The mixed-spins 1/2 and 3/2 Blume–Capel model with a random crystal field

Erhan Albayrak†

Erciyes University, Department of Physics, 38039, *Kayseri, Turkey*

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The random crystal field (RCF) effects are investigated on the phase diagrams of the mixed-spins 1/2 and 3/2 Blume–Capel (BC) model on the Bethe lattice. The bimodal random crystal field is assumed and the recursion relations are employed for the solution of the model. The system gives only the second-order phase transitions for all values of the crystal fields in the non-random bimodal distribution for given probability. The randomness does not change the order of the phase transitions for higher crystal field values, i.e., it is always second-order, but it may introduce first-order phase transitions at lower negative crystal field values for the probability in the range about 0.20 and 0.45, which is only the second-order for the non-random case in this range. Thus our work claims that randomness may be used to induce first-order phase transitions at lower negative crystal field values at lower probabilities.

Keywords: randomness, crystal field, Bethe lattice, mixed spin, bimodal

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1. Introduction

Mixed-spin models with different spins have been studied extensively, since they exhibit less translational symmetry than their single counterparts and may show many new phenomena that cannot be observed in the single-spin Ising models. These models are well adopted to study a certain type of ferrimagnetism which are of great interest because of their interesting and possible useful properties. Experimentally, it was shown that the MnNi (EDTA)–$6H_2O$ complex is a mixed-spin system.[1]

The mixed spin-1/2 and spin-1 models have been studied very extensively with a variety of theoretical techniques, but the case of spin-1/2 and spin-3/2 has not received enough attention so far. The mixed spin-1/2 and spin-3/2 model with a crystal field acting on all spin-3/2 sites, which corresponds to the case with a probability of $p = 1$, was studied with only a few techniques. Thus, just a few works could be reported for the study of the mixed spin-1/2 and spin-3/2 Ising system; the transverse Ising model with a crystal field within the framework of the effective field theory (EFT) with correlations on the honeycomb lattice,[2] on a square lattice by using the EFT,[3,4] again on a square lattice with a Monte Carlo (MC) algorithm,[5] in terms of the recursion relations on the Bethe lattice,[6] by establishing a mapping correspondence with the eight-vertex model on the Union Jack lattice[7] and in the Heisenberg model by the use of the Oguchi approximation.[8]

The inclusion of a crystal field into the system may change its critical behavior considerably. If it is strong enough, the energy difference between the split levels is large. Then, it is energetically more favorable to put as many electrons into the lower energy level before one starts to fill the higher energy level. Filling all the orbitals in the lower level means one has to pair them up within each orbital with opposite spins. The effect of pairing electrons with opposite spins makes no addition to the total spin. This results in a low-spin state. Thus its competition with the bilinear interaction parameter may lead to the first-order phase transitions. Lately, the random distribution of crystal fields with some probabilities instead of a constant one, i.e., $p = 1$, have become popular to investigate. The effect of randomness and the distribution type of the crystal field may change the critical behavior of the system considerably, therefore, the Blume–Capel (BC) model with a random crystal field (RCF) is going to be studied here on the Bethe lattice for the mixed spin-1/2 and spin-3/2 Ising model.

The first and only works for the mixed-spin models with RCF include only the spin-1/2 and spin-1. It was studied with effective-field theory with correlations,[9−11] within the mean field approach[12,13] and within the finite cluster approximation based on a single-site cluster theory.[14] It

†Corresponding author. E-mail: albayrak@erciyes.edu.tr

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is unfortunate that no other mixed-spin models with RCF have been investigated so far.

Therefore, in this work, the effects of the bimodal RCF in the form of $P(\Delta_i) = p\delta(\Delta_i - \Delta) + (1-p)\delta(\Delta_i)$ are investigated on the Bethe lattice for given coordination numbers $z = 3, 4, 5$, and 6. This distribution of the RCF either turns off or on the given crystal field values on the spin-3/2 sites of the Bethe lattice randomly with given probability. The phase diagrams of the model are obtained on the $(\Delta, kT/J)$ and $(p, kT/J)$ planes for given values of probabilities p and the reduced crystal field values $\Delta = D/J$, respectively. It was found that the randomness may change the type of phase transitions from the second-order to the first-order at lower negative Δ values for the probability values in the range about 0.20–0.45.

The remaining part of this work is organized as follows: The next section is devoted for the explanation and formulation of our model on the Bethe lattice and the last section includes our illustrations and findings in addition to a brief summary and conclusion.

2. The formulation

The Hamiltonian for the mixed spin-1/2 and 3/2 BC model[6] is given as

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} s_i \sigma_j + \sum_j D_j \sigma_j^2, \tag{1}$$

where J is the bilinear exchange interactions between the nearest neighboring (NN) spins, i.e., only between spin-1/2 and spin-3/2, and D_j is the site-dependent crystal field acting only to the spin-3/2 sites.

In the case of mixed spin-1/2 and spin-3/2, each s_i located at site i is a spin-1/2 and can take the values $\pm 1/2$ and each σ_j located at site j is a spin-3/2 which can take the values $\pm 3/2$ and $\pm 1/2$ on the Bethe lattice. In this formulation the Bethe lattice is arranged such that[6] the central-spin is spin-1/2, the next generation is spin-3/2, and the next generation is again spin-1/2, and so on to infinity (see Fig. 1). It is important to note here that the choice of the central-spin, i.e., whether it is spin-1/2 or spin-3/2, does not affect the results and both choices lead to the same physical conclusions.[15,16]

The formulation of the mixed spin-1/2 and spin-3/2 BC model has already been obtained in terms of recursion relations,[6] thus we do not go into details and give only the necessary equations. The recursion relations may serve as the equation of states of the problem. They are defined as the ratios of the partial partition functions of $g_n(S)$ for each of the separate branches of the tree. Thus for this model, one can obtain only one recursion relation for the sites with spin-1/2 which is found as

$$\begin{aligned} X_n = {} & [\,\mathrm{e}^{\beta'(0.75+2.25\Delta_i)} A_{n-1}^{z-1} + \mathrm{e}^{\beta'(-0.75+2.25\Delta_i)} B_{n-1}^{z-1} + \mathrm{e}^{\beta'(0.25+0.25\Delta_i)} C_{n-1}^{z-1} \\ & + \mathrm{e}^{\beta'(-0.25+0.25\Delta_i)}]/[\,\mathrm{e}^{\beta'(-0.75+2.25\Delta_i)} A_{n-1}^{z-1} + \mathrm{e}^{\beta'(0.75+2.25\Delta_i)} B_{n-1}^{z-1} \\ & + \mathrm{e}^{\beta'(-0.25+0.25\Delta_i)} C_{n-1}^{z-1} + \mathrm{e}^{\beta'(0.25+0.25\Delta_i)}], \end{aligned} \tag{2}$$

and three recursion relations for the spin-3/2 sites

$$\begin{aligned} A_{n-1} &= \frac{\mathrm{e}^{0.75\beta'} X_{n-2}^{z-1} + \mathrm{e}^{-0.75\beta'}}{\mathrm{e}^{-0.25\beta'} X_{n-2}^{z-1} + \mathrm{e}^{0.25\beta'}}, \\ B_{n-1} &= \frac{\mathrm{e}^{-0.75\beta'} X_{n-2}^{z-1} + \mathrm{e}^{0.75\beta'}}{\mathrm{e}^{-0.25\beta'} X_{n-2}^{z-1} + \mathrm{e}^{0.25\beta'}}, \\ C_{n-1} &= \frac{\mathrm{e}^{0.25\beta'} X_{n-2}^{z-1} + \mathrm{e}^{-0.25\beta'}}{\mathrm{e}^{-0.25\beta'} X_{n-2}^{z-1} + \mathrm{e}^{0.25\beta'}}, \end{aligned} \tag{3}$$

where $\beta' = \beta J = J/kT$ is the reduced temperature with k being the Boltzmann constant, $\Delta_i = D_i/J$ is the reduced crystal field and z is the number of nearest neighbors. n counts the number of the shells and goes to infinity in the thermodynamic limit on the Bethe lattice.

Since the spin-1/2 system is a two-state and one order-parameter system, one needs to define only one order-parameter which is the dipole moment or the magnetization $M_{1/2}$ and it is given in terms of the recursion relations as

$$M_{12} = \frac{1}{2}\left[\frac{X_n^z - 1.0}{X_n^z + 1.0}\right], \tag{4}$$

and spin-3/2 system is a four-state system for which one needs at least two order-parameters to define it, i.e., they are the magnetization $M_{3/2}$ and the quadrupolar moment $Q_{3/2}$, and are given in terms of the recursion relations as

$$M_{32} = \frac{1.5\,\mathrm{e}^{2.25\beta'\Delta_i}(A_{n-1}^z - B_{n-1}^z) + 0.5\,\mathrm{e}^{0.25\beta'\Delta_i}(C_{n-1}^z - 1.0)}{\mathrm{e}^{2.25\beta'\Delta_i}(A_{n-1}^z + B_{n-1}^z) + \mathrm{e}^{0.25\beta'\Delta_i}(C_{n-1}^z + 1.0)},$$

$$Q_{32} = \frac{2.25\,\mathrm{e}^{2.25\beta'\Delta_i}(A^z_{n-1} + B^z_{n-1}) + 0.25\,\mathrm{e}^{0.25\beta'\Delta_i}(C^z_{n-1} + 1.0)}{\mathrm{e}^{2.25\beta'\Delta_i}(A^z_{n-1} + B^z_{n-1}) + \mathrm{e}^{0.25\beta'\Delta_i}(C^z_{n-1} + 1.0)}. \tag{5}$$

After having given the formulation of the mixed spin-1/2 and spin-3/2 BC model on the Bethe lattice, we are now ready to introduce the random crystal field which acts only on the spin-3/2 sites and is distributed according to

$$P(\Delta_i) = p\delta(\Delta_i - \Delta) + (1-p)\delta(\Delta_i). \tag{6}$$

This is the bimodal random distribution of the crystal field, i.e., equation (6), either turns on or off the crystal field randomly for a given probability p on the shells of the Bethe lattice consisting of spin-3/2 sites only. If the crystal field is turned on, then, all the spins on that shell are under the effect of the given crystal field otherwise they are all turned off for all the spin-3/2 sites on that shell (See Fig. 1).

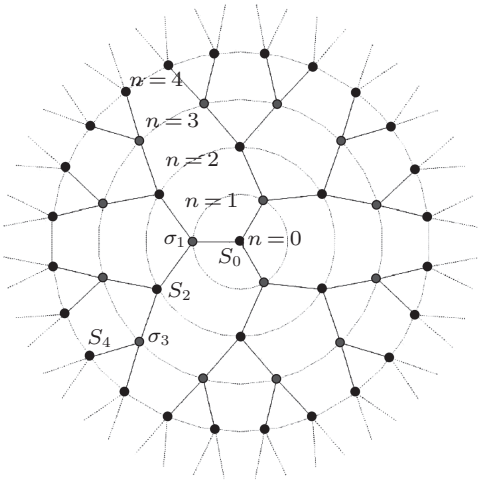


Fig. 1. The Bethe lattice of coordination number z=3. The black circles denote the spin-1/2 and the gray ones refer to the spin-3/2. n counts the number of shells which goes to infinity in the thermodynamic limit. The crystal field values are turned on or off randomly for given probability p.

The second-order phase transition temperatures are determined from the thermal variations of the order-parameters. In order to determine the first-order phase transition temperatures, one may also need the free energy expression in addition to the order-parameters. It can be calculated in terms of the recursion relations by using the definition $F = -kT\ln Z$ and it is obtained in thermodynamic limit, i.e., $n \to \infty$, as

$$\begin{aligned} F/J = -\frac{1}{\beta'}\Bigg[& \frac{1}{2-z}\ln[\,\mathrm{e}^{\beta'(-0.75+2.25\Delta_i)}A^{z-1}_{n-1} \\ & + \mathrm{e}^{\beta'(0.75+2.25\Delta_i)}B^{z-1}_{n-1} \\ & + \mathrm{e}^{\beta'(-0.25+0.25\Delta_i)}C^{z-1}_{n-1}] \\ & + \frac{z-1}{2-z}\ln\left[\,\mathrm{e}^{-0.25\beta'}X^{z-1}_n + \mathrm{e}^{-0.25\beta'}\right] \\ & + \ln\left[X^z_n + 1\right]\Bigg]. \end{aligned} \tag{7}$$

After obtaining the numerical values for the recursion relations, i.e., Eqs. (2) and (3), the order-parameters and free energy can be obtained easily by using an iteration scheme which include the effects of the RCF for the given system.

3. Results and conclusions

In order to obtain the critical behaviors of this model, i.e., the phase diagrams, we have studied the thermal variations of the order-parameters and free energy. Thus, the phase diagrams are obtained on the $(\Delta, kT/J)$ planes for given values of the probability p between 0 and 1 with the increment 0.1 and on the $(p, kT/J)$ planes for given values of Δ for the coordination numbers $z = 3, 4, 5$, and 6. In the phase diagrams, the solid lines, named as the critical lines, are constructed from either second- or first-order phase transition temperatures and separate the ferromagnetic (F) regions from the paramagnetic (P) ones.

Figures 2(a)–2(d) illustrate the phase diagrams on the $(\Delta, kT/J)$ planes for given p with the increment of 0.1. As seen from the figures and Eq. (6), the $p = 0$ lines correspond to the $\Delta = 0.0$ case for which the critical lines are straight lines as expected, since the Hamiltonian has only the interaction parameter J which enters into the formulation as a scaling parameter. The case with $p = 1$ corresponds to the mixed spin-1/2 and 3/2 BC model with all the spin-3/2 sites being under the influence of the crystal field.[6] The model is the RCF model for the intermediate values of the probability, i.e., for $0 < p < 1$. The critical lines start from higher temperatures at lower negative Δ for lower p, i.e., the lowest temperature is seen for $p = 1$. Then, as Δ increases towards zero the critical lines increase monotonically at lower p's but the increase gets sharper for higher p's. This is obvious as explained above for the cases of $p = 0$ and $p = 1$. All the critical lines for all p and each z combine at $\Delta = 0$ as expected which of course corresponds to the $p = 0$

case. The critical lines start spreading up with the further increase of Δ and they are seen at higher temperatures for higher p for $\Delta > 0.0$. As mentioned above, the temperatures of the critical lines become constant as $\Delta \to -\infty$ and $\Delta \to \infty$ at lower and higher temperatures, respectively, for all p values. The biggest temperature difference is seen for the $p = 1$ case and there is no temperature difference for the $p = 0$ case. The critical lines are seen at lower temperatures for a lower negative crystal field. Since the lower Δ values drive the system to the lowest spin states, i.e., to the $\pm 1/2$, therefore, they are seen at lower temperatures as explained in the introduction. We should also mention that the critical lines are seen at higher temperatures for higher z which is expected. The critical temperatures of the mixed spin-1/2 and 3/2 model are seen at a lower temperature when compared with the spin-3/2 RCF model,[17] which is caused by the existence of the spin-1/2 for the mixed-spin case.

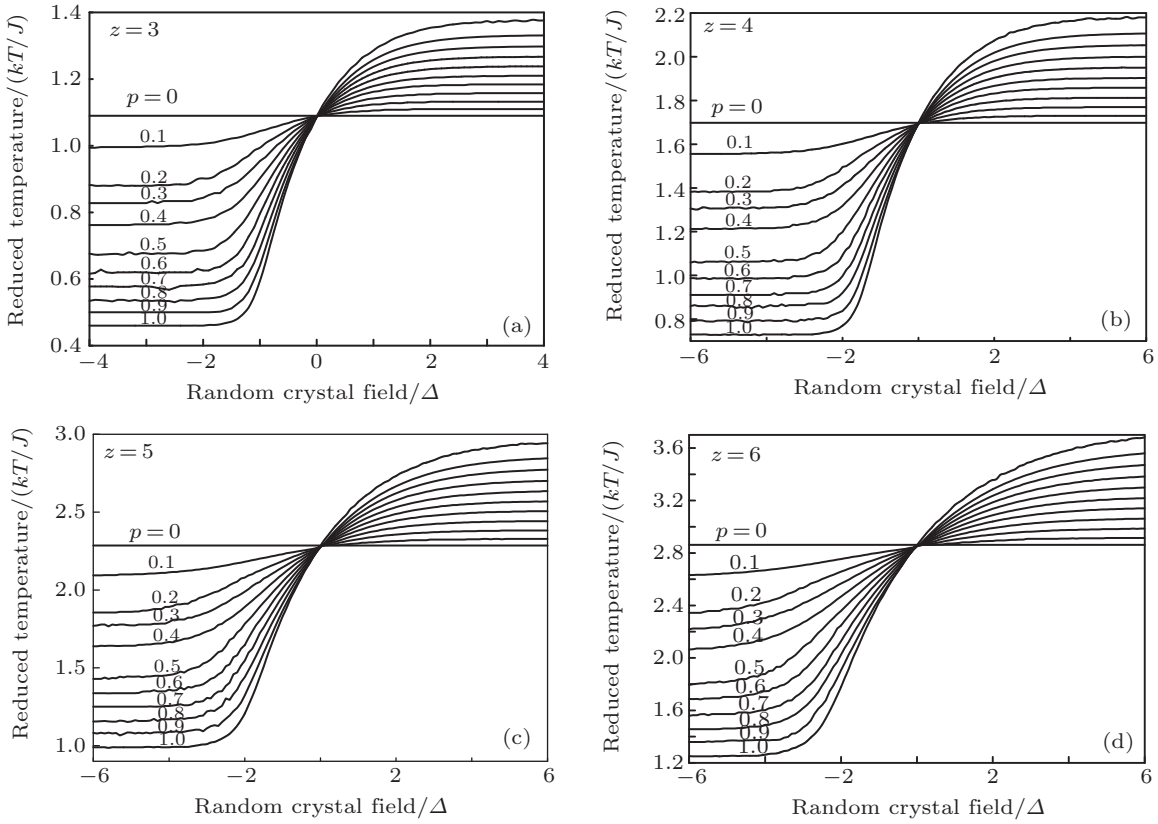


Fig. 2. The phase diagrams on the $(\Delta, kT/J)$ plane for given values of the probability p between 0 and 1 with the increment of 0.1 (a) $z = 3$, (b) $z = 4$, (c) $z = 5$, and (d) $z = 6$.

The next phase diagrams were obtained on the $(p, kT/J)$ planes for given values of Δ with $z = 3, 4, 5,$ and 6 as shown in Fig. 3. Again the $p = 0$ and $\Delta = 0$ cases have the same temperatures for each z. The critical lines below the $\Delta = 0$ lines for each z decreases in temperature with the decreasing negative crystal field values and above the $\Delta = 0.0$ lines for each z increases in temperature with the increasing positive crystal field values with the increasing p's. Figure 3 is in total agreement with Fig. 2. Note that as figure 2 suggests, when $\Delta \to -\infty$ and $\Delta \to \infty$, the critical lines do not exhibit anymore changes for each z.

Now we should emphasize that the randomness may induce the first-order phase transitions. When the crystal field is turned on in a non-random fashion, the phase transitions are of the second-order, but randomness may change it to first-order phase transitions at lower negative Δ values for the probability in the range at about $0.2 \sim 0.45$. This is indeed the case for $\Delta = -3.0$ for $z = 3$, $\Delta = -6.0, -2.0$ for $z = 4$ and 5, and $\Delta = -6.0$ for $z = 6$. Figure 4 is obtained for the thermal variations of the order-parameters $\Delta = -6.0$ for $z = 6$. For the non-random case, the crystal field is assumed to be of the 1000 (on–off–off–off) form, alternating. It was found that the phase transitions are of the second-order as indicated by the thermal

variations of the order-parameters (the black lines). But when the randomness is turned on the phase transition becomes the first-order almost at the same temperature of the non-random case (the gray lines). Therefore, the critical lines are of the second-order for the non-random case but they are a mixture of second- and first-order transitions at lower negative Δ values in the range about $p = 0.2 \sim 0.45$. For other values

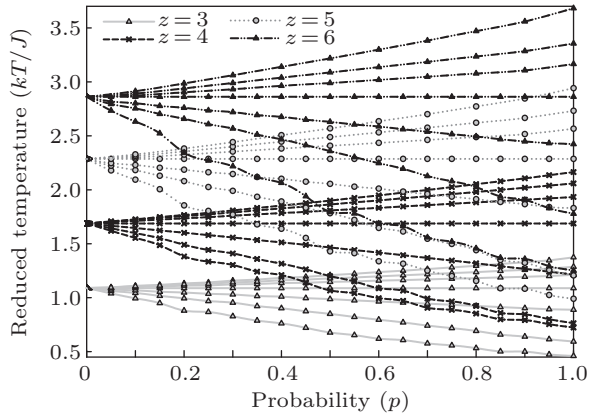


Fig. 3. The phase diagrams on the $(p, kT/J)$ planes for given values of $\Delta = -3.0,\ -1.0,\ -0.5,\ 0,\ 0.5,\ 1.0,\ 3.0$ for $z = 3$ and $\Delta = -6.0,\ -2.0,\ -1.0,\ 0,\ 1.0,\ 2.0,\ 6.0$ for $z = 4, 5$, and 6 from inside out.

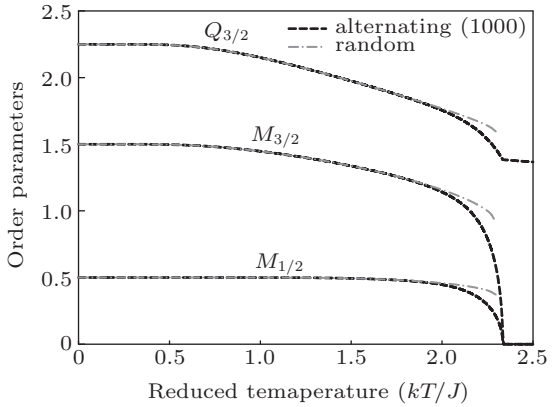


Fig. 4. The effect of the randomness was demonstrated on the thermal variations of the order parameters. The gray lines are obtained for the random case while the black lines were obtained for the non-random case, i.e., the spin-3/2 sites are alternating under the influence of the crystal field in the form 1000 (on–off–off–off) for $\Delta = -6.0$ and $z = 6$.

of p and higher values of Δ, the type of phase transitions are not effected by the randomness. All these conclude that the randomness may induce first-order phase transitions at lower Δ.

As a summary, we have studied the RCF effects on the phase diagrams of the mixed-spin 1/2 and 3/2 BC model on the Bethe lattice. The bimodal random crystal field was used and the problem was solved in terms of the recursion relations. It was found that the model gives only the second-order phase transitions for all values of the crystal fields in the non-random bimodal distribution for given probability. The randomness does not change the order of the phase transitions for higher crystal field values, i.e. it is always second-order, but it may introduce first-order phase transitions at lower negative crystal field values for the probability in the range about 0.20 and 0.45, which is only the second-order for the non-random case in this range. As a result, we claim that randomness may be used to induce first-order phase transitions at lower negative crystal field values at lower probabilities.

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