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Critical behaviour and logarithmic corrections of a quantum model with three-spin interaction

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Abstract. Extended finite-size scaling and series expansion methods are used to determine the critical properties of the one-dimensional quantum Ising model with three-spin interaction. Supposing the presence of logarithmic corrections the universality class of the model is investigated. Our results obtained by different methods support the conjecture that the model belongs to the same universality class as the four-state Potts model.

1. Introduction

Recently we have witnessed a growing interest in the study of models with multiparticle interactions. These models are thought to be relevant in various physical systems such as ^{3}He (Roger *et al* 1983), adsorbed systems (Kittler and Benneman 1979) and plasmas (Held and Deutsch 1981). The theoretical models with many-body interactions differ in some aspects from those with nearest-neighbour coupling. The critical properties generally depend on the range of the interaction. Due to the presence of long-range forces the numerical study of these models is more difficult. Therefore much less information is known about the critical behaviour of the multispin interaction models.

Recently Turban (1982), and independently Penson *et al* (1982), have introduced a class of multispin interaction models, which enables one to investigate systematically the role of the range of the interaction on the critical properties. The model is a generalisation of the one-dimensional quantum Ising model and defined by the following Hamiltonian:

$$H = -\lambda \sum_i \prod_{j=0}^{m-1} \sigma^x_{i+j} - \sum_i \sigma^z_i \tag{1.1}$$

where σ^x_i and σ^z_i are the Pauli matrices at the ith lattice site. The model is self-dual (Turban 1982, Penson *et al* 1982), the self-dual point is $\lambda^* = 1$ independently of the value of m. It is generally believed that only one phase transition takes place in the system (at which the degeneracy of the ground state is changing by a factor of 2^{m-1}). Thus λ^* coincides with the critical point of the system.

The model can be solved exactly in two cases:

(i) For $m = 2$ the model undergoes a second-order transition with Ising critical exponents (Pfeuty 1970).

(ii) In the limit $m \to \infty$ the mean-field solution becomes exact and shows a first-order transition (Turban 1982, Penson *et al* 1982, Maritan *et al* 1984).

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Consequently the transition should change from second order to first order at some intermediate value of $m = m_c$. In some two-dimensional models, and in their Hamiltonian version (like q-state Potts model, n-component cubic model) the transition turns from second order to first order, when the degeneracy of the ordered phase exceeds four (Baxter 1973, Nienhuis *et al* 1983, Iglói 1986a). In this analogy Debierre and Turban (1983) conjectured that $m_c = 3$. Furthermore Debierre and Turban (1983) also conjectured that the $m = 3$ model belongs to the same universality class as the four-state Potts model.

The first conjecture has recently been verified by Iglói *et al* (1986) using the strong and weak coupling expansion method, and by Blöte *et al* (1986b) using the Monte Carlo technique. However the situation in the verification of the second conjecture is more controversial. The results of the first numerical investigations by finite-size scaling (Penson *et al* 1982, Iglói *et al* 1983, Debierre and Turban 1983, Kolb and Penson 1986) by the renormalisation group method (Iglói *et al* 1983, Vanderzande 1984) and by series expansions (Iglói *et al* 1986) are significantly different from those of the four-state Potts model. However, very recently Blöte *et al* (1986b) have shown that there exists an exact mapping between the very anisotropic limits of the two models. They considered the classical Ising model on a square lattice with two-spin interaction in the horizontal direction and with three-spin interaction in the vertical one. Taking the time continuum limit (Kogut 1979) by using the horizontal direction as the time axis one reobtains the model in (1.1) for $m = 3$, while by choosing the other direction as time axis one obtains the Hamiltonian version of the four-state Potts model (Sólyom and Pfeuty 1981). Blöte *et al* (1986b) also performed MC simulation and by taking into account the effect of logarithmic corrections they obtained critical exponents which are approaching the four-state Potts values when the size of the system is increasing. However, due to the strong effect of the confluent logarithmic singularity the accuracy of the determination of the critical exponents was rather small. Therefore, there is a need to investigate the question of the universality class of the $m = 3$ model by other methods as well.

In this paper finite-size scaling is used for the specific heat, for the susceptibility and for the gap of the model. Furthermore the method of universal amplitudes is applied for the spin-spin and for the energy-energy correlation function. The strong and weak coupling expansion for the ground-state energy is extended up to sixteenth order. The results of the different methods are analysed by taking into account the presence of logarithmic corrections in the same form as in the four-state Potts model (Nauenberg and Scalapino 1980, Cardy *et al* 1980). The paper is organised as follows. The results of the finite-size scaling and the series expansion are presented in §§ 2 and 3, respectively. These sections also contain the results of the analysis by neglecting the effect of logarithmic singularities. In § 4 the analysis of the results is repeated by taking into account logarithmic corrections. Finally in § 5 there is a short discussion.

2. Finite-size scaling and the method of universal amplitudes

In the study of the critical properties of Hamiltonian systems the determination of the energy of the ground state ($E_0(\lambda)$) and the energy of the first excited state ($E_1(\lambda)$) is of great importance. The energy gap

$$\Delta(\lambda) = E_1(\lambda) - E_0(\lambda) \tag{2.1}$$

governs the correlation behaviour of the system, and shows a power law singularity in the vicinity of the critical point $\lambda^* = 1$:

$$\Delta(\lambda) \sim |\lambda - \lambda^*|^{-\nu}. \tag{2.2}$$

The specific heat behaves as

$$C(\lambda) = \frac{1}{L}\frac{\partial^2 E_0}{\partial \lambda^2} \sim |\lambda - \lambda^*|^{-\alpha} \tag{2.3}$$

(L is the number of lattice sites.)

The zero-field susceptibility is defined in the presence of a longitudinal field:

$$H_{\text{field}} = -h \sum_i \sigma_i^x \tag{2.4}$$

as

$$\chi(\lambda) = \frac{1}{L}\frac{\partial^2 E_0(\lambda, h)}{\partial h^2}\bigg|_{h=0} \sim |\lambda - \lambda^*|^{-\gamma}. \tag{2.5}$$

A powerful method to determine the critical properties of the infinite system is to perform the calculation for finite systems with linear size L and then use the finite-size scaling hypothesis (Barber 1983). According to this hypothesis a physical quantity $\psi(\lambda)$, which has a power law singularity at the critical point with exponent ϕ

$$\psi(\lambda) \sim |\lambda - \lambda^*|^{-\phi} \tag{2.6}$$

for finite systems asymptotically behaves as

$$\psi_L(\lambda) = L^{\phi/\nu} Q_\psi(L/\xi) \tag{2.7}$$

where ξ is the correlation length in the infinite system and Q_ψ is some function depending on ψ. In particular, at the critical point ψ_L should only depend on L through the power ϕ/ν.

Thus as special cases the specific heat and the susceptibility behave as

$$C_L(1) \sim L^{-d+2y_t} \tag{2.8}$$

$$\chi_L(1) \sim L^{-d+2y_h} \tag{2.9}$$

Here the hyperscaling relations

$$\begin{aligned} \alpha/\nu &= -d + 2y_t \\ \gamma/\nu &= -d + 2y_h \end{aligned} \tag{2.10}$$

are used. (In the present quantum system the effective dimension $d = 1 + z$, where $z = 1$ is the dynamical exponent.)

Another possibility of determining y_t is to calculate it from the derivative of the gap

$$\frac{\partial \Delta_L}{\partial \lambda}(1) \sim L^{y_t - 1}. \tag{2.11}$$

Finally we show that one may obtain a further independent relation between y_t and y_h by using the method of universal amplitudes (Luck 1982, Nightingale and Blöte 1983, Cardy 1984, Penson and Kolb 1984, Burkhardt and Guim 1985, Gehlen *et al* 1986). Let Θ be some operator (energy, spin, etc) of the system and define the gap $\Delta_L^\Theta(\lambda)$ between the ground state $|0\rangle$ and the first excited state $|\mu_1\rangle$ of the system for which

$$\langle \mu_1 | \Theta | 0 \rangle \neq 0. \tag{2.12}$$

This gap behaves at $\lambda = \lambda^*$ as

$$\lim_{L\to\infty} L\Delta_L^{\Theta}(1) = c2\pi x_{\Theta} \tag{2.13}$$

where x_{Θ} is the anomalous dimension, for which

$$x_{\Theta} + y_{\Theta} = d \tag{2.14}$$

and c is some constant. (If the system is conformally invariant—which is probably the case with the present model (Kolb and Penson 1986)—then $c = v_s$, where v_s is the sound velocity of the single-particle excitation spectrum $E_1(k) - E_0 = v_s k$ (Blöte *et al* 1986a).)

Now we focus on the gap of the energy operator (denoted by $\Delta_L^t(\lambda)$) and on that of the spin operator ($\Delta_L^h(\lambda)$). From (2.13) one can deduce that

$$R = \lim_{L\to\infty} R_L = \lim_{L\to\infty} \frac{\Delta_L^t(1)}{\Delta_L^h(1)} = \frac{x_t}{x_h} \tag{2.15}$$

obtaining an extra relation between y_t and y_h.

2.1. *Results for the multispin-coupling model*

In the calculation periodic boundary conditions were used. In order to maintain the symmetry of the Hamiltonian in (1.1) the system sizes were chosen as $L = 3 \times l$, where l is an integer.

The numerical calculation of $E_0(\lambda)$ and $E_1(\lambda)$ were performed for systems up to $L = 15$ by using the Lanczos algorithm (Wilkinson 1965, Whitehead *et al* 1977). The specific heat and the susceptibility were obtained by numerical differentiation according to (2.3) and (2.5).

The result for the critical exponents obtained by two-point fits from (2.8), (2.11) and (2.9) are given in table 1, together with the values of the four-state Potts model (den Nijs 1979, Pearson 1980, Nienhuis *et al* 1980). (For the largest system size the susceptibility is too big to be determined accurately from numerical differentiation.) As is seen in table 1, while y_h agrees with the four-state Potts value within the accuracy of the calculation, the values for y_t seem to tend to a significantly different value, which is close to $\frac{4}{3}$ obtained by other numerical methods as well (Penson *et al* 1982, Iglói *et al* 1983, 1986, Debierre and Turban 1983, Vanderzande 1984, Kolb and Penson 1986).

Similar conclusions may be deduced from the results of the method of universal amplitudes (table 2). The R_L ratios defined by (2.15) seem to tend to a value of close to 5, which would be compatible with $y_h = \frac{15}{8}$ and $y_t = \frac{11}{8}$.

Table 1. Critical exponents calculated by two-point fits from the finite-size data of the specific heat, the gap and the susceptibility.

$(L+3, L)$	y_t	y_t	y_h
(6, 3)	1.64	1.28	2.05
(9, 6)	1.47	1.32	1.89
(12, 9)	1.43	1.33	1.85
(15, 12)	1.41	1.33	
Potts $q = 4$	3/2	3/2	1.875

Table 2. Ratio of the universal amplitudes for finite systems.

L	R_L
3	7.856
6	5.310
9	5.219
12	5.148
15	5.089

Table 3. Thermal exponent y_t and logarithmic correction strength β obtained by three-point fit from finite-size data of the gap.

$(L+6, L+3, L)$	y_t	β
(9, 6, 3)	1.62	0.91
(12, 9, 6)	1.61	0.89
(15, 12, 9)	1.59	0.85
Potts $q=4$	3/2	3/4

Closing this section we present the results of the analysis supposing a general form for the confluent logarithmic singularity as

$$\frac{\partial \Delta_L}{\partial \lambda}(1) \sim L^{y_t-1}(\ln L)^{-\beta}. \tag{2.16}$$

The exponents y_t and β, calculated by three-point fit, are presented in table 3. According to these data it seems possible that the model belongs to the same universality class as the four-state Potts model. This question will be investigated in more detail in § 4, where the confluent logarithmic singularity is taken in the same form as in the four-state Potts model.

3. Analysis of the strong and weak coupling series

The critical properties of the model are now investigated by the analysis of the strong coupling series for the ground-state energy

$$E_0(\lambda) = -\sum_k a_k \lambda^k. \tag{3.1}$$

(Due to self-duality the coefficients of the strong and weak coupling series are identical.) In this paper the results of Iglói *et al* (1986) are extended up to sixteenth order.

The coefficients of the strong coupling series for the specific heat are given in table 4, together with the estimates for the α critical exponent obtained by the ratio method (Gaunt and Guttmann 1974). The analysis of the series by the Dlog Padé method (Gaunt and Guttmann 1974) gives similar results, as is seen in table 5. Finally the scaling method proposed by Iglói (1986b) is applied to determine the α exponent. In this method the relation is used that the series of the latent heat (Iglói *et al* 1986)

$$L^{(n)} = \sum_{k=0}^{n} (2k-1)a_k \tag{3.2}$$

Table 4. Strong-coupling series coefficients for the specific heat and estimates for the α exponent from the ratio method.

Order	Coefficient	
0	1/3	
		0.6667
2	2/9	
		0.5139
4	0.168 209 88	
		0.5095
6	0.140 706 16	
		0.5289
8	0.124 135 67	
		0.5129
10	0.112 042 23	
		0.5147
12	0.102 978 99	
		0.5156
14	0.095 851 20	

Table 5. Padé analysis of the logarithmic derivative of the specific heat.

M \ N	1	2	3	4	5
1	0.5783	0.5587	0.5552	0.5482	0.5444
2	0.5519	0.5544	0.5621	0.5396	0.5365
3	0.5542	0.5525	0.5282	0.5365	
4	0.5535	0.5954	0.5357		
5	0.5413	0.5377			
6	0.5315				

tends to zero as $n^{-(1-\alpha)}$ for large values of n. The evaluation table of the method for the α exponent is given in table 6. By comparing the results of the different methods of analysis one may conclude that the estimates lay in a region of $0.5<\alpha<0.55$. The corresponding y_t exponent from the hyperscaling relation (2.10) would be $y_t = 1.36\pm 0.03$, in accordance with the earlier estimate (Iglói *et al* 1986) and with the result obtained in the previous section by neglecting the logarithmic corrections. However the estimates of the different methods are somewhat different and the results within one method show some systematic alternation. These facts may signal the presence of some strong confluent singularities.

To investigate the possible presence of a logarithmic confluent singularity of the specific heat in the general form of

$$C(\lambda)\sim|\lambda-\lambda^*|^{-\alpha}\log^{\beta}|\lambda-\lambda^*| \tag{3.3}$$

Table 6. Analysis of the series of the latent heat by scaling method: estimates for the α exponent.

n_1 \ n_2	2	3	4	5	6	7
1	0.5270	0.5314	0.5324	0.5338	0.5352	0.5365
2		0.5391	0.5367	0.5379	0.5392	0.5404
3			0.5332	0.5377	0.5402	0.5419
4				0.5438	0.5448	0.5457
5					0.5460	0.5469
6						0.5480

(similar to (2.16)) the method of Adler and Privman (1981) is applied. In this procedure the β exponent is determined by the Dlog Padé method for fixed values of α. The different Padé approximants for β as a function of α are plotted in figure 1. One can see that within the region denoted by the broken line the error in the Padé table is minimal. The possible estimate $\alpha = 0.48 \pm 0.02$ and $\beta = 0.18 \pm 0.05$ are different from those of the four-state Potts model: $\alpha = \frac{2}{3}$ and $\beta = -1$, and is in contrast to the results obtained by finite-size scaling in the end of the last section. The possible reason is that the structure of the confluent singularities is different in the two methods and it is very important to choose the accurate form of the logarithmic singularity in the series analysis method. It will be shown in the next section that one may obtain better agreement, if the form of the logarithmic correction is taken more accurately.

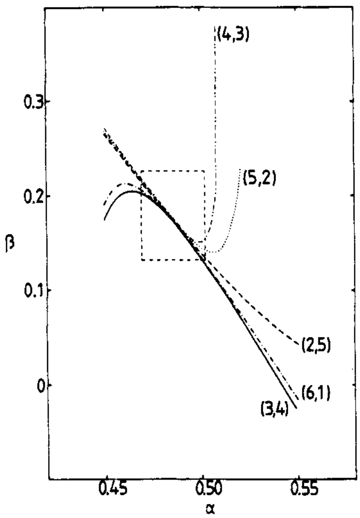

Figure 1. The method of Adler and Privman (1981) applied to the series of the specific heat. The various Padé approximants for the strength of the logarithmic correction β is plotted as a function of α. Within the rectangle the error in the Padé table is minimal.

4. Logarithmic corrections

The equivalence of the three-spin coupling model to the four-state Potts model implies the presence of similar logarithmic corrections. In the case of the Potts model these logarithmic corrections are associated with a marginal scaling field (denoted by ψ), which appears besides the two relevant scaling fields: temperature (t) and magnetic field (h).

According to Nauenberg and Scalapino (1980), Cardy *et al* (1980) and Blöte and Nightingale (1982) the scaling form of the free energy in a finite system close to the critical point obeys the following scaling relation:

$$f(t, h, \psi, L) \sim b^{-2} f(z^{3/4} b^{3/2} t, z^{1/16} b^{15/8} h, z\psi, L/b) \tag{4.1}$$

where b is the rescaling factor and

$$z = \left(1 - \frac{\psi(0)}{\pi} \ln L\right)^{-1}. \tag{4.2}$$

The non-universal constant $\psi(0)$ stands for the value of ψ at the critical point of the Potts model. Similarly any gap of the spectrum should obey the following scaling relation:

$$\Delta(t, h, \psi, L) \sim b^{-1}\Delta(z^{3/4}b^{3/2}t, z^{1/16}b^{15/8}h, z\psi, L/b). \tag{4.3}$$

From relations (4.1) and (4.3) it is easy to deduce that the specific heat, the susceptibility and the gap scales at the critical point as

$$\begin{aligned} C_L(1) &\sim L^{-d+2y_t}\left(1-\frac{\psi(0)}{\pi}\ln L\right)^{-3/2} \\ \chi_L(1) &\sim L^{-d+2y_h}\left(1-\frac{\psi(0)}{\pi}\ln L\right)^{-1/8} \\ \frac{\partial\Delta_L}{\partial\lambda}(1) &\sim L^{y_t-1}\left(1-\frac{\psi(0)}{\pi}\ln L\right)^{-3/4}. \end{aligned} \tag{4.4}$$

(In the Hamiltonian version the inverse of the coupling λ^{-1} plays the role of the temperature.)

The critical exponents obtained from these relations can be expanded in powers of $1/\ln L$ in the following way:

$$\begin{aligned} y_t(L) &= y_t - \frac{3}{4}\frac{1}{\ln L} + \frac{a_2}{(\ln L)^2} + \ldots \\ y_h(L) &= y_h - \frac{1}{16}\frac{1}{\ln L} + \frac{b_2}{(\ln L)^2} + \ldots. \end{aligned} \tag{4.5}$$

Here $y_t(L)$ and $y_h(L)$ denote the result of the two-point fit. For example

$$y_t(L) = \frac{1}{2}\left(\frac{\log(C_{L+3}(1)/C_L(1))}{\log(L+3/L)} + d\right) \tag{4.6}$$

and a_2 and b_2 are non-universal constants.

Similarly one may also expand the ratio of the universal amplitudes in (2.15):

$$R_L = R + \frac{4}{\ln L} + \frac{C_2}{(\ln L)^2} + \ldots. \tag{4.7}$$

A convenient way to apply relations (4.5) and (4.7) is to plot $y_t'(L) = y_t(L) + \frac{3}{4}(\ln L)^{-1}$ and $R_L' = R_L - 4(\ln L)^{-1}$ against $(\ln L)^{-2}$, and then to extrapolate to the $L \to \infty$ case. (Such an extrapolation is not performed for y_h, since the $y_h'(L)$ values show oscillatory behaviour. Furthermore the effect of logarithmic corrections in this case is much smaller.)

In figure 2 the $y_t'(L)$ exponents calculated from the specific heat and from the gap are plotted. As it is seen $y_t'(L)$ obeys the relation (4.5) in both cases and the extrapolated values $y_t = 1.50 \pm 0.02$ are consistent with the Potts value. A sinilar plot of the R_L quantities are given in figure 3. The extrapolated value is $R = 4.0 \pm 0.05$ which is also in agreement with the four-state Potts value $R = 4$.

Finally the specific heat series given in § 3 is reanalysed using the accurate form of the confluent singularity (Nauenberg and Scalapino 1980):

$$C(\lambda) \sim |\lambda - \lambda^*|^{-\alpha}\left(\frac{3\pi}{2\psi(0)} + \log|\lambda - \lambda^*|\right)^{-1}. \tag{4.8}$$

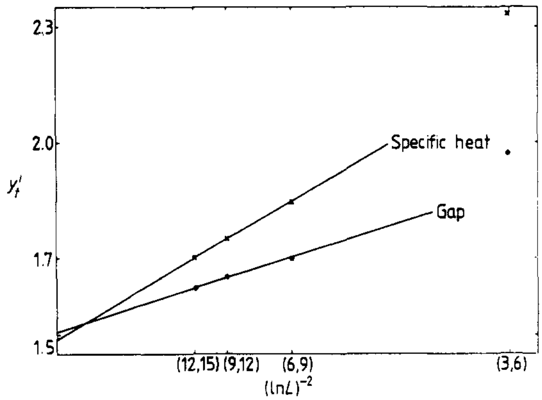

Figure 2. The $y_t' = y_t(L) + \frac{3}{4}(\ln L)^{-1}$ effective exponent as a function of $(\ln L)^{-2}$. Crosses and circles denote the values obtained from specific heat data and from the derivative of the gap, respectively.

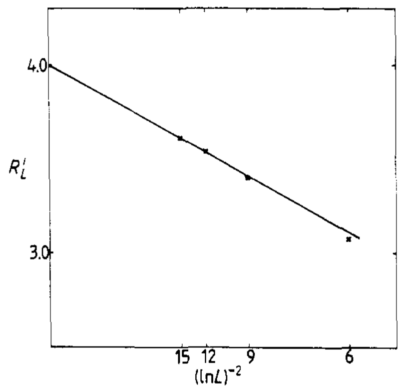

Figure 3. The $R_L' = R_L - 4(\ln L)^{-1}$ ratio as a function of $(\ln L)^{-2}$.

Taking the estimate $\psi(0) = -3.0 \pm 1.0$ that one may obtain from the finite size scaling data, the Padé analysis predicts

$$\alpha = 0.71 \pm 0.03 \tag{4.9}$$

which lays close to the four-state Potts value $\alpha = \frac{2}{3}$.

5. Discussion

In this paper the critical properties of the quantum Ising model with three-spin interaction is studied by finite-size scaling and series expansion. The earlier investigations were extended to other quantities, larger system sizes and longer series. Furthermore the method of universal amplitudes was also applied. The central problem of the paper is to determine the universality class of the model, whether it can be characterised with the same critical exponents as that of the four-state Potts model. To answer to this question the results of the calculations were analysed by different methods: (i) neglecting the confluent logarithmic singularities, (ii) supposing a general form for these corrections, or (iii) taking these singularities in the same form as in the four-state Potts model.

The results of the standard analysis ($y_t = 1.37$, $y_h = 1.87$) are in accordance with the findings of the earlier investigations. However, supposing a general form for the logarithmic corrections, one may predict the presence of strong corrections from the finite-size scaling results. Repeating the analysis with corrections in the same form as in the four-state Potts model the exponents become consistent with the four-state Potts critical behaviour. Since all methods used in this paper (finite size scaling, method of universal amplitudes, series expansion) give consistent results, we consider our findings as support to the validity of the mapping of the two models (Blöte *et al* 1986b) and supporting evidence for the conjecture that the three-spin coupling model belongs to the four-state Potts universality class.

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Note added in proof. After this work was completed, we received a paper by Alcaraz and Barber (1987) in which the present model is also studied. The result of that work agrees with our results. However, the authors did not study the influence of logarithmic corrections.

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