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A discussion of some magnetic properties of the square Ising lattice with a fluctuating exchange integral

J Mielnicki†, T Balcerzak‡ and G Wiatrowski‡

† Institute of Physics, Polish Academy of Sciences, Al. Lotników 32, PL 02-668 Warsaw, Poland

‡ Institute of Physics, University of Łódź, Nowotki 149/153, PL 90-236 Łódź, Poland

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Abstract. The magnetisation curve and the critical temperature of the square Ising lattice with a fluctuating exchange integral has been investigated using the Matsudaira method. Particular attention has been drawn to the re-entrant ferromagnetism phenomenon and it has been shown that it strongly depends on the accuracy of calculations with a tendency to disappear when the accuracy is improved.

1. Introduction

In recent years, great effort has been made to describe the so-called re-entrant magnetism phenomenon in disordered magnetic systems. This phenomenon was observed experimentally (see, e.g., [1]) and since then a number of theoretical papers have appeared, where both two- and three-dimensional systems have been discussed. For instance, in a series of papers, diluted ferromagnetic and ferrimagnetic systems with a random exchange parameter have been considered [2–4]. A recent paper [5] in which a discussion of the re-entrant ferromagnetism resulting from one- and two-spin cluster models and from a finite-cluster approximation have been presented should also be noted. In all these papers the fluctuations of the exchange integral have been taken into account by means of the distribution function $P(I_{ij})$

$$P(I_{ij}) = p\delta(I_{ij} - I) + (1 - p)\delta(I_{ij} - I') \tag{1}$$

which takes into account various possibilities. For instance, with $p = 1$ we get the perfect crystal case, while $I' = 0$ corresponds to the case of a diluted ferromagnetic alloy. Then, if $I > 0$ and $I' > 0$, all interactions are ferromagnetic; hence no frustration of the lattice appears. However, if $I > 0$ and I' becomes negative, then some interactions are antiferromagnetic which can lead to frustration and, as a result, re-entrant ferromagnetism can be expected. In all the above papers, calculations were made in the framework of the first-order Matsudaira approximation [6] where spin–correlation functions are neglected. The common result is that, for I' negative, the phase diagrams predict the existence of re-entrant magnetism in some range of I'-values. Some improvement in the above theory was achieved when the mean spin–correlation function was taken into account in the magnetisation equations [7]. The phase diagram with this

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correction predicts a large reduction in the re-entrant phenomenon when compared with the predictions of theories with the correlations neglected (see figure 7 of [7]).

Thus, it is seen that, when considering re-entrant magnetism, rather a high accuracy of the calculations is necessary. For this reason we have performed calculations using the Matsudaira method where in successive approximations the number of correlations is taken into account. This method, although rather sophisticated, gives better results than that in [7], which can be seen from a comparison of the $k_B T_c/I$-values for the perfect-crystal case.

In the present paper we consider a square lattice with a distribution function of the type given by equation (1) but used in a particularly simple form:

$$P(I_{ij}) = \tfrac{1}{2}[\delta(I_{ij} - I - \delta_1) + \delta(I_{ij} - I + \delta_1)]. \tag{2}$$

As a result, first of all the phase diagram has been obtained in various Matsudaira approximations. Then, also the magnetisation curve together with various correlations have been calculated. The main conclusion is that the range of δ_1 where re-entrant magnetism exists strongly reduces with increase in the calculation accuracy, and it is possible that in our model given by the distribution function (2) it does not occur at all.

2. The theory

We shall consider below the magnetisation curve and in particular the critical temperature of the disordered Ising ferromagnet with the fluctuating exchange integral

$$I_{ij} = I + \Delta_{ij} \tag{3}$$

where Δ_{ij} is the random value. Thus, in the calculations, not only the thermodynamic but also the configurational averages should be found. This can be done by means of the method given, for example, in [8], where some function $F(I_{ij})$ is presented in the form

$$F(I_{ij}) = \int F(E)\delta(E - I_{ij})\,\mathrm{d}E \tag{4}$$

and the Dirac delta function is given by the relation

$$\delta(E - I_{ij}) = (\mathrm{i}/2\pi)[(E - I_{ij} + \mathrm{i}\varepsilon)^{-1} - (E - I_{ij} - \mathrm{i}\varepsilon)^{-1}]_{\varepsilon\to 0+} \qquad -I_{ij} = I + \Delta_{ij} \tag{5}$$

where

$$(E - I \pm \mathrm{i}\varepsilon - \Delta_{ij})^{-1} = (E - I \pm \mathrm{i}\varepsilon)^{-1} \sum_{\nu=0}^{\infty} \frac{\Delta_{ij}^{\nu}}{(E - I \pm \mathrm{i}\varepsilon)^{\nu}}. \tag{6}$$

For further calculations the Handrich–Kaneyoshi approximation will be used, according to which we have

$$\langle\Delta_{ij}^{2\nu}\rangle_r \simeq \langle\Delta_{ij}^{2}\rangle_r^{\nu} \qquad \langle\Delta_{ij}^{2\nu+1}\rangle_r \simeq 0 \tag{7}$$

with $\langle\ldots\rangle_r$ denoting the configurational average. With the above approximation, one can find that

$$\langle\delta(E - I_{ij})\rangle_r = \tfrac{1}{2}[\delta(E - I - \delta_1) + \delta(E - I + \delta_1)] \tag{8}$$

where

$$\delta_1 = \sqrt{\langle\Delta_{ij}^{2}\rangle_r}.$$

Hence, the probability distribution function of the exchange integral is given by equation (2), and also from equation (4) we obtain the general relation

$$\langle F(I_{ij})\rangle_r = \tfrac{1}{2}[F(I + \delta_1) + F(I - \delta_1)]. \tag{9}$$

On the basis of equation (9) we shall consider below the square crystallographic lattice with $S = \frac{1}{2}$. The magnetisation of such a ferromagnet in the framework of the Ising model can be found by means of the generalised Callen relation

$$R \equiv \langle\!\langle S_i \rangle\!\rangle_r = \left\langle\!\!\left\langle \tanh\left(\beta \sum_{j\in i} I_{ij} S_j\right)\right\rangle\!\!\right\rangle_r \qquad S_j = \pm 1 \quad \beta = \frac{1}{k_B T} \tag{10}$$

together with a similar relation for the two-spin correlation function

$$\langle\!\langle S_i S_k \rangle\!\rangle_r = \left\langle\!\!\left\langle S_k \tanh\left(\beta \sum_{j\in i} I_{ij} S_j\right)\right\rangle\!\!\right\rangle_r . \tag{11}$$

To calculate the right-hand sides of (10) and (11), the integral representation method will be used (for details see, e.g., [9, 10]), according to which equation (10) takes the form

$$R = \int \mathrm{d}\omega \tanh(\beta\omega) \frac{1}{2\pi} \int \mathrm{d}t \exp(\mathrm{i}\omega t) \left\langle\!\!\left\langle \exp\left(-\mathrm{i}t \sum_{j\in i} I_{ij} S_j\right)\right\rangle\!\!\right\rangle_r \tag{12}$$

and a similar representation can be used for equation (11). For the $S_i = \pm 1$ case considered, we also have

$$\exp(-\mathrm{i}tI_{ij}S_j) = \cos(tI_{ij}) - \mathrm{i}S_j \sin(tI_{ij}). \tag{13}$$

As a result of the straightforward calculations of the right-hand sides of equations (10) and (11) in the integral representation, we finally obtain the following two relations:

$$R = X \sum \langle\!\langle S_j \rangle\!\rangle_r + Y \sum \langle\!\langle S_{j1} S_{j2} S_{j3} \rangle\!\rangle_r \tag{14}$$

$$\langle\!\langle S_i S_k \rangle\!\rangle_r = X \sum \langle\!\langle S_j S_k \rangle\!\rangle_r + Y \sum \langle\!\langle S_{j1} S_{j2} S_{j3} S_k \rangle\!\rangle_r \tag{15}$$

where the notation introduced in [6] has been used, and the coefficients X and Y are given by the equations

$$X = -\mathrm{i} \int \mathrm{d}\omega \tanh(\beta\omega) \frac{1}{2\pi} \int \mathrm{d}t \exp(\mathrm{i}\omega t) \langle \sin(tI_{ij})\rangle_r \langle \cos(tI_{ij})\rangle_r^3 \tag{16}$$

$$Y = \mathrm{i} \int \mathrm{d}\omega \tanh(\beta\omega) \frac{1}{2\pi} \int \mathrm{d}t \exp(\mathrm{i}\omega t) \langle \sin(tI_{ij})\rangle_r^3 \langle \cos(tI_{ij})\rangle_r . \tag{17}$$

In the above we have assumed that the functions of the different exchange integrals can be averaged independently. Thus, we see that we have obtained two equations enabling the magnetisation calculations to be made in the general form analogous to the Matsudaira equations, with the only difference that coefficients X and Y given by (16) and

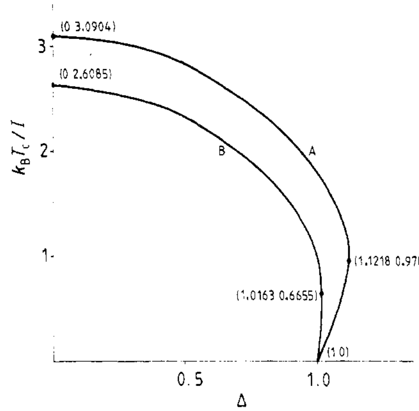

Figure 1. k_BT_c/I plotted against Δ $(=\delta_1/I)$ for the square crystallographic lattice: curve A, curve obtained in the first-order Matsudaira approximation; curve B, curve obtained in the third-order approximation. The coordinates of the corresponding points are given in parentheses. In particular, $\Delta_1 = 1.1218$ and $\Delta_3 = 1.0163$, where Δ_1 and Δ_3 are the maximal values of Δ resulting from the first- and third-order approximation, respectively.

(17) should be calculated now using equation (9). On the basis of this equation, one can obtain

$$\langle\cos(tI_{ij})\rangle_r = \cos(tI)\cos(t\delta_1) \tag{18}$$

$$\langle\sin(tI_{ij})\rangle_r = \sin(tI)\cos(t\delta_1). \tag{19}$$

Then, on the basis of (16) and (17), we have

$$X = A + B \tag{20}$$

$$Y = A - B \tag{21}$$

where

$$A = 2^{-7}\{6\tanh(4\beta I) + 4\tanh[4\beta I(1+\Delta/2)] + 4\tanh[4\beta I(1-\Delta/2)] + \tanh[4\beta I(1+\Delta)] + \tanh[4\beta I(1-\Delta)]\} \tag{22}$$

$$B = 2^{-6}\{6\tanh(2\beta I) + 4\tanh[2\beta I(1+\Delta)] + \tanh[2\beta I(1-\Delta)] + \tanh[2\beta I(1+2\Delta)] + \tanh[2\beta I(1-2\Delta)]\} \tag{23}$$

and $\Delta = \delta_1/I$. It should be noted here that, for $\Delta = 0$, equations (14) and (15) reduce to the corresponding Matsudaira equations. Further calculations are exactly the same as those given in [6] (with only the X and Y parameters changed) and hence we shall present below only the numerical results obtained for the disordered ferromagnet.

3. Numerical results and discussion

In figure 1 the phase diagrams of k_BT_c/I against Δ obtained in the first- and third-order Matsudaira approximation are presented.

As can be seen from this figure in the case of the first-order approximation there is rather a wide Δ range $(1 < \Delta < 1.1218)$ where two critical temperatures occur, which corresponds to the re-entrant phenomenon. On increase in the calculation accuracy this range is strongly reduced ($1 < \Delta < 1.04$ in the approach in [7] and $1 < \Delta < 1.0163$ resulting from the third-order Matsudaira approximation). We have also carried out the calculations in the fourth-order approximation. As a result, only a small modification of

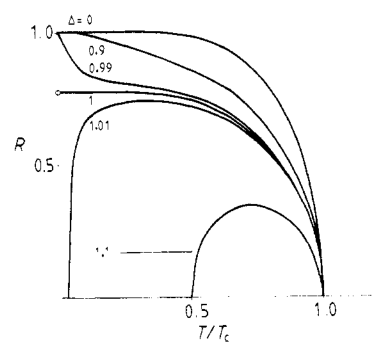

Figure 2. The magnetisation curves obtained in the first-order approximation for several values of Δ. For $\Delta = 1.01$ and $\Delta = 1.1$, re-entrant magnetism is shown.

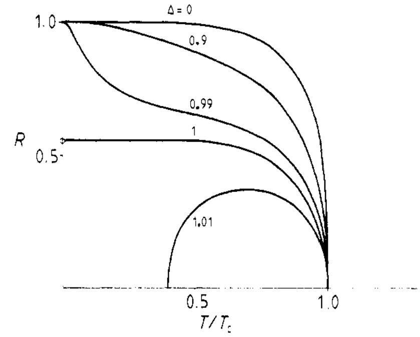

Figure 3. The magnetisation curves obtained in the third-order approximation for several values of Δ. Re-entrant magnetism still appears for $\Delta = 1.01$.

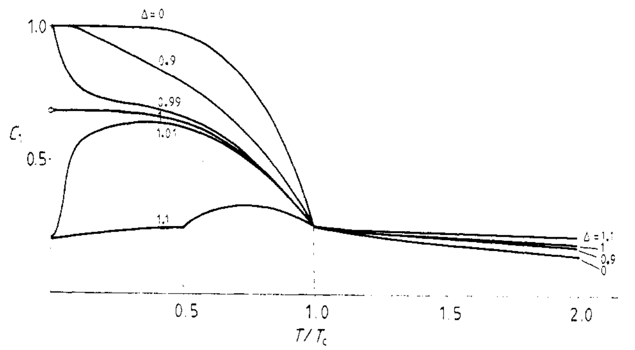

Figure 4. The nearest-neighbour spin–correlation function C_1 plotted against the reduced temperature T/T_c, resulting from the first-order approximation for the same Δ-values as those in figure 2.

curve B in figure 1 has been obtained with re-entrant magnetism appearing for $1 < \Delta < 1.0133$. Thus, because the results of the Matsudaira method are still far from the results of the exact Onsager model (see, e.g., [11]), it is possible that, in the ferromagnet considered here, the predicted re-entrant phenomenon is simply due to the calculation inaccuracy.

It should be noted also that in all the Matsudaira approximations used here for the square lattice, we get $T_c = 0$ for $\Delta = 1$.

The general behaviour of re-entrant magnetism discussed above is illustrated also in figures 2 and 3, where the magnetisation curves for several Δ-values resulting from first- and third-order approximations have been presented. As can be seen, the re-entrant magnetism in figure 3 is strongly reduced compared with that presented in figure 2 (compare for instance the curves for $\Delta = 1.01$). The same result is also shown in figures 4 and 5, where the nearest-neighbour spin–correlation functions C_1 obtained in the first- and third-order approximations for various values of Δ are shown. Note that the correlation C_1 is of primary importance, because it is closely related to the internal energy and to the magnetic contribution to the specific heat.

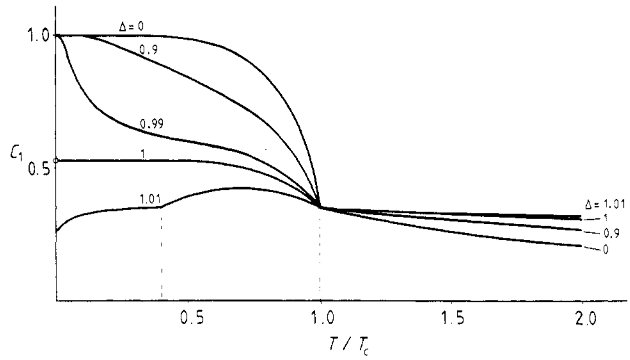

Figure 5. The same as in figure 4 but for the third-order approximation. The Δ-values are the same as those in figure 3.

The numerical results presented in figures 2–5 have shown that, for $0 \leqslant \Delta < 1$ and for $T \to 0$, both the magnetisation and the correlation function tend to unity. The particularly interesting shape of these curves have been obtained for Δ close to unity (e.g. $\Delta = 0.99$), where abrupt decreases in the magnetisation and correlation functions in the low-temperature range are observed. This effect was not reported in other papers (see, e.g., [2]).

From equations (22) and (23) we see that, for $\Delta = 1$, we have no precisely defined X and Y functions in the $T \to 0$ limit; hence this point was excluded from numerical calculations. Nevertheless, calculations made for temperatures very close to zero predict no variation in both the magnetisation and the correlation functions.

For $\Delta > 1$ the magnetisation becomes equal to zero at low temperatures and re-entrant magnetism appears. Also in this Δ range a strong reduction in the correlation functions is observed.

When comparing our results with the results obtained in [5], first of all it should be mentioned that the parameter p in [5] is equal to 0.5 in our considerations and the parameter α is related to our parameter Δ by the equation

$$\alpha = (1 - \Delta)/(1 + \Delta). \tag{24}$$

Then, from the comparison of our figure 1 with figure 2 of [5], it is seen that the results obtained in [5] are in agreement with our results obtained in the first-order approximation. For instance our Δ_1-value of 1.1218 corresponds to $\alpha \simeq -0.057$ (see figures 2 and 3 of [5] for $p = 0.5$). However, $\Delta_3 = 1.0163$ corresonds to $\alpha \simeq -0.008$.

Thus it is seen that in the third-order approximation, which is likely to be better than the first-order approximation, the range where re-entrant behaviour occurs is considerably reduced and hence the work in [5] overestimates the occurrence of this phenomenon. The same tendency is observed when the fourth-order approximation is used. However, all the results of the fourth-order approximation are only slightly changed in comparison with the results given in this paper. It should also be remembered that the Matsudaira method produces results still far from the exact Onsager method and is therefore not too reliable for the re-entrant phenomenon. Moreover, as the accuracy of the calculations plays so important a role in the problems considered, other assumptions of the theory should also be improved. For instance the Handrich–Kaneyoshi distribution function should be substituted by a Gaussian distribution of exchange integrals.

To conclude, this paper should not be regarded as a demonstration of the existence of a re-entrant phenomenon for certain parameters within a particular model. Rather it serves to show that its occurrence is highly dependent on the accuracy of the calculation, and the tendency is for it to disappear altogether when the accuracy of a calculation is improved.

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