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Mixed spin-$\frac{1}{2}$ and spin-S Ising ferrimagnets with a crystal field

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Abstract

The mixed spin-$\frac{1}{2}$ and spin-S ($S = 1, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$) Ising ferrimagnetic systems with a crystal field are studied within the framework of the exact recursion relations on the Bethe lattice. The phase diagrams and thermal behaviors of magnetizations are investigated numerically for the different values of lattice coordination numbers. We find that the present system shows behaviors different from pure Ising systems. The results show that there is no compensation points for the system with half-integer values.

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Keywords: Mixed-spins; Compensation temperature; Phase diagrams; Bethe lattice

1. Introduction

In recent years, much attention has been directed to two-sublattice mixed spin Ising systems. There are many new phenomena in these systems, which cannot be observed in their single-spin counterparts. These systems have less translational symmetry and are well adopted to study a certain type of ferrimagnetism [1]. An important property of a ferrimagnetic material is the possibility of the existence,

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under certain conditions, of a compensation temperature T_{comp} at which the total magnetization vanishes below its transition temperature T_c. The appearance of a compensation temperature is due to the fact that the magnetic moments of the sublattices compensate each other completely at $T = T_{comp}$, owing to the different temperature dependencies of the sublattice magnetizations. 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. This property is very useful in thermomagnetic recording. Since the pioneering work of Neél [1], the conditions for the appearance of a compensation point as well as the composition dependencies of the transition and the compensation temperatures have been extensively investigated. Important advances have been made in the synthesis of two- and three-dimensional ferrimagnets, such as organometallic ferrimagnets [2], networks of the mixed-metal material [3] and ferrimagnetic amorphous oxides containing Fe^{3+} ions [4]. From a theoretical point of view, the two-sublattice mixed Ising spin systems consisting of spin-$\frac{1}{2}$ and spin-S ($S > \frac{1}{2}$) have been introduced as a simple model showing ferrimagnetic behavior. These mixed spin systems have been studied by a variety of techniques. Many authors have investigated the magnetic properties of a mixed spin-$\frac{1}{2}$ and spin-1 Ising model with crystal-field or transverse field by various techniques. The most extensively studied mixed spin Ising model consists of half-integer and integer spins, i.e. spin-$\frac{1}{2}$ and spin-1: For example, the effective-field theory with correlations (EFT) [5–14],mean-field approximation (MFA) [15], the Monte-Carlo simulation [16,17], the renormalization group method [18–20], the cluster variation method [21], Bethe–Peierls approximation [22] and the Bethe lattice solution [23,24]. The existence of tricritical behavior is controversial among different approximate and exact results. Very recently, we have examined the mixed spin-$\frac{1}{2}$ and spin-1 Ising model on the Bethe lattice and two-fold Cayley tree [25,26], respectively. The results indicate the existence of compensation points for the lattice coordinations $q \geqslant 4$.

On the other hand, the magnetic properties of a mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising system without and with a crystal-field or a transverse field have been examined by the effective field theory [27–35], Monte-Carlo simulation [36] and exact treatments [37–40]. A convenient way to qualitatively discuss such systems is through a Bethe lattice approach. The Bethe lattice, traditionally viewed as graphs embedded in infinite-dimensional spaces, has been used to model a variety of problems. However, it has been pointed out by Mosseri and Sadoc [41] that this structure can be considered as regular lattices of fixed bond angles and lengths if they are embedded in a two-dimensional space of constant negative curvature. If one also ignores the boundary sites, the deep sites of a very large Cayley tree may be seen as a regular lattice, which is usually called a Bethe lattice [42–44]. As far as we know, the properties of mixed spin-$\frac{1}{2}$ and spin-S ($S = 1, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$) Ising systems with a crystal-field have not been examined on the Bethe lattice in detail. The purpose of this paper is to investigate whether a compensation point exists or not in the mixed spin-$\frac{1}{2}$ and spin-S Ising system by using the exact recursion relations on the Bethe lattice.

The rest of the paper is arranged as follows. The description of the model and its formulation are given in Section 2. Namely, we give the exact expressions of the partition function, the sublattice and total magnetizations on the Bethe lattice. The thermal variations of magnetizations, the total magnetizations and phase diagrams for $q = 3, 4, 6$ and 8 are presented in Section 3. The effect of crystal-field interaction and coordination numbers on the magnetic properties of the model is elucidated. Finally, we give concluding remarks in Section 4.

2. Model formulation on the Bethe lattice

We consider the mixed Ising spin-$\frac{1}{2}$ and spin-1 ferrimagnetic system ($J>0$) with crystal-field interaction, described by the Hamiltonian

$$\mathscr{H} = J \sum_{\langle ij \rangle} S_i \sigma_j + \Delta \sum_i S_i^2 \, . \tag{1}$$

A Bethe lattice is obtained by the following geometrical construction: From a site, chosen initially as the central site, q bonds emanate and connect 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 infinite. 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 solution we will obtain is for the deep interior of the infinite Cayley tree, which is called the Bethe lattice [42–44]. The constructed Bethe lattice has two 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-$\frac{1}{2}$ magnetic atoms at site j. Δ is the

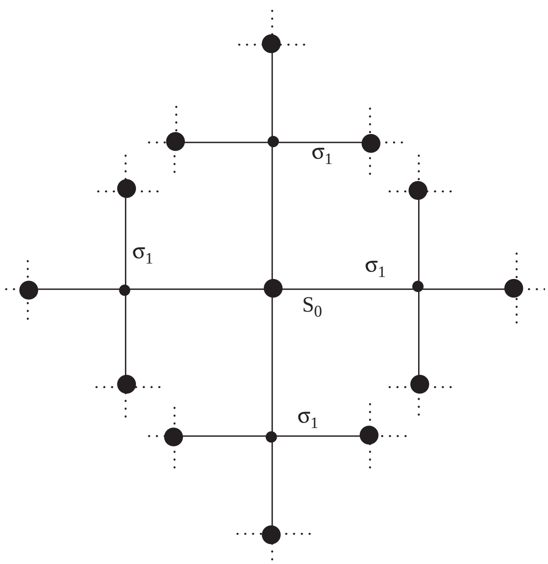

Fig. 1. The mixed-spin Ising system consisting of two kinds of magnetic atoms A (●) and B (•) with spin values $S_i = 1, \frac{3}{2}, \frac{5}{2}$ and $\frac{7}{2}$ and $\sigma_j = \frac{1}{2}$, respectively, on the Bethe lattice with coordination number $q = 4$.

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. In this section, the formulation of the problem only will be made for $S=\frac{5}{2}$ and $\sigma=\frac{1}{2}$. The partition function can be written as

$$Z=\sum\exp(-\beta\mathscr{H}) \\ =\sum_{(S,\sigma)}\exp\left[\beta\left(-J\sum_{\langle ij\rangle}S_i\sigma_j-\Delta\sum_i S_i^2\right)\right]. \tag{2}$$

From Fig. 1 it is obvious that if the Bethe lattice is cut at the central site 0 with a spin value S_0, the lattice splits into q identical branches. Each of these is a rooted tree at the central spin S_0. Thus the partition function on the Bethe lattice can be written as

$$Z=\sum_{(S_0)}\exp[-\beta(\Delta S_0^2)][g_n(S_0)]^q, \tag{3}$$

where S_0 is the central spin value on the lattice, and the partition function of an individual branch, namely $g_n(S_0)$ is

$$g_n(S_0)=\sum_{\sigma_1}\exp\left[\beta\left\{-JS_0\sigma_1-J\sum_{\langle ij\rangle}S_i\sigma_j-\Delta\sum_i S_i^2\right\}\right]. \tag{4}$$

Each branch can be cut on the site σ_1, which is nearest to the central point, respectively. Thus we can obtain the expressions for $g_n(S_0)$ and $g_{n-1}(\sigma_1)$:

$$g_n(S_0)=\sum_{\sigma_1}\exp[\beta\{-JS_0\sigma_1\}][g_{n-1}(\sigma_1)]^{q-1} \tag{5}$$

and

$$g_{n-1}(\sigma_1)=\sum_{S_2}\exp[\beta(-J\sigma_1S_2-\Delta S_2^2)][g_{n-2}(S_2)]^{q-1}. \tag{6}$$

Let us introduce the following variables w_{n-1} (for spin-$\frac{1}{2}$ magnetic atoms) and x_n, y_n, z_n, t_n, v_n (for spin-$\frac{5}{2}$ magnetic atoms), respectively,

$$w_{n-1}=\frac{g_{n-1}(+\frac{1}{2})}{g_{n-1}(-\frac{1}{2})} \tag{7}$$

and

$$x_n=\frac{g_n(\frac{5}{2})}{g_n(-\frac{1}{2})},\quad y_n=\frac{g_n(-\frac{5}{2})}{g_n(-\frac{1}{2})},\quad z_n=\frac{g_n(\frac{3}{2})}{g_n(-\frac{1}{2})},\quad t_n=\frac{g_n(-\frac{3}{2})}{g_n(-\frac{1}{2})},\quad v_n=\frac{g_n(\frac{1}{2})}{g_n(-\frac{1}{2})}. \tag{8}$$

Since S_0 can take the values $\pm\frac{5}{2},\pm\frac{3}{2},\pm\frac{1}{2}$, one can obtain six different $g_n(S_0)$ for two possible values of σ_1. Thus

$$g_n(\pm\tfrac{5}{2})=\sum_{\sigma_1}\exp(\beta(\mp\tfrac{5}{2}J\sigma_1))[g_{n-1}(\sigma_1)]^{q-1},$$

$$g_n(\pm\tfrac{5}{2}) = \exp(\beta(\mp\tfrac{5}{4}J))[g_{n-1}(\tfrac{1}{2})]^{q-1} + \exp(\beta(\pm\tfrac{5}{4}J))[g_{n-1}(-\tfrac{1}{2})]^{q-1} , \tag{9}$$

$$g_n(\pm\tfrac{3}{2}) = \sum_{\sigma_1} \exp(\beta(\mp\tfrac{3}{2}J\sigma_1))[g_{n-1}(\sigma_1)]^{q-1} ,$$

$$g_n(\pm\tfrac{3}{2}) = \exp(\beta(\mp\tfrac{3}{4}J))[g_{n-1}(\tfrac{1}{2})]^{q-1} + \exp(\beta(\pm\tfrac{3}{4}J))[g_{n-1}(-\tfrac{1}{2})]^{q-1} \tag{10}$$

and

$$g_n(\pm\tfrac{1}{2}) = \sum_{S_1} \exp(\beta(\mp\tfrac{1}{2}J\sigma_1))[g_{n-1}(\sigma_1)]^{q-1} ,$$

$$g_n(\pm\tfrac{1}{2}) = \exp(\beta(\mp\tfrac{1}{4}J))[g_{n-1}(\tfrac{1}{2})]^{q-1} + \exp(\beta(\pm\tfrac{1}{4}J))[g_{n-1}(-\tfrac{1}{2})]^{q-1} . \tag{11}$$

On the other hand, since σ_1 can take the values $\pm\frac{1}{2}$, one can obtain two different $g_{n-1}(\sigma_1)$ for two possible values of σ_1:

$$g_{n-1}(\pm\tfrac{1}{2}) = \sum_{S_2} \exp(\beta(\mp\tfrac{1}{2}JS_2 - \Delta S_2^2))[g_{n-2}(S_2)]^{q-1} ,$$

$$\begin{aligned} g_{n-1}(\pm\tfrac{1}{2}) = {} & \exp(\beta(\mp\tfrac{5}{4}J - \tfrac{25}{4}\Delta))[g_{n-2}(\tfrac{5}{2})]^{q-1} + \exp(\beta(\pm\tfrac{5}{4}J - \tfrac{25}{4}\Delta))[g_{n-2}(-\tfrac{5}{2})]^{q-1} \\ & \times \exp(\beta(\mp\tfrac{3}{4}J - \tfrac{9}{4}\Delta))[g_{n-2}(\tfrac{3}{2})]^{q-1} + \exp(\beta(\pm\tfrac{3}{4}J - \tfrac{9}{4}\Delta))[g_{n-2}(-\tfrac{3}{2})]^{q-1} \\ & \times \exp(\beta(\mp\tfrac{1}{4}J - \tfrac{1}{4}\Delta))[g_{n-2}(\tfrac{1}{2})]^{q-1} + \exp(\beta(\pm\tfrac{1}{4}J - \tfrac{1}{4}\Delta))[g_{n-2}(-\tfrac{1}{2})]^{q-1} . \end{aligned} \tag{12}$$

Thus we can obtain a set of six recursion relations from which the sublattice magnetizations can be found. The recursion relations are found by substituting Eqs. (9)–(12) into Eqs. (7)–(8). The values of x_n, y_n, z_n, t_n, v_n and w_{n-1} have no direct physical meaning, but one can express the magnetizations and other thermodynamic quantities. Thus, we can say that in the thermodynamic limit ($n \to \infty$) the above variables determine the states of the system. The sublattice magnetizations of the mixed ferrimagnetic system are expressed in terms of recursion relations by

$$M_{5/2} = Z_{5/2}^{-1} \sum_{S_0} S_0 \exp\{-\beta\Delta S_0^2)\}[g_n(S_0)]^q ,$$

$$\begin{aligned} M_{5/2} = {} & Z_{5/2}^{-1}\{\tfrac{5}{2}\mathrm{e}^{-(25/4)\beta\Delta}([g_n(\tfrac{5}{2})]^q - [g_n(-\tfrac{5}{2})]^q) + \tfrac{3}{2}\mathrm{e}^{-(9/4)\beta\Delta}([g_n(\tfrac{3}{2})]^q - [g_n(-\tfrac{3}{2})]^q) \\ & + \tfrac{1}{2}\mathrm{e}^{-(1/4)\beta\Delta}([g_n(\tfrac{1}{2})]^q - [g_n(-\tfrac{1}{2})]^q)\} , \end{aligned}$$

$$M_{5/2} = \frac{\tfrac{5}{2}\mathrm{e}^{-(25/4)\beta\Delta}(x_n^q - y_n^q) + \tfrac{3}{2}\mathrm{e}^{-(9/4)\beta\Delta}(z_n^q - t_n^q) + \tfrac{1}{2}\mathrm{e}^{-(1/4)\beta\Delta}(v_n^q - 1)}{\mathrm{e}^{-(25/4)\beta\Delta}(x_n^q + y_n^q) + \mathrm{e}^{-(9/4)\beta\Delta}(z_n^q + t_n^q) + \mathrm{e}^{-\frac{1}{4}\beta\Delta}(v_n^q + 1)} \tag{13}$$

and

$$M_{1/2} = Z_{1/2}^{-1} \sum_{\sigma_1} \sigma_1[g_{n-1}(\sigma_1)]^q ,$$

$$M_{1/2} = \frac{1}{2}\frac{[g_{n-1}(+\frac{1}{2})]^q - [g_{n-1}(-\frac{1}{2})]^q}{[g_{n-1}(+\frac{1}{2})]^q + [g_{n-1}(-\frac{1}{2})]^q}$$

$$M_{1/2} = \frac{1}{2}\frac{w_{n-1}^q - 1}{w_{n-1}^q + 1} \ . \tag{14}$$

Here, we define the averaged total magnetization per site as

$$M = \tfrac{1}{2}(M_{5/2} + M_{1/2}) \ . \tag{15}$$

It should be mentioned here that within the present framework we can investigate the crystal-field and coordination number effects of Bethe lattice on the phase diagram and magnetization curves for the ferrimagnetic (if $J>0$) or ferromagnetic (if $J<0$) mixed Ising spin systems. However, we will discuss below the physical quantities of the ferrimagnetic system only, since from an experimental point of view the study may be very important.

3. Results and discussions

In this section, we show some typical results for the mixed spin-$\frac{1}{2}$ and spin-S Ising systems with the presence of the crystal field on the Bethe lattice.

3.1. Phase diagrams ($S = 1$ and $\frac{3}{2}$)

Let us investigate the phase diagrams of the mixed spin Ising systems with $S = 1$ and $\frac{3}{2}$ on the Bethe lattice with $q = 4$ and 5 by solving the general expressions given in Section 3 numerically. The phase diagrams of the system with $S = 1$ and $\frac{3}{2}$ are shown in Fig. 2 by changing the value of coordination q, in order to see the difference between $q = 4$ and 5. The solid lines represent the second-order phase transition and separate the ferrimagnetic phase from the disordered phase. As seen from Fig. 2(a),

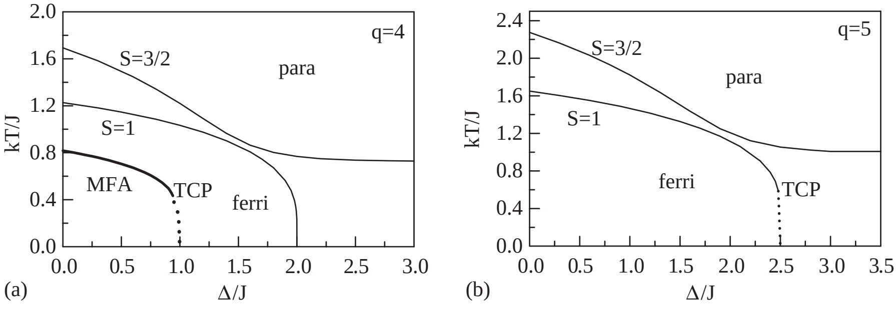

Fig. 2. The phase diagrams of the ferrimagnetic mixed spin Ising system with $S = 1$ and $S = \frac{3}{2}$ when $\sigma = \frac{1}{2}$. Solid and dotted lines denote the continuous and first-order transitions, respectively. (a) $q = 4$ and (b) $q = 5$.

the system with $S = 1$ does not exhibit a tricritical point (TCP) in the phase diagram for $q = 4$, although the Bethe lattice with $q = 5$ can show a tricritical point [23,24], seen in Fig. 2(b). A mean-field analysis (MFA) of the ferromagnetic spin-$\frac{1}{2}$ and spin-1 Ising system exhibits a tricritical point, seen in Fig. 2(a). This result is not surprising since MFA, in general, does not describe correctly low-dimensional systems. On the other hand, the behavior of the mixed spin system with $S = \frac{3}{2}$ is completely different from the system with $S = 1$. For all coordination numbers, the transition line between the ferrimagnetic and disordered phase is always of second-order (Fig. 2). Furthermore, the curves in Fig. 2 change continuously from a constant value for a large negative Δ to a constant value for a large positive Δ. It comes from the following fact: For a large negative value of $\Delta(\Delta/J = -2.5)$ the spin state of S_i^z is in the $S_i^z = \pm\frac{3}{2}$ at the ground state $T = 0$. But, it is in the $S_i^z = \pm\frac{1}{2}$ state for a large positive $\Delta(\Delta/J = 3.0)$. Thus, from Fig. 2(a) and (b) one may imagine that the tricritical behavior (where the phase transition changes from the second-order to the first-order) does not exist in the system with $S = \frac{3}{2}$, in contrast to the system with $S = 1$.

3.2. Compensation points ($S = 1$ and $\frac{3}{2}$)

A compensation point corresponds to the temperature T_{comp} below the transition temperature such that the sublattice magnetizations compensate each other and the total magnetization M_T (Eq. (15)) vanishes. The total and sublattice magnetization curves are shown in Fig. 3 for ferrimagnetic mixed spin Ising system. From Fig. 3(a), we see that only one compensation point can exist for the ferrimagnetic system with $S = 1$. However, when $S = \frac{3}{2}$ the system does not exhibit a compensation point for all values of Δ (Fig. 3(b)). Thus, it is very important that the role of the crystal field Δ, coordination number q, and spin value on the existence of the compensation point and tricritical point. When only the nearest-neighbor interaction and the crystal-field term are included our results indicate no compensation temperature at finite temperature. The obtained result is reasonable in comparison with the approximate [27–35], Monte-Carlo simulation [36] and exact results [37–40].

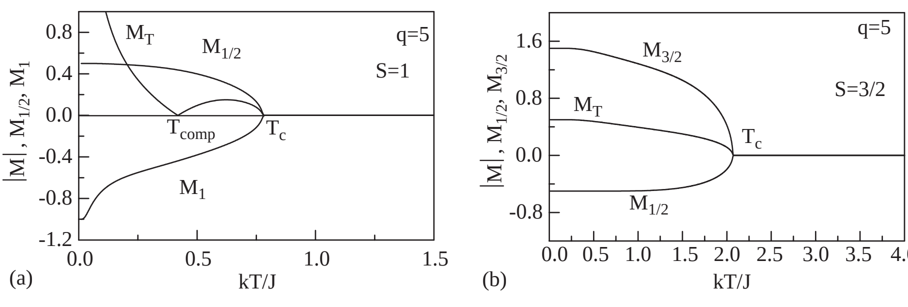

Fig. 3. The temperature dependence of the total magnetization for the ferrimagnetic system with $S = 1$ and $S = \frac{3}{2}$ when $\sigma = \frac{1}{2}$. (a) The system with $S = 1$ exhibits only one compensation point. (b) The system with $S = \frac{3}{2}$ does not exhibit any compensation point.

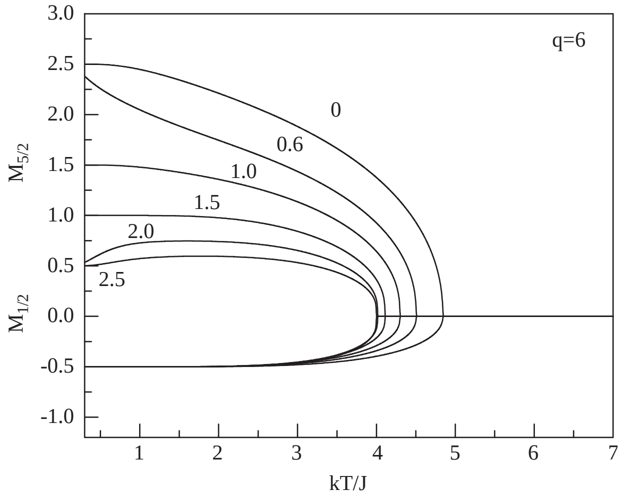

Fig. 4. The temperature dependence of the sublattice magnetizations of the system with $S = \frac{5}{2}$ and $\sigma = \frac{1}{2}$. The numbers at the curves are the crystal field Δ/J.

3.3. *Magnetization curves and phase diagrams* ($S = \frac{5}{2}, \frac{7}{2}$)

In order to see the effects of the spin values on the compensation point and phase diagrams of the mixed spin ferrimagnetic system more clearly, the sublattice and total magnetization curves are presented in Figs. 4 and 5, respectively, for selected values of Δ/J when $q = 6$. Looking at Figs. 4 and 5, the behavior of sublattice and total magnetization curves is similar to those of Fig. 3(b). As a consequence, the compensation point does not exist in the system with half-integer spin values ($S = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \ldots$). We also considered other integer values of S and we found that only one compensation point can exist for integer spins and any compensation point is not possible when S is an integer.

Finally, Fig. 6 shows the phase diagrams of the mixed ferrimagnetic Ising system with $S = \frac{5}{2}$ for $q = 3, 4, 6$ and 8. The present system exhibits only second-order phase transition. It should also be mentioned that as the coordination number increases the second-order phase transitions occur at higher critical temperatures.

4. Concluding remarks

In this work, we have studied a mixed spin-$\frac{1}{2}$ and spin-S ($S = 1, \frac{3}{2}, \frac{5}{2}, \ldots$) Ising system on the Bethe lattice within the exact recursion relations. In Section 2, only the formulation of the model for $\sigma = \frac{1}{2}$ and $S = \frac{5}{2}$ has been presented. The systems with $S = 1, \frac{3}{2}$ and $\frac{7}{2}$ are easily formulated. In Section 3, we have investigated a mixed spin-$\frac{1}{2}$ and spin-S Ising system by solving the recursion relations of the mixed spin-$\frac{1}{2}$ and spin-S systems on the Bethe lattice with arbitrary coordination numbers q,

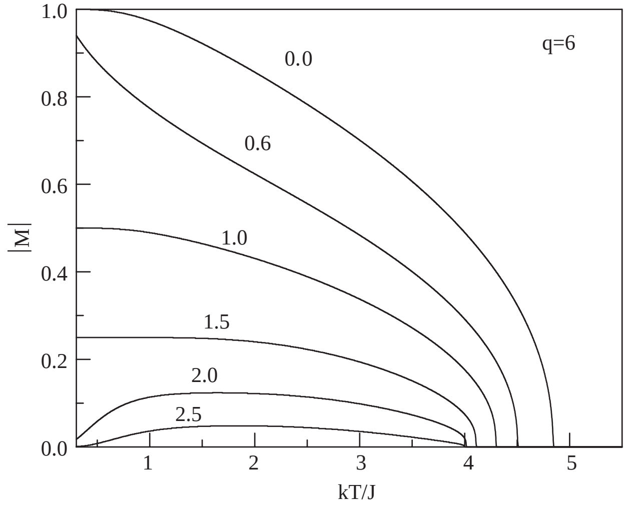

Fig. 5. The total magnetization M versus kT/J curves when $S = \frac{5}{2}$. The numbers at the curves are the crystal-field Δ/J.

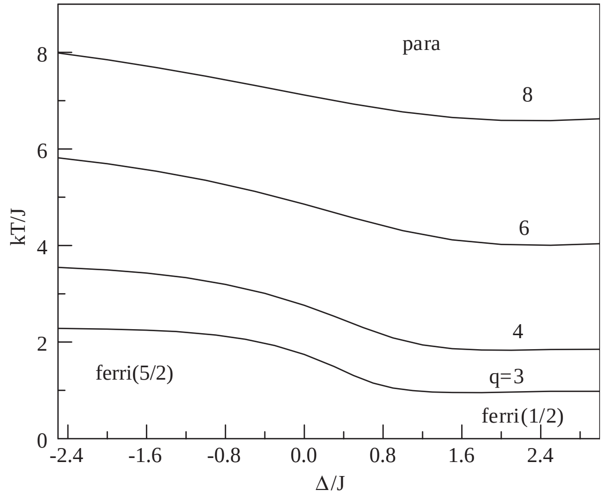

Fig. 6. The phase diagrams of the ferrimagnetic Ising system with $S = \frac{5}{2}$ for different values of q. The solid lines represent the continuous transition temperature.

numerically. In general, the solution of the problem on the arbitrary lattices is obtained through the evaluation of fixed points of a set of recursion relations. We have also given the sublattice, total magnetization curves and phase diagrams in Section 3.

To make a comparison with other methods such as EFT [27–35], Monte-Carlo simulation [36] and exact solutions [37–40], the effect of the coordination number and crystal-field on the compensation temperatures and tricritical point was examined. We have shown that the mixed spin-$\frac{1}{2}$ and spin-S (If S is an half-integer value) Ising systems on the Bethe lattice with coordination number q do not exhibit any compensation point, depending on the values of Δ/J, in contrast to mixed spin-$\frac{1}{2}$ and spin-1 system with $q\geqslant 4$. Moreover, the mixed spin-$\frac{1}{2}$ and spin-S Ising system exhibits different behavior from the corresponding spin-$\frac{1}{2}$ and spin-1 system, where for coordination number $q\geqslant 5$ the tricritical point has been found in different methods [21–26].

Finally, the present framework provides qualitative and to a certain extent also quantitative confidence. The solution of the problem on the deep sites may be viewed as approximations to the exact solutions on the regular lattices such as honeycomb, square and simple cubic lattices. We believe that these results may be helpful in the analysis of the experimental data for ferrimagnetic materials.

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