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Effect of crystal-field potential on compensation temperature of a mixed spin-1/2 and spin-1 Ising ferrimagnetic system

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Abstract

The magnetic properties of the mixed spin-1/2 and spin-1 Ising ferrimagnetic system with nearest-neighbor and crystal-field interaction on the Bethe lattice are investigated within the framework of exact recursion relations. Particular interest is given to the coordination numbers q = 3, 4, 5 and 6. The existence and dependence of compensation temperature on crystal-field interaction and coordination number is also investigated. If $q \ge 4$, we find that the compensation temperature point is obtained in a restricted region of crystal-field interaction Δ . © 2005 Elsevier B.V. All rights reserved.

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The phenomenon of ferrimagnetism has been intensively studied in recent years, because of their potential device applications in technologically important materials. In contrast to ferromagnets and antiferromagnets, there is in ferrimagnets an important possibility of the existence, under certain conditions, of a compensation temperature $T_{\rm comp}$, at which the resultant magnetization vanishes below the transition temperature T_c [1]. The existence of a compensation point is due to the fact that the magnetic moments of the sublattices compensate each other completely at $T = T_{comp}$. The occurrence of a compensation point is of great technological importance, since at this point only a small driving field is required to change the sign of the resultant magnetization. Just below the compensation point the coercivity falls to a minimum before rising again at low temperature. The increasing interest in this matter is mainly related to the potential technological applications of these systems in the area of thermomagnetic recording [2].

Mixed-spin Ising systems provide good models to study ferrimagnetism. These systems have less translational symme-

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0375-9601/\$ - see front matter © 2005 Elsevier B.V. All rights reserved. doi:10.1016/j.physleta.2005.12.037 try than their "single-spin" counterparts and are well adopted to study a certain type of ferrimagnetism. Experimentally, the MnNi(EDTA)– $6H_2O$ complex has been shown to be an example of a mixed-spin system [3].

In order to examine the magnetic properties, these systems have been studied by various theoretical methods [4–18]. More recently, the effect of coordination number on the compensation temperature in the mixed Ising system on the two-fold Cayley tree has been discussed within the framework of exact recursion method [8].

Since the mixed Ising spin systems consist of two interpenetrating inequivalent sublattices, they exhibit unusual behaviors not observed in single-spin Ising models. The existence of compensation temperature is controversial in different approximate methods [5–10]. The studies based on mean-field approximation [5], effective-field theory [6], cluster variation method [7] and two-fold Cayley tree consideration [8] claim for the existence of compensation temperature with a Hamiltonian model that includes only nearest-neighbor couplings and crystal-fields. On the other hand, studies based on Monte Carlo simulations, transfer matrix methods [9] and renormalization group method [10] indicate that the compensation temperature exists only for the Hamiltonian model that includes also nextnearest-neighbor bonds. It is very important for the ferrimagnet to have the compensation temperature points, because of the high coercivity around this point.

Our aim in this Letter is to give an answer whether a compensation point is possible or not in the mixed-spin Ising ferrimagnetic system with only antiferromagnetic interaction J between pairs of nearest-neighbor spins σ and s and a crystal-field interaction Δ in the framework of exact Bethe lattice calculations. We focus on the existence predicted by mean-field and effective-field theories [5,6], cluster variation method [7] and two-fold Cayley tree treatment [8] and not found in Monte Carlo and transfer matrix studies [9] and renormalization group method [10]. The Bethe lattice consideration is an adequate starting point. Within this theoretical framework we determine some outstanding features in the temperature dependences of sublattice and total magnetizations. Gujrati [19] has shown that in many cases the behavior of spin models on hierarchical graphs is qualitatively correct even when conventional meanfield theories fail. The correlations are present on the Bethe-like lattices and the advantage introduced is that for the models formulated on it, the exact recursion relations can be derived. It should be mentioned that the recursion method in this study is an exact method only on the Bethe lattice. However, the results of Bethe lattice are approximate for the physical Bravais lattices such as two-dimensional square and three-dimensional simple cubic lattice. The solution we will obtain is for the deep interior of the infinite Cayley tree, which is called the Bethe lattice [20].

We consider the mixed spin-1/2 and spin-1 Ising system with crystal-field interaction, described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i \sigma_j + \Delta \sum_i s_i^2. \tag{1}$$

A Bethe lattice is obtained by the following geometrical construction [20]: from a site, chosen initially as the central site, q bonds are emanated and connected to the central site with its q nearest-neighbors. Each of these nearest-neighbors are connected similarly to q - 1 distinct new sites, each of which, in turn, is connected to yet another new set of q - 1 sites, and so on to infinity. In other words, each parent site is connected to its q-1 offsprings through q-1 bonds and another bond connects it to its own parent site. The smallest nontrivial value of qis 3 because q = 2 corresponds to a one-dimensional chain. In the case of mixed spins, the Bethe lattice is composed of two different kinds of sublattices A and B, seen in Fig. 1. One is occupied by spin-1 magnetic atoms at site i, while the other is occupied by spin-1/2 magnetic atoms at site j. Δ is the parameter of crystal-field, assumed to be positive. J defines the exchange interaction between the spin at site *i* and its neighbor at site *j*. The analysis will be performed only for the simple case of the antiferromagnetic nearest-neighbor interaction. The partition function will be written as

$$Z = \operatorname{Trexp}(-\beta \mathcal{H})$$

= $\operatorname{Trexp}\left[\beta \left(J \sum_{\langle ij \rangle} s_i \sigma_j - \Delta \sum_i s_i^2\right)\right].$ (2)



Fig. 1. The mixed-spin Ising system consisting of two different kinds of magnetic atoms A (\bullet) and B (\bullet) with spin values $s_i = 1$ and $\sigma_j = 1/2$, respectively, on the Bethe lattice with coordination number q = 3.

As seen in Fig. 1, each s_i located at site *i* is a spin of kind 1 and each σ_j located at site *j* is a spin of another kind, i.e., kind 2, on the bipartite Bethe lattice. In the case of mixed spins, the bipartite Bethe lattice is arranged such that the central spin is spin-1, the next generation spins are the spin-1/2, and the next generation spins are again spin-1, and so on to infinity. From Fig. 1 it is obvious that if the Bethe lattice is cut at the central site 0, the lattice splits into *q* disconnected pieces or branches. Thus the partition function for the central site on the Bethe lattice can be written as

$$Z = \sum_{(s_0)} \exp[-\beta \Delta s_0^2] [g_n(s_0)]^q,$$
(3)

where s_0 is the central spin value on the lattice, and $g_n(s_0)$ is the partition function of an individual branch. The suffix *n* denotes the fact that the sub-tree has *n* shells, i.e., *n* steps from the root to the boundary sites. Each branch can be cut on the site σ_1 , which is the nearest to the central point, respectively. Thus we can obtain the expressions for $g_n(s_0)$ and $g_{n-1}(\sigma_1)$:

$$g_n(s_0) = \sum_{\sigma_1} \exp[\beta(Js_0\sigma_1)] [g_{n-1}(\sigma_1)]^{q-1},$$
(4)

and

$$g_{n-1}(\sigma_1) = \sum_{s_2} \exp\left[\beta \left(J\sigma_1 s_2 - \Delta s_2^2\right)\right] \left[g_{n-2}(s_2)\right]^{q-1}.$$
 (5)

Let us introduce the following variables w_{n-1} (for spin-1/2 magnetic atoms) and x_n , y_n (for spin-1 magnetic atoms) respectively,

$$w_{n-1} = \frac{g_{n-1}(+\frac{1}{2})}{g_{n-1}(-\frac{1}{2})},\tag{6}$$

and

$$x_n = \frac{g_n(+1)}{g_n(0)}, \qquad y_n = \frac{g_n(-1)}{g_n(0)}.$$
 (7)

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