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LETTER TO THE EDITOR

Critical properties of an $S = 1$ multispin coupling Ising model

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Abstract. Strong and weak coupling series expansions are used to investigate the critical properties of the $S = 1$ multispin coupling Ising chain in the presence of a transverse field. The order of the transition goes from second order to first order when more than three spins are coupled. According to the numerical results the two-spin and three-spin coupling models belong to the Ising and the four-state Potts universality classes, respectively. Thus the critical properties of the model do not depend on the value of the spin, even when three spins are coupled.

In this letter we investigate the critical properties of a simple one-dimensional quantum model, described by the Hamiltonian

$$H = -\frac{1}{S^m}\sum_i S_i^z S_{i+1}^z \ldots S_{i+m-1}^z - \frac{h}{S}\sum_i S_i^x \tag{1}$$

where the S^x and S^z are quantum spin S operators. The model for $S = \frac{1}{2}$ has been introduced by Turban (1982) and Penson *et al* (1982) and has been investigated in several papers (Iglói *et al* 1983, 1986, Maritan *et al* 1984, Alcaraz 1986, Kolb and Penson 1986, Blöte *et al* 1986, Alcaraz and Barber 1987, Vanderzande and Iglói 1987). On the other hand, the two-spin coupling model for general values of the spin has been studied by Penson and Kolb (1984).

The classical statistical mechanical equivalent of model (1) may be obtained by following the work of Suzuki (1976) and Oitmaa and Coombs (1981). For the $S = 1$ model it is a two-dimensional square lattice $S = 1$ Ising model with m-spin interactions in the horizontal direction, and with two-spin interactions as well as with single site anisotropy terms and biquadratic pair interactions in the vertical. For larger values of the spin the form of the interaction in the vertical direction, besides the two-spin interaction terms, becomes more and more complicated. These terms, however, are irrelevant in determining the critical properties of the system for $m = 2$, and presumably they remain irrelevant also for $m > 2$.

The phase structure of the model in (1) is the same for all values of the spin. In the strong coupling regime, when $h < h^*$ the system exhibits a 2^{m-1}-fold degenerate ground state with non-vanishing order parameter $\langle S_i^z \rangle \neq 0$ while in the weak coupling regime for $h > h^*$ the system is in a non-degenerate ground state with $\langle S_i^z \rangle = 0$. At $h = h^*$, at the critical value of the coupling, a phase transition takes place in the system.

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For the two-spin coupling model the phase transition is of second order with two-dimensional Ising critical exponents independent of the value of the spin. This statement is exact for $S=\frac{1}{2}$ (Pfeuty 1970) and for $S>\frac{1}{2}$ it is numerically justified (Oitmaa and Coombs 1981, Penson and Kolb 1984). On the other hand, the mean-field solution predicts a first-order transition for $m>2$, which becomes exact in the $m\to\infty$ limit. Consequently, for all S the transition should go from second order to first order at some finite $m_c(S)$ value.

The prediction of the mean-field theory, $m_c(S)=2$, probably underestimates this critical value. It is possible, however, to make another conjecture on the analogy of the q-state Potts model (Debierre and Turban 1983, Maritan *et al* 1984). Supposing that the degeneracy of the ground state in the ordered phase determines the order of the transition in both models in a similar way, then the critical value of m should be $m_c(S)=3$, independent of the value of the spin. For $S=\frac{1}{2}$ recent numerical investigations (Iglói *et al* 1986, Alcaraz 1986, Blöte *et al* 1986) justify the validity of this conjecture. Furthermore the $S=\frac{1}{2}$, $m=3$ model presumably belongs to the four-state Potts universality class (Blöte *et al* 1986, Vanderzande and Iglói 1987, Alcaraz and Barber 1987).

In this letter the investigation of the model is extended for the $S=1$ case. We use strong and weak coupling series expansions, which have turned out to be very useful in the study of many systems (Hamer *et al* 1979, Elitzur *et al* 1979, Marland 1981, Hamer and Irving 1984) and also for the $S=\frac{1}{2}$ model in (1) (Iglói *et al* 1986).

In the strong coupling expansion the transverse field is taken as a perturbation, and a series in powers of h is generated. The ground-state energy per site yields the form:

$$E/N=-\sum_i a_i h^i. \qquad (2)$$

On the other hand, in the weak coupling expansion the multispin coupling term is taken as a perturbation, and a series in powers of $1/h$ is generated:

$$E/N=-h\sum_i b_i h^{-i}. \qquad (3)$$

The coefficients of these series were calculated up to tenth order for $m=2$ and 3, and up to eighth order for $m=4$. They are presented in table 1. The numerical calculation of these coefficients needed about one hundred hours CPU time on a Masscomp-500 computer. Since for the $S=1$ models self-duality does not hold (in contrast to the $S=\frac{1}{2}$ models), there is no connection between the coefficients of the strong and weak coupling series and the phase transition point is not known exactly. Now supposing second-order transitions, the phase transition point and the α critical exponent might be estimated independently from strong and weak coupling series. However, these series contain strong confluent singularities and it is impossible to make a reasonable estimate from the relatively short series in this way.

Much more accurate results may be obtained, however, by following the analysis used in the $S=\frac{1}{2}$ case (Iglói 1986, Iglói *et al* 1986). Let us denote by E_n^{S} and E_n^{W} the ground-state energies calculated by strong and weak coupling expansions, respectively, keeping terms up to nth order. Then the phase transition point in the nth order (denoted by h_n^*) is defined as the crossing point of these two expressions:

$$E_n^{\mathrm{S}}(h_n^*)=E_n^{\mathrm{W}}(h_n^*). \qquad (4)$$

Obviously $h_n^*\to h^*$ when $n\to\infty$. Furthermore the order of the transition may be determined from the difference in the slopes at the crossing point. More precisely the

Table 1. Coefficients of the strong coupling (a) and of the weak coupling (b) series for the ground-state energy for $m = 2$, 3 and 4.

Order	$a_i(2)$	$a_i(3)$	$a_i(4)$
(a)			
2	$\frac{1}{4}$	$\frac{1}{6}$	$\frac{1}{8}$
4	0.005 208 333	0.008 333 333	0.006 454 613
6	0.000 325 521	0.001 638 595	0.001 264 989
8	0.000 209 780	0.000 525 128	0.000 388 008
10	0.000 050 521	0.000 204 099	
Order	$b_i(2)$	$b_i(3)$	$b_i(4)$
(b)			
2	0.125 000 000	0.041 666 667	0.015 625 000
4	0.058 593 750	0.018 373 843	0.005 462 646
6	0.036 254 883	0.012 068 269	0.002 932 599
8	0.026 372 910	0.009 778 305	0.001 969 105
10	0.021 608 243	0.008 995 761	

nth order latent heat, defined by

$$L_n = \frac{1}{N}\left(\frac{\partial E_n^{\mathrm{S}}(h)}{\partial h}\bigg|_{h=h_n^*} - \frac{\partial E_n^{\mathrm{W}}(h)}{\partial h}\bigg|_{h=h_n^*} \right) \tag{5}$$

goes to zero for second-order transitions, while it approaches a non-zero value for first-order transitions.

The series for the phase transition points and for the latent heat are presented in table 2. From the series of phase transition points it is possible to make estimates with relatively small errors, which are also presented in table 2. This estimate for $m = 2$ agrees well with the finite-size scaling result of Penson and Kolb (1984): $h^* = 1.326$.

To analyse the latent heat series the following asymptotic relation valid for second-order transitions (Iglói 1986) is used:

$$L_n \propto n^{-(1-\alpha)}. \tag{6}$$

Table 2. Phase transition points (h_n^*) and latent heats (L_n) in nth order of the expansion for $m = 2$, 3 and 4. In the last row the estimated values for $n \to \infty$ are given.

	$m = 2$		$m = 3$		$m = 4$	
Order	h_n^*	L_n	h_n^*	L_n	h_n^*	L_n
2	1.403 032	0.234 984	1.209 263	0.568 419	1.152 464	0.700 120
4	1.395 301	0.135 174	1.224 709	0.478 251	1.164 500	0.647 670
6	1.353 557	0.112 612	1.227 365	0.432 263	1.167 356	0.624 551
8	1.343 903	0.084 412	1.228 297	0.400 972	1.168 454	0.610 973
10	1.335 929	0.068 408	1.228 778	0.377 427		
Estimate	1.32 ± 0.01	0.0	1.230 ± 0.002	0.0	1.172 ± 0.002	0.47 ± 0.05

According to this relation a plot of $\log(L_n)$ against $\log(n)$ should approach a straight line with slope $-(1-\alpha)$ for second-order transitions, while for first-order transitions the points bend off a straight line, signalling an $\alpha=1$ exponent, characteristic of first-order transitions (Fisher and Berker 1982). This plot is given in figure 1 for $m=2$, 3 and 4. In this figure the estimates for the $(1-\alpha)$ exponents obtained by a two-point fit are also presented. From these data one can conclude that the results for $m=2$ are consistent with the Ising critical behaviour ($\alpha=0$). However, the effect of the confluent singularity is still strong. In the $m=3$ model the estimates for the $(1-\alpha)$ exponent are continuously increasing with increasing n, while for the $m=4$ model they are monotonically decreasing. Thus the order of the transitions turns from second order to first order at $m_c=3$. In order to make an estimate for the latent heat of the $m=4$ model in figure 2 the L_n latent heats are plotted against $n^{-1/3}$ for $m=3$ and 4. As is seen in this figure for $m=4$ the L_n values lie well on a straight line and one may estimate the latent heat as $L(m=4)=0.47\pm0.05$. This is roughly twice as large as the latent heat of the same model for $S=\frac{1}{2}$ (Iglói *et al* 1986).

Finally we turn to the question of the transition in the $m=3$ model. In this case we conjecture that the model belongs to the four-state Potts universality class. This conjecture is based on the degeneracy of the ordered ground state of the model and supported by the results of the series analysis. Supposing that the correction to the $(1-\alpha)$ exponent obtained by a two-point fit is of the form of constant/$\log(n)$, then the estimated value is close to the four-states Potts value (den Nijs 1979) $1-\alpha=\frac{1}{3}$, as is seen in figure 3. Thus it seems to be very probable that the universality class of the model in (1) does not depend on the value of the spin.

To summarise the phase transition in the multispin coupling Ising models shows similar behaviour for $S=\frac{1}{2}$ and $S=1$. In both cases the transition turns from second order to first order when more than three spins are coupled. Furthermore the critical

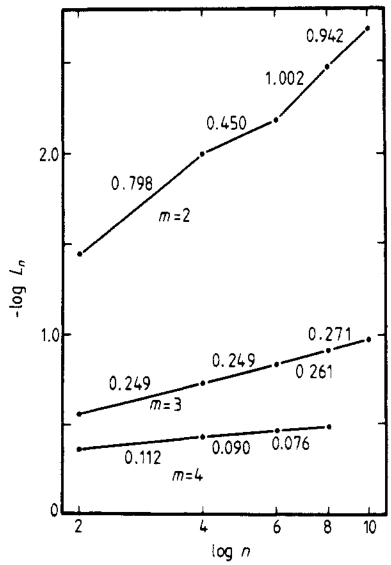

Figure 1. The nth-order latent heat L_n against n on a log–log plot for different values of the coupled spins. The estimates for the $1-\alpha$ exponent obtained from the slopes between two neighbouring points are also given.

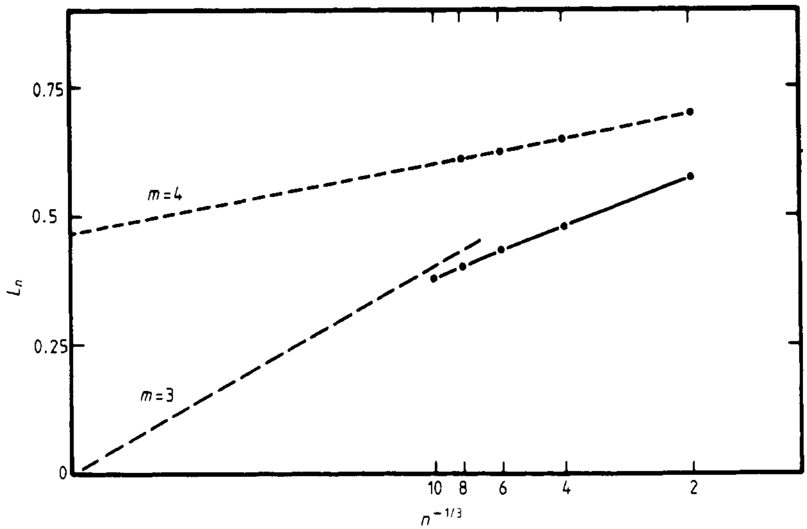

Figure 2. The nth-order latent heat L_n against $n^{-1/3}$ for $m=3$ and 4. The broken lines indicate the possible asymptotic behaviours.

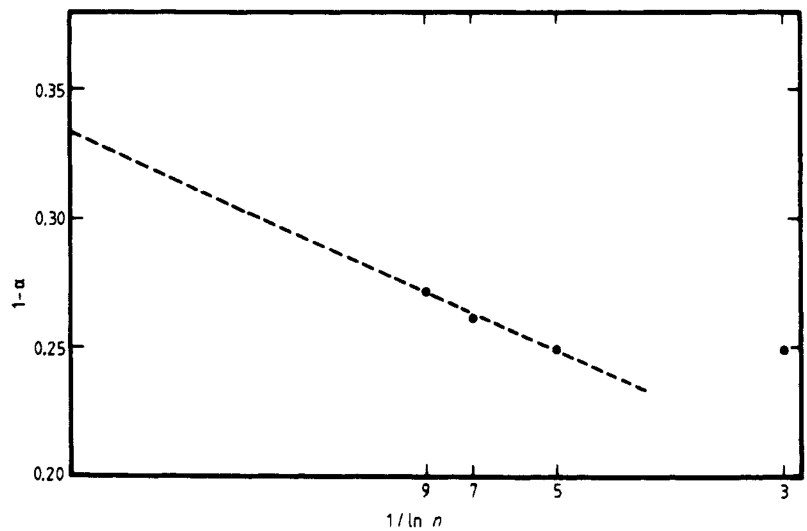

Figure 3. The $(1-\alpha)$ exponent obtained by a two-point fit against $1/\log(n)$ for the $m=3$ model.

properties of the models for $m=2$ and $m=3$ do not depend on the value of the spin. The $m=3$ model presumably belongs to the four-state Potts universality class, giving a further example for the relation that the degeneracy of the ordered ground state may determine the universality class of the model.

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