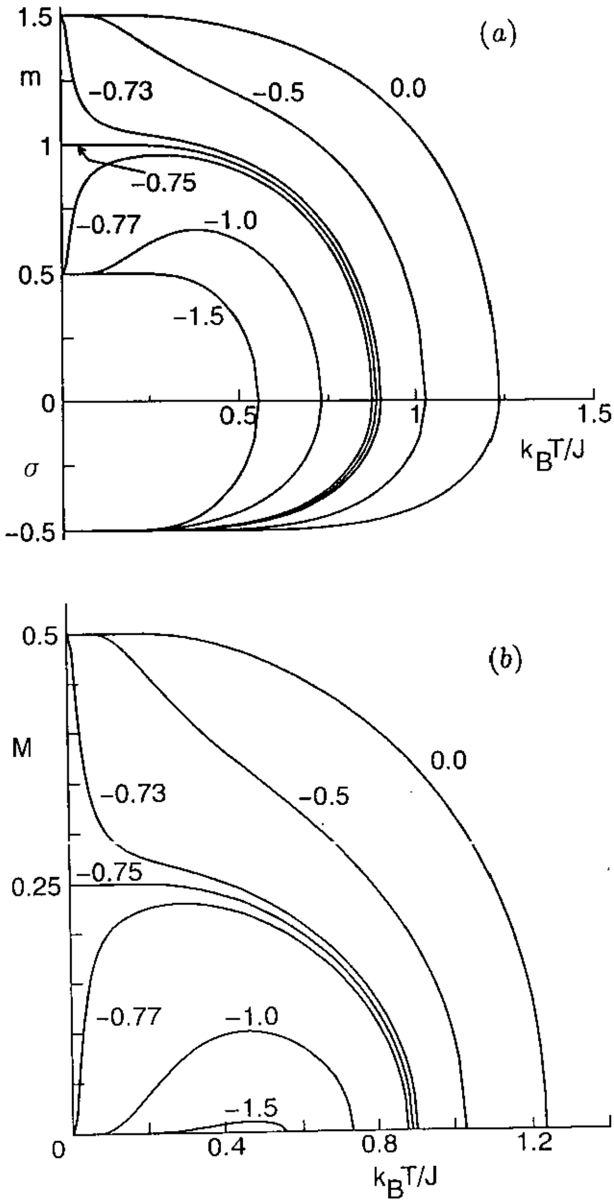

Figure 2. (*a*) The temperature dependences of the sublattice magnetizations m, σ in the mixed-spin system with $z = 3$, when the value of D/J is changed. (*b*) The thermal variations of M in the same systems as those of (*a*).

Before discussing the numerical results, it is necessary to comprehend the ground state. By comparing the values of the ground-state energies for the mixed-spin system with $S_j^z = \pm\frac{3}{2}$ or $S_j^z = \pm\frac{1}{2}$, the possible ordered phases at $T = 0$ K are separated at the critical value D_c of D, namely

$$D_c/J = -z/4 = -0.75 \qquad \text{for } z = 3. \tag{13}$$

That is to say, at the critical value the ordered phases at $T = 0$ K may show the first-order transition; from the $S_j^z = \pm\frac{3}{2}$ state to the $S_j^z = \pm\frac{1}{2}$ state, when the value of D decreases.

As shown in figure 2(*a*), when $D/J \geqslant 0$, the sublattice magnetization m shows normal thermal-variation behaviour. As D decreases from $D = 0.0$, however, the temperature dependence of m may exhibit a rather rapid decrease from its saturation value at $T = 0$ K. The phenomenon is further enhanced when the value of D approaches the critical value D_c. In particular, at the critical value D_c and for $T =$ 0 K, the saturation value of m is $m = 1$, which indicates that in the ground state the spin configuration of S_j^z in the system consists of the mixed phase; the S_j^z are randomly in the $S_j^z = \pm\frac{3}{2}$ or $S_j^z = \pm\frac{1}{2}$ state with equal probability. As noted above, when $D/J <= 0.75$, the spin state of S_j^z is in the $S_j^z = \pm\frac{1}{2}$ state at $T = 0$ K and hence the saturation magnetization is given by $m = 0.5$. Even in the region $D/J < -0.75$, the thermal variation of m exhibits different behaviours depending on the value of D. For a value of D in the region $-1.5 < D/J < -0.75$, the temperature dependence of m may increase from the saturation value with increase in T. But, for $D/J \leqslant -1.5$, the thermal variation of m displays normal behaviour. On the other hand, for all values of D the sublattice magnetization σ may show normal behaviour, even though it is coupled to m.

In figure 2(*b*), the thermal variations of M for the same systems as those of figure 2(*a*) are also depicted. As is seen from the figure, the present system with $S = \frac{3}{2}$ cannot exhibit N-type behaviour in the thermal variation of M (or the compensation point) for any value of D, although it does show Q-type (the curves of $D/J \geqslant 0.0$ and $D/J = -0.75$) and L-type behaviours (the curves of $D/J < -0.75$). In particular, the non-existence of the N-type in the present system is in sharp contrast to the case of $S = 1$ [6]. At this point, one should notice that a new phenomenon not predicted in the Néel theory of ferrimagnetism [1] is obtained in the present system; when the value of D/J approaches the critical value $D_c/J = -0.75$, the temperature dependence of M has an outstanding feature. As shown for the curve labelled $D/J = -0.73$, one observes a rapid drop from the saturation value with increasing T at very low temperatures and then the variation of M with T is somewhat similar to that expected for Q-type ferrimagnetic materials. Such a characteristic thermal variation of M is similar to that observed in amorphous ferrites [8], although in the present system any disorder in the spin configuration is not taken into account.

In conclusion, the temperature dependence of the total magnetization in the ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system may exhibit some characteristics different from the corresponding spin-$\frac{1}{2}$ and spin-1 system, as shown in figure 2. These results may be helpful when the experimental data of ferrimagnetic materials are analysed.

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