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Series expansion study of first- and second-order phase transitions in a model with multispin coupling

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Abstract. The type of phase transition in a chain of Ising spins with multispin interaction is studied in a transverse field, using strong- and weak-coupling expansions. The transition is shown to be of first order if more than three spins are coupled. The critical exponents for the three-spin coupling model are estimated.

1. Introduction

While second-order phase transitions can be studied conveniently by using various formulations of the renormalisation group transformation, the situation is much less satisfactory for first-order phase transitions. Although the concept of a discontinuity fixed point (Nienhuis and Nauenberg 1975) is useful in describing first-order phase transitions, these are not always associated with a discontinuity fixed point. Similarly, although detailed studies have been performed in finite-size scaling for systems with first-order phase transitions (Imry 1980, Fisher and Berker 1982, Blöte and Nightingale 1982, Iglói and Sólyom 1983, Hamer 1983, Cardy and Nightingale 1983, Privman and Fisher 1983, Binder and Landau 1984), in many practical cases it is not easy to decide from the data for finite systems, whether the transition is of first or second order. This is the case for the multispin coupling model studied in this paper.

The model was introduced by Turban (1982) and Penson *et al* (1982). The Hamiltonian can be written in the form

$$H = -\lambda \sum_i \sigma_i^z \sigma_{i+1}^z \ldots \sigma_{i+m-1}^z - h \sum_i \sigma_i^x \tag{1.1}$$

where σ_i^x and σ_i^z are Pauli operators on site i. The value of m determines the number of neighbouring spins that are coupled. At zero temperature the system has a phase transition as the transverse field increases. Since it seems that there is a single phase transition in the system, the self-duality of the model predicts that it should be at $(h/\lambda)^* = 1$, independently of the number of coupled spins m. For $m = 2$ the model is the standard Ising model in transverse field which has a second-order phase transition. For $m \to \infty$, however, mean field theory should be exact and the transition turns out to be of first order. There are controversial predictions for the critical value of m, above which the transition should be of first order. Mean field theory gives $m_C = 2$. However renormalisation group calculations (Iglói *et al* 1983) give the usual second-order behaviour for $m = 3$. The analysis of finite-size scaling results lead Penson *et al* (1982) to conclude that $m_C = 4$. From a conjectured criterion for distinguishing between continuous and discontinuous transitions (Livi *et al* 1983), Maritan *et al* (1984) predicted that for $m = 4$ the transition is already of first order. Since finite-size scaling is not very sensitive in deciding when the character of the transition changes, other methods should be used.

In this paper we use the series expansion method to determine the critical value of m_C. The paper is organised as follows. The series obtained for the ground-state energy in the weak- and strong-coupling limits are presented in § 2. The series are analysed in § 3, where we find that in fact $m_C = 3$, and for this case, where the transition is still of second order, the critical exponents are also determined. The results are discussed in § 4.

2. Series expansion

The weak- and strong-coupling series expansions for quantum spin systems, which are analogous to the high- and low-temperature expansions in classical statistical mechanics, and the analysis of the series by using different methods to determine the critical behaviour, have been proved to be very useful in the study of many systems (Hamer *et al* 1979, Elitzur *et al* 1979, Hamer and Kogut 1980, Marland 1981). We will apply this procedure to the multispin coupling model.

The Hamiltonian of equation (1.1) can be split in two ways. If the multispin coupling λ is stronger than the transverse field h, the latter can be treated in perturbation and an expansion in powers of h/λ can be generated. This strong-coupling expansion for the ground-state energy per site will have the form

$$E/N = -\lambda \sum_n a_n (h/\lambda)^n \qquad \text{for } \lambda \geqslant h. \tag{2.1}$$

On the other hand, if the multispin coupling is weaker than the transverse field, a weak-coupling expansion in powers of λ/h can be generated. Due to the self-duality of the model, the series expansion coefficients will be the same in the two cases, i.e.

$$E/N = -h \sum_n a_n (\lambda/h)^n \qquad \text{for } \lambda \leqslant h \tag{2.2}$$

and at $\lambda = h$ the two expressions match. This is valid even if only a few finite-order terms are calculated in the expansion.

If the transition is of second order, then the two expressions give not only the same energy at $\lambda = h$, but the left and right derivatives, calculated from the two expressions in their regions of validity respectively, are also identical at this point. Only the second derivatives will differ. On the other hand, if the transition is of first order, the weak- and strong-coupling expansions give different first derivatives on the two sides of the transition point, indicating a finite latent heat.

If the expansion coefficients are calculated up to a finite order, the two expansions always give differing left and right derivatives at the transition point, although after extrapolating to $n \to \infty$ the difference may disappear, indicating a second-order phase transition. If, however, the transition is of first order, the difference between the two derivatives should remain finite even when $n \to \infty$.

We have performed the weak- and strong-coupling series expansions for the ground-state energy of the model given in equation (1.1) up to tenth order for $m = 2$, 3 and 4, while for $m = 5$, 6 and 7 up to eighth order. The series expansion coefficients are given in table 1.

Table 1. Series expansion coefficient $a_n(m)$ for the model with m coupled spins in nth order of perturbation.

Order	$a_n(2)$	$a_n(3)$	$a_n(4)$	$a_n(5)$	$a_n(6)$	$a_n(7)$
2	$\frac{1}{4}$	$\frac{1}{6}$	$\frac{1}{8}$	$\frac{1}{10}$	$\frac{1}{12}$	$\frac{1}{14}$
4	0.001 562 500	0.018 518 52	0.014 973 96	0.011 833 33	0.009 490 74	0.007 762 39
6	0.003 906 25	0.005 607 00	0.004 573 68	0.003 466 19	0.002 628 71	0.002 026 79
8	0.001 525 88	0.002 512 61	0.002 051 43	0.001 484 76	0.001 061 45	0.000 769 53
10	0.000 747 68	0.001 379 29	0.001 124 33			

3. Analysis of the series

As discussed in the previous section, finite-order perturbation theory always gives a finite latent heat, a finite difference between the derivatives of the ground-state energy at $\lambda = h$, when calculated from the weak- or strong-coupling expansions. This nth-order latent heat L_n is defined as

$$L_n = \frac{1}{N}\left(\frac{\partial E_n^{\mathrm{s}}(h,\lambda)}{\partial h}\bigg|_{h=\lambda} - \frac{E_n^{\mathrm{w}}(h,\lambda)}{\partial h}\bigg|_{h=\lambda}\right). \tag{3.1}$$

Here E_n^{s} and E_n^{w} are the ground-state energies calculated in the strong- and weak-coupling expansion, respectively, keeping terms up to nth order. The values obtained using the results of the previous section are given in table 2.

In the extrapolation to $n \to \infty$ the exact solution of the $m = 2$ case (Pfeuty 1970) can be used as a guide. It is easily seen that for the Ising case the expansion coefficients can be written in the form

$$a_{2n} = \prod_{i=1}^{n} [(2i-3)/2i]^2. \tag{3.2}$$

After summing up the series with these coefficients one recovers the exact result of Pfeuty (1970). The latent heat in nth order can be approximated by

$$L_n \approx (2/\pi)(n+\tfrac{1}{2})^{-1}. \tag{3.3}$$

One can see that the latent heat goes to zero roughly as $1/n$. This expression is the special case of the general scaling form valid for second-order transitions (Iglói 1986)

$$L_n \propto n^{-(1-\alpha)}. \tag{3.4}$$

Here α is the specific heat exponent. This kind of scaling behaviour has been used by one of us to determine the critical exponents of various physical quantities from series expansions.

Table 2. The latent heat $L_n(m)$ in nth order of perturbation theory calculated from equation (3.1) for the model with m coupled spins.

Order	$L_n(2)$	$L_n(3)$	$L_n(4)$	$L_n(5)$	$L_n(6)$	$L_n(7)$
2	0.25	0.5	0.625	0.7	0.75	0.7857
4	0.1406	0.3704	0.5202	0.6172	0.6836	0.7314
6	0.0976	0.3087	0.4699	0.5790	0.6546	0.7091
8	0.0748	0.2710	0.4391	0.5568	0.6387	0.6975
10	0.0606	0.2448	0.4178			

According to equations (3.3) and (3.4), a plot of $\log L_n$ against $\log(n+\frac{1}{2})$ should give a straight line for second-order phase transitions, with a slope $-(1-\alpha)$. This plot is shown in figure 1 for different values of the number of coupled spins. The points lie very well on a straight line for $m=2$ and 3, while for $m \geqslant 4$ there are considerable deviations. The slope of the line for $m=3$ is approximately $\frac{1}{2}$. Therefore we plot in figure 2 the value of L_n as a function of $(n+\frac{1}{2})^{-1/2}$. As is seen, the values are on a straight line not only for $m=3$, but for larger m values as well. For $m=3$ the extrapolated latent heat vanishes, and thus the transition is of second order. The error in the extrapolation of the latent heat is smaller than 0.005. For $m \geqslant 4$, however, the latent heat differs significantly from zero. In these cases the transition is of first order. The accuracy of the extrapolation is rather good. This is due to the fact that the ratio of the coefficients $a_n(m)/a_n(m+1)$ varies only slowly with n, as can be read off from table 1. This quantity is smaller than one for $m=2$, but it is larger than unity for $m \geqslant 3$. This ratio is extremely stable for $m=3$. Supposing that this ratio is the same in higher orders of the expansion as well, i.e. $a_n(3)/a_n(4) \approx 1.227$, independently of n, we estimate the latent heat for the case $m=4$ to be

$$L(m=4) = L_{10}(m=4) - L_{10}(m=3)[a_n(4)/a_n(3)] = 0.218. \tag{3.5}$$

This value is in good agreement with the estimate from figure 2. The latent heat for larger values of m can be extrapolated in the same way, however, and in this case the accuracy is somewhat smaller. The calculated latent heats are shown in figure 3, together with the series expansion results. The latent heat for large values of m behaves

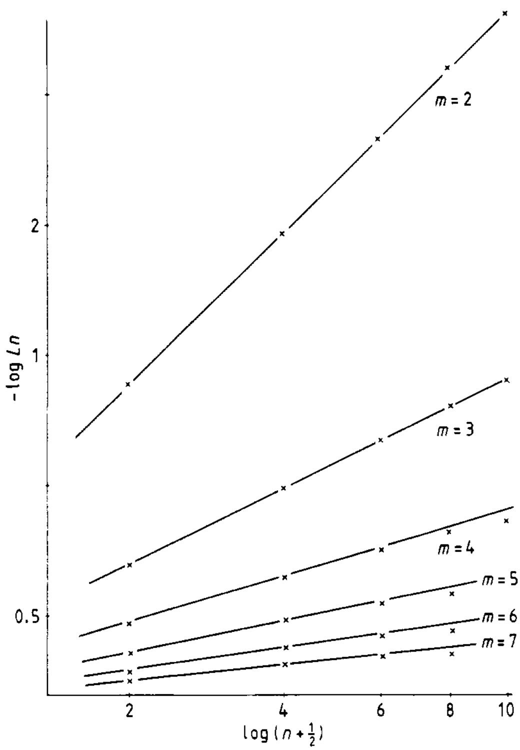

Figure 1. The nth-order latent heat L_n against $n+\frac{1}{2}$ on a log-log plot for different values of the number of coupled spins.

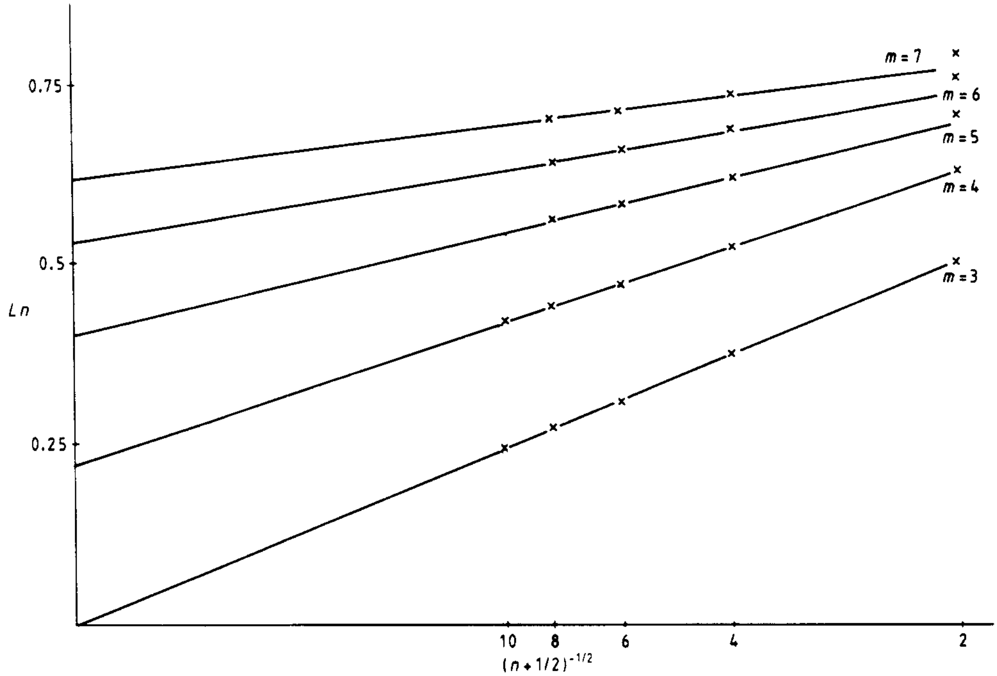

Figure 2. The nth-order latent heat L_n against $(n+\frac{1}{2})^{-1/2}$ for the models with $m \geqslant 3$.

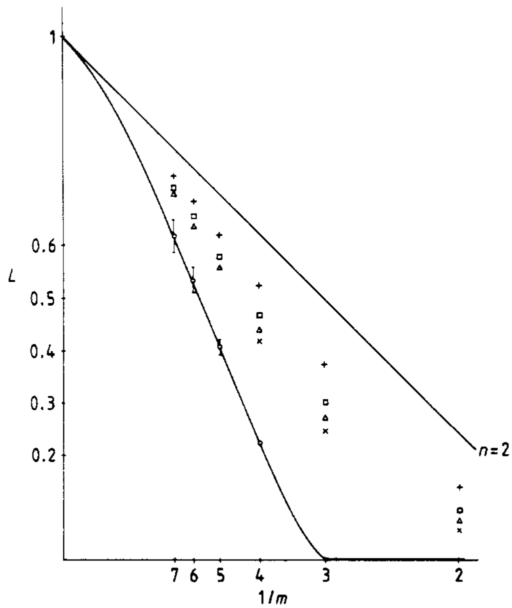

Figure 3. The nth-order latent heat and the extrapolated value for $n \to \infty$ plotted for different m values; $n = 4$ denoted by $+$, $n = 6$ by $\square$, $n = 8$ by $\triangle$ and $n = 10$ by $\times$.

as $L = 1 - 3/2m$. At $m = 3$ the latent heat becomes zero and remains identically zero for smaller values of m.

Next we estimate the critical properties of the model for $m = 3$. Since we have calculated the ground-state energy only, the specific heat exponent α can be obtained from the second derivative. The series is rather short and therefore different methods have been used to get a best estimate. The result of the ratio method (Gaunt and Guttmann 1974) is $\alpha = 0.53 \pm 0.03$. By using the scaling relation (3.4) we obtain $\alpha = 0.54 \pm 0.02$. The best result is achieved by Padé analysis (Gaunt and Guttmann 1974) of the series. According to the Padé approximants (table 3) we obtain $\alpha = 0.554 \pm 0.001$. Thus all these estimates are consistent with the prediction

$$\alpha = 0.55 \pm 0.01. \tag{3.6}$$

The critical exponent of the correlation length can be calculated from the hyperscaling relation $d\nu = 2 - \alpha$, and we get $\nu = 0.73 \pm 0.01$. This value is somewhat smaller than the result obtained by Iglói *et al* (1983) from the renormalisation group calculation and is close to the value determined by Penson *et al* (1982) from finite-size scaling.

Table 3. Padé analysis of the series for the logarithmic derivative of the specific heat in the $m = 3$ model.

M \ N	1	2	3
1	0.5783	0.5587	0.5552
2	0.5519	0.5544	
3	0.5542		

4. Discussion

In the present paper the phase transition in a chain of Ising spins coupled by a multispin interaction and submitted to a transverse field has been studied. The weak- and strong-coupling series expansions for the ground-state energy have been performed up to tenth order in the perturbation. It has been shown that in the cases when more than three neighbouring spins are coupled, the transition is of first order. This method is thus more sensitive than finite-size scaling to determine the order of transition. By the latter method the $m = 4$ case still seemed to behave as having a second-order phase transition (Penson *et al* 1982). As shown by Iglói and Sólyom (1983) and Hamer (1983) the finite latent heat in a first-order transition can be determined from finite-size scaling calculations as well but the limits $L \to \infty$, where L is the length of the system, and $\lambda \to \lambda^*$ cannot be interchanged.

The analysis of the series allowed us to estimate the critical exponents α and ν for the case $m = 3$. The values obtained differ from the values known for the four-state Potts model indicating once more that these models do not belong to the same universality class (Iglói *et al* 1983), although in both cases a fourfold degeneracy is lifted at the transition.

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