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Ising model with two-, three- and four-spin interactions

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Abstract. The two-state Ising model with nearest-neighbour bilinear exchange constant $J^{(2)}$, three-spin coupling constant $J^{(3)}$ and four-spin coupling constant $J^{(4)}$ is studied using the effective-field approximation. The temperature variation in spontaneous magnetization is studied for different coordination numbers z and for various values of the parameters $\alpha = J^{(3)}/J^{(2)}$ and $\alpha' = J^{(4)}/J^{(2)}$. It is seen that, in the absence of three-spin coupling, there exists a critical value of α' (say, α'_c) above which the magnetization becomes double valued at and beyond the Curie temperature T_C, forming a bulge near T_C which indicates the occurrence of a first-order transition. The expressions for α'_c for $z = 3, 4, 6$ are derived and it is found that α'_c increases as z increases. In the absence of four-spin coupling it is found that first-order transitions appear for $\alpha \geqslant 0$. The magnetization curves are also studied for the case when all the interactions are present. The results are discussed with reference to those obtained from the molecular-field approximation.

1. Introduction

The Ising model with higher-order interactions has been the subject of considerable attention during the past few years owing to some peculiarities observed in the results of calculations of thermodynamic properties of such models. An interesting example is the Blume–Emery–Griffiths (1971) model in which some novel features were noticed (Chakraborty 1988, Tucker 1987, 1988, 1989). Another useful model is the two-state Ising model described by a Hamiltonian which consists of a bilinear interaction term and a four-spin coupling term. Such a model might be important for explaining the first-order phase transitions which appear in a squaric acid crystal. Wang *et al* (1989, 1990) studied such a model in the molecular-field approximation (MFA) and found that the first-order phase transitions can occur when the ratio of the strength of the four-spin coupling to that of that two-spin coupling exceeds a critical value. However, it is well known that in the MFA the dimensionality of the lattice is not taken into account and the quantitative accuracy of the result is questionable. It is, therefore, worthwhile to carry out the calculations using a more rigorous approximation method. On the other hand, it was demonstrated by Baxter and Wu (1973) that the exact solution of the Ising model on a triangular lattice with three-spin coupling exhibits a critical behaviour which differs markedly from that of the Ising model with two-spin coupling. The Ising model with both three-spin and four-spin coupling was studied by Wood (1972), Wood and Griffiths (1973, 1974a, 1974b) and Griffiths and Wood (1973, 1974) using dual transformation and series analysis.

The purpose of the present paper is to employ the effective-field approximation (EFA) of Honmura and Kaneyoshi (1978, 1979) to study a two-state Ising model with both three-spin and four-spin interactions along with the usual two-spin coupling. We concentrate on the temperature variation in the spontaneous magnetization and on the search for the possibility of first-order phase transitions for different lattices. The results have been discussed with reference to the MFA results.

2. The Hamiltonian and the effective-field approximation

The Hamiltonian appropriate for the model under consideration may be expressed as

$$H = -\sum_{ij} J_{ij}^{(2)} S_i S_j - \sum_{ijk} J_{ijk}^{(3)} S_i S_j S_k - \sum_{ijkl} J_{ijkl}^{(4)} S_i S_j S_k S_l \tag{2.1}$$

where $i \neq j \neq k \neq l$ for $z > 3$ and any two are equal for $z = 3$. S_i is the Ising spin having the eigenvalues $+1$ and -1. $J_{ij}^{(2)}$ is the two-spin exchange, $J_{ijk}^{(3)}$ is the three-spin exchange and $J_{ijkl}^{(4)}$ is the four-spin exchange. In the case of a triangular lattice the last term is to be considered as the three-site, four-spin interaction so that any two sites have to be considered as equivalent.

To apply the effective-field theory of Honmura and Kaneyoshi (1978, 1979) to the above model, one starts with the Callen (1963) identity for the two-state Ising model:

$$\langle S_i \rangle = \langle \tanh(\beta E_i) \rangle \tag{2.2}$$

where E_i is a suitably defined effective field appropriate for the model and the angular brackets denote the thermal averages:

$$\langle A \rangle = \mathrm{Tr}[A \exp(-\beta H)]/\mathrm{Tr}[\exp(-\beta H)]. \tag{2.3}$$

Honmura and Kaneyoshi (1978, 1979) used the identity

$$\langle \tanh \theta \rangle = \langle \exp(\mathrm{D}\theta) \rangle \tanh(x)|_{x \to 0} \tag{2.4}$$

with $\mathrm{D} \equiv \partial/\partial x$.

In the present problem we introduce the following effective field:

$$E_i = \sum_j J_{ij}^{(2)} S_j + \sum_{jk} J_{ijk}^{(3)} S_j S_k + \sum_{jkl} J_{ijkl}^{(4)} S_j S_k S_l. \tag{2.5}$$

Considering the nearest neighbour two-, three-, and four-spin exchange constants defined by $J^{(2)}$, $J^{(3)}$ and $J^{(4)}$ respectively the above expression may be approximated by

$$E_i = J^{(2)} \sum_j S_j + J^{(3)} \sum_j S_j \langle S_k \rangle + J^{(4)} \sum_j S_j \langle S_k \rangle \langle S_l \rangle \tag{2.6}$$

which can be written in the form

$$E_i = J^{(2)}(1 + \alpha m + \alpha' m^2) \sum_{j=1}^{z} S_j \tag{2.7}$$

where z is the number of nearest neighbours, $\alpha = J^{(3)}/J^{(2)}$ and $\alpha' = J^{(4)}/J^{(2)}$. The symbol m stands for the magnetization $m = \langle S_i \rangle$.

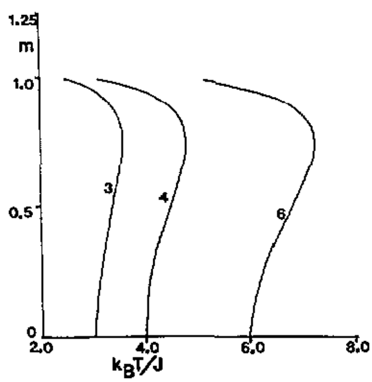

Figure 1. Spontaneous magnetization m plotted against $k_BT/J^{(2)}$ using the MFA. We have considered only the $\alpha' = 1$ case. The number attached to each curve refers to the value of z ($J^{(2)} \equiv J$).

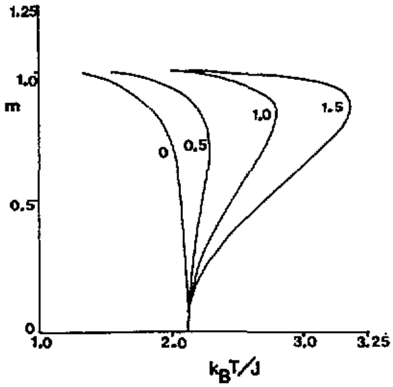

Figure 2. Magnetization curves for the model in the absence of three-spin coupling. The triangular lattice is considered. The value attached to each curve refers to the value of the four-spin coupling strength α' ($J^{(2)} \equiv J$).

Defining a parameter $K = \beta J^{(2)}(1 + \alpha m + \alpha' m^2)$ and using the Van der Waerden identity for the spin-$\frac{1}{2}$ case, i.e.

$$\exp(KS_iS_j) = \cosh K + S_iS_j \sinh K$$

one gets

$$m = \left\langle \sum_{j=1}^{z} [\cosh(\mathrm{D}K) + S_j \sinh(\mathrm{D}K)] \right\rangle \tanh(x) \bigg|_{x\to 0}. \tag{2.8}$$

3. Results and discussion

The explicit expressions for m for various values of z may be obtained readily from equation (2.8). These expressions will coincide with those of Taggart and Fittipaldi (1982) if one substitutes the present definition of K in their equations. We do not write here these expressions; rather we concentrate on the computation of these expressions for various values of the parameters. The computation of magnetization for different lattices $z = 3, 4, 6$ has been carried out and the results for several values of α and α' are critically analysed.

Firstly, we consider the case of four-spin coupling only, i.e. $\alpha = 0$. The magnetization curves obtained from the MFA for $z = 3, 4, 6$ are shown in figure 1. The curves refer to the case $\alpha' = 1$. The magnetization curves obtained from EFA for $z = 3, 4, 6$ and for different values of α' are shown in figures 2–4. The general qualitative feature which is evident from these figures is that there exists a critical value of α' (say, α'_c) such that beyond α'_c the spontaneous magnetization m becomes double valued at and above the Curie temperature T_C. Each curve bends round from a limiting point to the Curie point, thus forming a bulge in the neighbourhood of T_C.

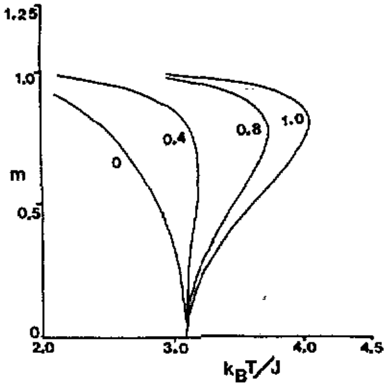

Figure 3. Same as for figure 2 but for a square lattice.

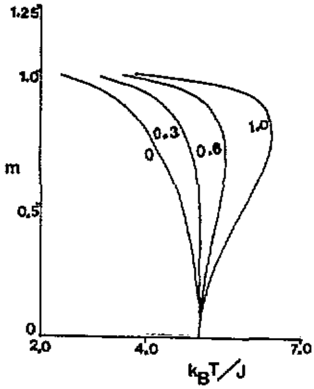

Figure 4. Same as for figure 2 but for a cubic lattice.

Table 1. The values of $k_BT_C/J^{(2)}$ and α'_c for different z.

	$k_BT_C/J^{(2)}$		α'_c	
z	MFA	EFA	MFA	EFA
3	3.0	2.1038	1/3	0.198
4	4.0	3.0899	1/3	0.231
6	6.0	5.0733	1/3	0.257

The values of α'_c for different lattices obtained from computation agree with those obtained from the following conditions for first-order transitions:

$$\partial T/\partial m = 0 \qquad \partial^2 T/\partial m^2 = 0 \tag{3.1}$$

as m tends to zero. T in equation (3.1) is the temperature. The Curie temperature T_C is obtained from the first condition in (3.1).

Using the above conditions we get the following expressions for α'_c:

$$\alpha'_c = \frac{3\tanh(\beta_c J^{(2)}) - \tanh(3\beta_c J^{(2)})}{\beta_c J^{(2)}[8 - 5\tanh^2(3\beta_c J^{(2)}) - 3\tanh^2(\beta_c J^{(2)})]} \tag{3.2}$$

for $z = 3$;

$$\alpha'_c = \frac{2\tanh(2\beta_c J^{(2)}) - \tanh(4\beta_c J^{(2)})}{4\beta_c J^{(2)}[2 - \tanh^2(4\beta_c J^{(2)}) - \tanh^2(2\beta_c J^{(2)})]} \tag{3.3}$$

for $z = 4$;

$$\alpha'_c = \frac{15\tanh(2\beta_c J^{(2)}) - 5\tanh(6\beta_c J^{(2)})}{3\beta_c J^{(2)}[16 - 3\tanh^2(6\beta_c J^{(2)}) - 8\tanh^2(4\beta_c J^{(2)}) - 5\tanh^2(2\beta_c J^{(2)})]} \tag{3.4}$$

for $z = 6$. In the above equations, $\beta_c J^{(2)} = J^{(2)}/k_B T_C$.

The values of α'_c obtained from the above equations are shown in the table 1.

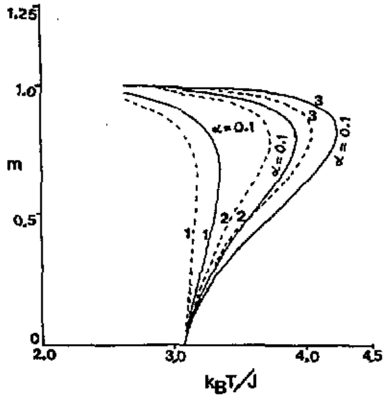

Figure 5. Magnetization curves for a square lattice ($J^{(2)} \equiv J$): curve 1, ----, $\alpha = 0$, $\alpha' = 0.4$; curve 1, ——, $\alpha = 0.1$, $\alpha' = 0.4$; curve 2, ----, $\alpha = 0$, $\alpha' = 0.8$; curve 2, ——, $\alpha = 0.1$, $\alpha' = 0.8$; curve 3, ----, $\alpha = 0$, $\alpha' = 1.0$; curve 3, ——, $\alpha = 0.1$, $\alpha' = 1.0$.

In the MFA we get, for $\alpha = 0$,

$$m = \tanh[\beta J^{(2)} zm(1 + \alpha' m^2)].$$

The above equation yields $\beta_c J^{(2)} = 1/z$ and the critical value of α'_c obtained using the conditions (2.1) is the same for all z and is equal to $\frac{1}{3}$.

On the other hand, when we consider only the three-spin coupling, the conditions (3.1) yield $\alpha_c = 0$. Indeed we have found from computations that, for $\alpha \geqslant 0$ and for all z, the magnetization curves show bulges in the vicinity of Curie temperature.

Figure 5 shows some of the results of computation when both the three-spin and the four-spin interactions are taken into account. In the first place we see that, as the three-spin coupling strength or the four-spin coupling strength increases, the bulge in the magnetization curve increases. Secondly, when α is kept constant and α' is allowed to increase, the same result is obtained. The problem of calculations regarding the inclusion of still higher-order interactions and consideration of more rigorous evaluation of the effective field will be taken up in future investigations.

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