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An exact formulation of the Blume-Emery-Griffiths model on a two-fold Cayley tree model

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Abstract. A two-fold Cayley tree graph with fully q-coordinated sites is constructed and the spin-1 Ising Blume-Emery-Griffiths model on the constructed graph is solved exactly using the exact recursion equations for the coordination number $q = 3$. The exact phase diagrams in (kT/J, K/J) and (kT/J, D/J) planes are obtained for various values of constants D/J and K/J, respectively, and the tricritical behavior is found. It is observed that when the negative biquadratic exchange (K) and the positive crystal-field (D) interactions are large enough, the tricritical point disappears in the (kT/J, K/J) plane. On the other hand, the system always exhibits a tricritical behavior in the phase diagram of (kT/J, D/J) plane.

PACS. 05.70.Fh Phase transitions: general studies – 64.60.Cn Order-disorder transformations; statistical mechanics of model systems – 75.10.Hk Classical spin models

1 Introduction

The Ising systems have been one of the most actively studied systems in statistical physics. After the exact solution of the simple spin-1/2 Ising model for two-dimensional lattice [1] several attempts were made to arrive at the exact solution of the spin-1/2 Ising model in three dimensions, but all attempts led only to a partial success. However, in the course of these studies many powerful approximation methods with gradually increasing sophistications have arised and flourished in the literature [2–4]. Various attempts were also made to devise models and propose pseudolattices for which the exact solution can readily be obtained. Cayley tree and cactus tree are two such examples of pseudolattices [2,5]. The incorporation of the boundary sites in the exact treatment of the spin-1/2 Ising model on the Cayley tree were investigated by Runnels [6], Eggarter [7], Müller-Hartmann and Zittartz [8] and Thompson [9] shows unusual properties. Moreover, a two-fold Cayley tree graph with fully q-coordinated sites is constructed and the ferromagnetic spin-1/2 Ising model on the constructed graph is solved exactly by Delale [10]. It is shown that a phase transition results in zero field at the critical Bethe temperature with spontaneous magnetization below the critical Bethe temperature.

On the other hand, it is well-known that the spins greater than one-half are quite interesting in view of the appearance of some complicated interactions in addition to a simple isotropic dipolar interaction. Therefore, spin-1 Ising systems [11] have been used to study the thermodynamical behavior of many cooperative physical systems, such as He^3-He^4 mixtures, multicomponent fluids, microemulsions, semiconductor alloys, magnetic materials, martensitic transformation to quote only a few. The above investigations were done by different approximations [2–4]. The exact solutions of the spin-1 Ising systems have been given on the honeycomb lattices for the bilinear (J) and biquadratic (K) exchange interactions in the subspace $e^{\beta K}\mathrm{Cosh}\,\beta J = 1$, where $\beta = 1/(kT)$, k is the Boltzmann constant and T is the absolute temperature, by Horiguchi [12], Wu and Wu [13] and Shankar [14]. Moreover, Rosengren and Häggkvist [15] solved the spin-1 Ising model with bilinear (J), biquadratic (K) nearest-neighbor exchange interactions and the crystal-field interaction (D), also known as the Blume-Emery-Griffiths (BEG) [16] or spin-1 Ising BEG model, exactly for the two-dimensional honeycomb lattice for $e^{\beta K}\mathrm{Cosh}\,\beta J = 1$. Furthermore, the exact solution of the spin-1 Ising model with J and K exchange interactions was given by Chakraborty and Morita [17,18] and J, K and D interactions by Chakraborty and Tucker [19,20] using a generalization of the method of Katsura and Takizawa [21]. The critical properties of the spin-1 Ising BEG model on the Bethe lattice were studied (using exact recursion equations [22]) by Ananikian *et al.* [23], Akheyan and Ananikian [24] and Izmailian and Hu [25].

In this paper, we use the exact recursion equations [22] to obtain exact expressions for the free energy, the Curie temperature, the dipolar and the quadrupole moment order parameters of the BEG model on a two-fold Cayley tree with fully q-coordinated sites. We obtained the

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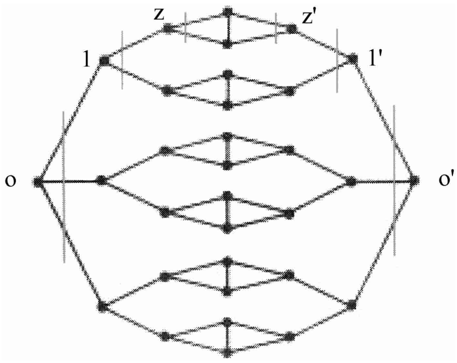

Fig. 1. The construction of the Cayley tree with the coordination number $q = n = 3$. Each point z on the $(n-1)$th left shell there exists a point z' on the $(n-1)$th right shell such that they share the same number of neighbors. In this way, the points z and z' and each vertex of the polygon will have precisely q nearest-neighbors.

exact phase diagrams in $(kT/J, D/J)$ and $(kT/J, K/J)$ planes for the system and found the tricritical behavior.

The organization of the remaining part of the paper is as follows. In Section 2, we present the construction of the two-fold Cayley tree graph and give exact formulation of the BEG model on the constructed graph. The exact expressions for the critical temperatures or the second-order phase transition temperatures and the free energy, which is used to find the first-order phase transition temperatures, are obtained and the phase diagrams are presented in Section 3. A summary and discussion of the phase diagrams are given in Section 4.

2 The BEG model on the two-fold Cayley tree graph

In this section, first we construct a hierarchical graph which is called the two-fold Cayley tree graph with fully q-coordinated sites and then we solve the BEG model on the two-fold Cayley tree graph. Since a detailed description of the two-fold Cayley tree model is given in reference [10], we shall only give a brief summary here. We take two points, *i.e.* O and O$'$, as the central points of the graph, seen in Figure 1. We connect q different points to each central point and call each of the q points "the first shell". To distinguish between the two first shell, we call the one connected to the central point O "the first left shell" and that connected to the central point O$'$ "the first right shell". We continue by joining $(q-1)$ new points to every point in the left and right shells ending in a set of q $(q-1)$ points, called "the second left shell", all connected to the points of the first left shell and a set of q $(q-1)$ points, called "the second right shell", all connected to the points of the first right shell. In this way, we establish further shells by joining each point on the mth right (left) shell to new $(q-1)$ points to obtain the $(m+1)$th right (left) shell. We repeat this procedure for $m = 2, 3, \ldots, (n-1)$ for some positive integer n ending in two yet disconnected Cayley tree graphs each of which contains $(n-1)$ shells. If N_{s} is the number of the sites on the graph under construction, then there is a positive integer n such that for each point on the $(n-1)$th right (left) shell there will be a corresponding point on the $(n-1)$th left (right) shell that has the same $(q-1)$ neighboring points. The construction of the graph terminates with that of the nth shell, called the frontier shell which connects the two disconnected Cayley trees each containing $(n-1)$ shells.

N_{s}, the number of sites and N_{b}, the number of the bonds in this two-fold Cayley tree graph, are found by Delale [10] as

$$N_{\mathrm{s}} = \frac{q^2(q-1)^{n-1}-4}{q-2}, \qquad q > 2, \tag{1}$$

and

$$N_{\mathrm{b}} = \frac{q^3(q-1)^{n-1}-4q}{2(q-2)}, \qquad q > 2. \tag{2}$$

We should also mention that a two-fold Cayley tree is not a Bethe lattice because the graph contains closed loops due to the existence of the frontier shell which are absent in the Bethe lattice.

Now we are ready to study the Blume-Emery-Griffiths (BEG) model on such a two-fold Cayley tree graph. The BEG model is just a spin-1 Ising model with the Hamiltonian

$$H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - K\sum_{\langle i,j\rangle}\sigma_i^2\sigma_j^2 - D\sum_i \sigma_i^2, \tag{3}$$

where $\langle i, j\rangle$ indicates summation over nearest-neighbor pairs and σ_i and σ_j take the values ± 1, 0. J, K and D are the bilinear exchange, biquadratic exchange and crystal-field (or single-ion anisotropy) interactions, respectively. The calculation on the two-fold Cayley tree graph is done recursively [22]. On the other hand, the partition function of the model can be written

$$\begin{aligned} Z &= \sum \exp(-\beta H) \\ &= \sum_{\sigma} \exp\left[\beta\left\{J\sum_{\langle i,j\rangle}\sigma_i\sigma_j + K\sum_{\langle i,j\rangle}\sigma_i^2\sigma_j^2 + D\sum_i\sigma_i^2\right\}\right], \end{aligned} \tag{4}$$

where $\beta = 1/(kT)$, k is the Boltzmann constant and T is the absolute temperature.

The model has two long-range order parameters, namely the magnetization M which is the excess of one orientations over the other, also called the dipole moment and the quadrupolar order parameter Q. The order parameters at site O are given by

$$\begin{aligned} M = \langle\sigma_0\rangle = Z^{-1}\left\{\sum_{\sigma}\sigma_0 \exp\left[\beta\left\{J\sum_{\langle i,j\rangle}\sigma_i\sigma_j\right.\right.\right. \\ \left.\left.\left. + K\sum_{\langle i,j\rangle}\sigma_i^2\sigma_j^2 + D\sum_i\sigma_i^2\right\}\right]\right\}, \end{aligned} \tag{5}$$

and

$$Q = \langle \sigma_0^2 \rangle = Z^{-1} \left\{ \sum_{\sigma} \sigma_0^2 \exp \left[\beta \left\{ J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + K \sum_{\langle i,j \rangle} \sigma_i^2 \sigma_j^2 + D \sum_i \sigma_i^2 \right\} \right] \right\} \cdot \quad (6)$$

As it is the case in all statistical physics models, the evaluation of the partition function solves the problem. For this reason we utilize a factorization property of the exponential in equation (4) similar to that given in reference [22]. From Figure 1, it is easily seen that if the two-fold Cayley tree graph is cut at the central sites O and O′, the graph splits into q disconnected pieces. Thus the exponential in equation (4) factorizes as

$$\exp \left[\beta D \left(\sigma_0^2 + \sigma_0'^2 \right) \right] \prod_{j=1}^{q} Q_n \left(\sigma_0 + \sigma_0' | s^{(j)} \right), \quad (7)$$

where

$$Q_n \left(\sigma_0 + \sigma_0' | s^{(j)} \right) = \exp \left[\beta \left\{ J \left(\sigma_0 s_1 + \sigma_0' s_1' \right) + K \left(\sigma_0^2 s_1^2 + \sigma_0'^2 s_1'^2 \right) + J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + K \sum_{\langle i,j \rangle} \sigma_i^2 \sigma_j^2 + D \sum_i \sigma_i^2 \right\} \right] \cdot \quad (8)$$

and σ_i denotes the spin at the site i of the subgraph (other than the central sites O and O′ which have spins σ_0 and σ_0', respectively) and where the first two summations in equation (8) is over all unbroken bonds of the subgraph and the third summation is over all sites (other than the central sites). Moreover, suffix n ($n > 1$ by definition) for Q_n denotes that each subgraph consists of two Cayley trees each has $(n-1)$ shells joined to the nth (frontier) shell. Now if any of the q equivalent subgraphs, say the upper subgraph, is cut at sites 1 and 1′, it decomposes into $(q-1)$ equivalent subgraphs each consisting of two Cayley tree graphs with $(n-2)$ shell joined to the frontier shell. Thus the reccurence relation for Q_n is obtained as

$$Q_n \left(\sigma_0 + \sigma_0' | s \right) = \exp \left[\beta \left\{ J \left(\sigma_0 s_1 + \sigma_0' s_1' \right) + K \left(\sigma_0^2 s_1^2 + \sigma_0'^2 s_1'^2 \right) + D \left(s_1^2 + s_1'^2 \right) \right\} \right] \prod_{j=1}^{q-1} Q_{n-1} \left(s_1, s_1' | t^{(j)} \right), \quad (9)$$

where $t^{(j)}$ indicates all the spins other than s_1 and s_1' on the jth of the $(q-1)$ newly constructed subgraphs. From these factorization relations in equations (7–9), one can easily calculate the magnetization (dipolar) M and quadrupolar Q order parameters at site O. For this calculation we define

$$g_n \left(\sigma_0, \sigma_0' \right) = \sum_s Q_n \left(\sigma_0, \sigma_0' | s \right), \quad (10)$$

and using this definition in equation (7), we find the partition function from equations (4, 8) as

$$Z = \sum_{\sigma_0, \sigma_0'} \exp \left[\beta D \left(\sigma_0^2 + \sigma_0'^2 \right) \right] \left[g_n \left(\sigma_0, \sigma_0' \right) \right]^q . \quad (11)$$

On the other hand, using equation (5) magnetization at site O can be written as

$$M = Z^{-1} \sum_{\sigma_0, \sigma_0'} \sigma_0 \exp \left[\beta D \left(\sigma_0^2 + \sigma_0'^2 \right) \right] \left[g_n \left(\sigma_0, \sigma_0' \right) \right]^q , \quad (12)$$

and the quadrupolar order parameter Q, from equation (6), at the same site as

$$Q = Z^{-1} \sum_{\sigma_0, \sigma_0'} \sigma_0^2 \exp \left[\beta D \left(\sigma_0^2 + \sigma_0'^2 \right) \right] \left[g_n \left(\sigma_0, \sigma_0' \right) \right]^q . \quad (13)$$

At this point, it should be noticed that the two-fold Cayley tree graph is symmetric about the frontier shell by the construction, seen in Figure 1. This symmetry can be expressed as a symmetry relation for Q_n as

$$Q_n \left(\sigma_0, \sigma_0' | s^{(j)} \right) = Q_n \left(\sigma_0', \sigma_0 | s^{(j)} \right). \quad (14)$$

The function g_n, *i.e.* equation (10), also reflects this symmetry relation as

$$g_n \left(\sigma_0, \sigma_0' \right) = g_n \left(\sigma_0', \sigma_0 \right). \quad (15)$$

Summing over all s in equation (8) and using equation (10), the recursion relations for g_n is obtained as

$$g_n \left(\sigma_0, \sigma_0' \right) = \sum_{s_1} \sum_{s_1'} \exp \left[\beta \left\{ J \left(\sigma_0 s_1 + \sigma_0' s_1' \right) + K \left(\sigma_0^2 s_1^2 + \sigma_0'^2 s_1'^2 \right) + D \left(s_1^2 + s_1'^2 \right) \right\} \right] \left[g_{n-1} \left(s_1, s_1' \right) \right]^{q-1} . \quad (16)$$

Since $\sigma_0, \sigma_0' = \pm 1, 0$, we can define x_n, y_n, z_n, w_n and v_n by

$$x_n = \frac{g_n(+,+)}{g_n(-,0)}, \quad y_n = \frac{g_n(-,-)}{g_n(-,0)}, \quad z_n = \frac{g_n(+,-)}{g_n(-,0)}, \quad w_n = \frac{g_n(+,0)}{g_n(-,0)}, \quad v_n = \frac{g_n(0,0)}{g_n(-,0)} \cdot \quad (17)$$

We should also mention that $g_n(+,-) = g_n(-,+)$, $g_n(0,+) = g_n(+,0)$ and $g_n(0,-) = g_n(-,0)$ due to equation (15). The explicit expressions for x_n, y_n, z_n, w_n and v_n can be found by using equations (16, 17) with

$\sigma_0, \sigma_0' = \pm 1$, 0 and utilizing the symmetry relation, *i.e.* equation (15).

In order to solve equation (17) one needs to find the initial values of x_1, y_1, z_1, w_1 and v_1 which can be determined as follows: Since the subgraph under consideration is a polygon with $(q-1)$ vertices all connected pairwise, it follows from equations (8–10) that

$$g_1(s_z, s_z') = \sum_t Q_1(s_z, s_z'|t), \tag{18}$$

with

$$Q_1(s_z, s_z'|t) = \exp\left[\beta\left\{J\sum_{\langle i,j\rangle} t_i t_j + K\sum_{\langle i,j\rangle} t_i^2 t_j^2 + J(s_z, s_z') \times \sum_{i=1}^{q-1} t_i + \left[D + K\left(s_z^2, s_z'^2\right)\right]\sum_{i=1}^{q-1} t_i^2\right\}\right], \tag{19}$$

where t_i indicates the spin on the ith vertex of the polygon with values ± 1,0 referring to Figure 1. The initial values of x_1, y_1, z_1, w_1 and v_1 can be found explicitly by using equations (18, 19) for the coordination number $q = 3$ and the boundary graph looks like t_1 ●⟺● t_2.

It should be mentioned that the values x, y, z, w, and v have no direct physical meaning, but one can express all the thermodynamic functions of interest in terms of these quantities. Thus the order parameters are obtained by using the equation (17) and equations (11–13)

$$M = \{\exp[2\beta' d]\, x_n^q - \exp[2\beta' d]\, y_n^q + \exp[\beta' d]\, w_n^q - \exp[\beta' d]\}/\{\exp[2\beta' d]\, x_n^q + \exp[2\beta' d]\, y_n^q + 2\exp[2\beta' d]\, z_n^q + 2\exp[\beta' d]\, w_n^q + v_n^q + 2\exp[\beta' d]\}, \tag{20}$$

$$Q = \{\exp[2\beta' d]\, x_n^q + \exp[2\beta' d]\, y_n^q + 2\exp[2\beta' d]\, z_n^q + \exp[\beta' d]\, w_n^q + \exp[\beta' d]\}/\{\exp[2\beta' d]\, x_n^q + \exp[2\beta' d]\, y_n^q + 2\exp[2\beta' d]\, z_n^q + 2\exp[\beta' d]\, w_n^q + v_n^q + 2\exp[\beta' d]\}, \tag{21}$$

where $\beta' = \beta J$, $\alpha = K/J$ and $d = D/J$.

3 The transition temperatures and the phase diagrams

We are now in a position to obtain the exact expressions for the critical (Curie) temperatures or the second-order phase transition temperatures of the BEG model on the two-fold Cayley tree graph. In order to find the exact expression for the critical temperature one searches for the temperature at which the magnetization goes to zero. In this way the following exact expressions of the critical temperature is found:

$$\exp[\beta_{\mathrm{C}} d]\, x_n^q - \exp[\beta_{\mathrm{C}} d] y_n^q + w_n^q - 1 = 0, \tag{22}$$

where $\beta_{\mathrm{C}} = J/(kT_C)$. It is easily seen that this equation is satisfied when $x_n = y_n$ and $w_n = 1$, *i.e.* $g_n(+,+) = g_n(-,-)$ and $g_n(+,0) = g_n(-,0)$. The physical insight of these latter conditions is the following. At the critical temperature the magnetization must be equal to zero, therefore the probability of spins being up and spins being down has to be equal to each other. We should also mention that n characterizes how far the arbitrary chosen central sites of the graph lie from each other. In the limit $N_s \to \infty$ (thereby $N_b \to \infty$ with $N_b/N_s = (1/2)q$, compare Eq. (1) with Eq. (2)) the central sites O and O′ will be such that if one starts from any one of the two points the other is not reachable after finite steps, *i.e.* $n \to \infty$. Thus the thermodynamic limit $N_b \to \infty$ corresponds to the limit $n \to \infty$ (see also Eq. (1)). In the thermodynamic limit a significant fraction resides on the boundary (now at infinity) and only sites in the finite domain become all equivalent. Thus magnetization becomes the magnetization per site for sites in the finite domain, hence we can omit the suffix n. Now the exact expression for the critical temperature is written

$$\exp[\beta_{\mathrm{C}} d]\, x^q - \exp[\beta_{\mathrm{C}} d]\, y^q + w^q - 1 = 0, \tag{23}$$

where x, y, and w are given in equation (17). The solution of this equation gives us the critical or the second-order phase transition temperatures. It is obvious that this equation has a simple and special solution when $x = y$ and $w = 1$. However, we determine the second-order phase transition temperature as follows: The equations (17, 20) are solved simultaneously by iteration for given values of α and d, and the temperature is varied. The temperature at which the magnetization disappears, *i.e.* $M = 0$, is the critical temperature. It should also be mentioned that one can also determine the critical temperature for given values of α and d from equation (23). In this way one has to solve equations (17, 23) simultaneously by iteration. The temperature at which equation (23) is satisfied is the second-order phase transition or the critical temperature.

In order to determine the first-order phase transition temperatures we need the free energy expression ($F = -kT\ln Z$). So using equations (11, 16) and (17), and in the thermodynamic limit $n \to \infty$, one can obtain the exact free energy expression as

$$F = -\frac{1}{\beta'}\Big\{\frac{q}{2-q}[\ln[\exp[\beta'(-1+\alpha+2d)]\, x^{q-1} + \exp[\beta'(1+\alpha+2d)]\, y^{q-1} + 2\mathrm{Cosh}[\beta']\exp[\beta'(\alpha+2d)]\, z^{q-1} + (\exp[\beta' d] + \exp[\beta'(-1+\alpha+d)])\, w^{q-1} + v^{q-1} + (\exp[\beta' d] + \exp[\beta'(1+\alpha+d)])] + \ln[\exp[2\beta' d](x^q + y^q + 2z^q) + \exp[\beta' d](w^q+1) + v^q]\Big\}\cdot \tag{24}$$

The first-order phase transition temperatures are determined by matching the values of the two branches of the free energy followed while increasing and decreasing the temperature. The temperature at which the free energy values are equal to each other is the first-order phase transition temperature.

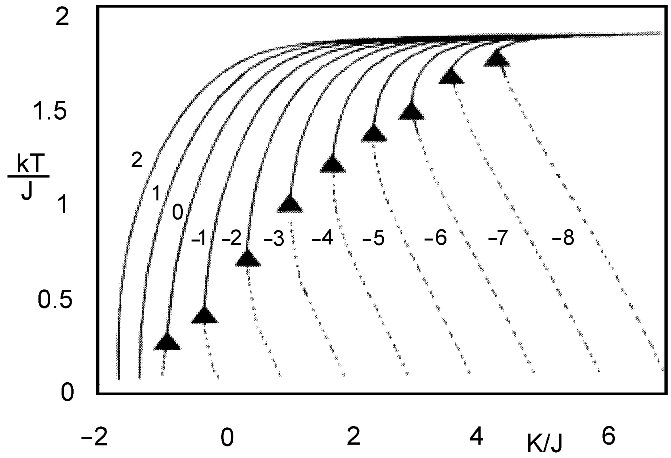

Fig. 2. The phase diagram in the $(kT/J, K/J)$ plane for various values of the D/J. The dashed and solid lines represent the first- and second-order phase transitions respectively. Tricritical points are indicated with a filled triangle. The lines are labelled with the values of D/J.

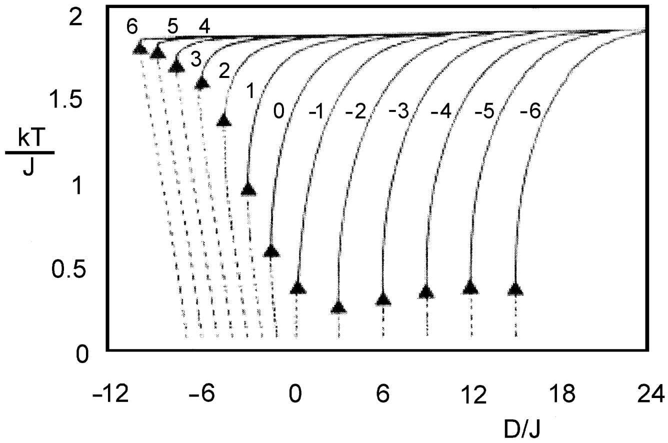

Fig. 3. The phase diagram in the $(kT/J, D/J)$ plane for various values of the K/J. The dashed and solid lines represent the first- and second-order phase transitions respectively. Tricritical points are indicated with a filled triangle. The lines are labelled with the values of K/J.

We can now obtain the phase diagram of the BEG model in $(kT/J, D/J)$ and $(kT/J, K/J)$ planes for various values of constants K/J and D/J respectively. In the phase diagrams the dashed and solid lines corresponds to the first- and second-order phase transition temperatures, respectively. The system also exhibits a tricritical point at which the lines of second- and first-order phase transitions meet, marked with the filled triangle.

4 Summary and discussion of the results

We construct a hierarchical graph called the two-fold Cayley tree with fully q-coordinated sites and we solve the BEG model on the constructed graph. Exact expressions for the magnetization and the quadrupolar order parameters and also the critical or the second-order phase transition temperature and the free energy are obtained. The first-order phase transition temperatures are determined by matching the values of the two branches of the free energy followed while increasing and decreasing the temperature. The temperature at which the free energy values are equal to each other is the first-order phase transition temperature. We presented the phase diagrams in the $(kT/J, K/J)$ and $(kT/J, D/J)$ planes for various values of constants D/J and K/J respectively, seen in Figures 2–3. In the phase diagrams the dashed and solid lines correspond to the first- and second-order phase transition temperatures respectively and filled triangles indicate the tricritical points.

In Figure 2, the phase diagram in $(kT/J, K/J)$ plane is shown for various values of D/J. For $D/J > 0.025$ the system always undergoes a second-order phase transition but for $D/J \leq 0.025$ either a first- or a second-order phase transition depending on the values of the order parameters, therefore the tricritical behavior appears in this range. The tricritical points occur at high temperatures for larger values of K. Similar phase diagrams have been obtained for only $D > 0$ by Chakraborty and Tucker [20] for the BEG model on the Bethe lattice. However, for $D \leq 0$ Chakraborty and Tucker found that the system undergoes only the second-order phase transition but in our case the system undergoes both second- and first-order phase transitions, compare Figure 2 of the present paper with Figure 2 of the reference [20]. This discrepancy is due to the fact that Chackraborty and Tucker have used Bethe lattice but we have used the two-fold Cayley tree. On the other hand, a similar phase diagram was also obtained by Wang *et al.* [26] for a two-dimensional BEG model using the Monte Carlo simulations (compare Fig. 2 of the present paper with Fig. 1 in Ref. [26]). Moreover, the phase diagram for the positive values of the quadrupolar coupling is very similar to the phase diagram of the BEG model Hamiltonian with transverse field interactions obtained by us [27] recently, compare Figure 2 with Figure 8 of reference [27]. We did not obtain the phase diagram for the negative values of coupling parameter in reference [27].

Figure 3 illustrates the phase diagram in the $(kT/J, D/J)$ plane for various values of K/J. The system always undergoes a first- and second-order phase transition, hence the system always exhibits a tricritical behavior. A similar phase diagram is obtained by Ananikian *et al.* [23] for the BEG model on the Bethe lattice. However they found that their system only undergoes a second-order phase transition for small negative values of K/J, *e.g.* $K = -1.5$. On the other hand, the phase diagram for the negative values of crystal-field interaction is similar to the phase diagram of reference [27] in which the phase diagram for positive values of the crystal-field interaction is not presented. Finally, it should be mentioned that the similar first- and second-order phase transition lines for $K/J = 0$ have been seen in many different approximations such as the mean-field approximation [16], series-extrapolation techniques [28], the renormalization group theory [29], the Monte Carlo simulation [30].

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