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The critical behaviour of a quantum spin problem with three-spin coupling

F Iglói†, D V Kapor‡, M Škrinjar‡ and J Sólyom†

† Central Research Institute for Physics, Budapest, Hungary
‡ Department of Physics, University of Novi Sad, Novi Sad, Yugoslavia

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Abstract. The critical behaviour of an Ising like model with three-spin coupling is studied in a transverse field. A self-dual renormalisation group transformation can be applied which gives well converging results for the critical exponents when large enough cells are taken. Finite size scaling on the same model gives comparable results.

1. Introduction

In a recent paper by Turban (1982) an Ising like model in a transverse field with multispin interaction has been introduced:

$$\mathcal{H}^{(m)}(\lambda) = -\lambda \sum_i \prod_{l=0}^{m-1} \sigma_{i+l}^z - \sum_i \sigma_i^x, \tag{1.1}$$

where σ^x and σ^z are the Pauli operators.

The same Hamiltonian has been considered independently by Penson *et al* (1982). Both papers show that the model is self-dual and address the question of whether for $m \geqslant 3$ the transition is of first order, as suggested by the mean field theory, or can be of second order. Penson *et al* (1982), using finite size scaling arguments, conclude that the critical value of m above which the transition is of first order is probably $m_c = 4$ in the one-dimensional case.

In this paper we report the results of a renormalisation group calculation for the $m = 3$ case. We have chosen a procedure which preserves the self-duality. As will be seen, our calculation suggests a second-order transition for the $m = 3$ case. The values for the critical exponents converge quite well as larger and larger cells are taken in the renormalisation procedure. Finite size scaling in a somewhat different form than that used by Penson *et al* (1982) confirms the results of the renormalisation group treatment.

2. Renormalisation procedure

The renormalisation group procedure for quantum spin systems has been formulated originally for the Ising model in a transverse field by Pearson *et al* (unpublished) and Drell *et al* (1977). This block method has been recently applied to a variety of quantum problems; for a review see Pfeuty *et al* (1982). An alternative procedure,

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the decimation transformation, has been proposed by Fradkin and Raby (1979). It has been shown by Sólyom (1981) that the two methods are dual to each other for self-dual models with pairwise interaction.

The present model of equation (1.1) is self-dual, but contains multispin interactions and therefore the duality of the two renormalisation procedures will not hold. It can easily be seen, however, that for the $m=3$ case the decimation transformation conserves the self-duality and therefore this procedure will be used in the present paper.

After choosing a scale factor b, the spins at sites $i=nb+1$, $n=0, 1, 2, \ldots$ are fixed arbitrarily while the intermediate spins are integrated out. For convenience the sites are relabelled as $i=(j,\alpha)$ where $j=1, 2, \ldots$ denotes the cell and $\alpha=0, 1, \ldots, b-1$ labels the sites in a cell. The fixed spins are at sites $j, 0$. The Hamiltonian is split into

$$\mathcal{H}=\mathcal{H}_0+V \tag{2.1}$$

where

$$\mathcal{H}_0=-\lambda\sum_j\sum_{\alpha=0}^{b-2}\sigma^z_{j,\alpha}\sigma^z_{j,\alpha+1}\sigma^z_{j,\alpha+2}-\sum_j\sum_{\alpha=1}^{b-1}\sigma^x_{j,\alpha} \tag{2.2}$$

and

$$V=-\lambda\sum_j\sigma^z_{j-1,b-1}\sigma^z_{j,0}\sigma^z_{j,1}-\sum_j\sigma^x_{j,0} \tag{2.3}$$

contains the transverse field acting on the selected spins and the couplings which couple the different cells.

The eigenvalues of $\mathcal{H}_0$ can be calculated for any fixed configuration of the selected spins. Keeping for any configuration the lowest lying level only, the matrix elements of V between these states will give the renormalised couplings.

For the model with three-spin coupling this procedure can be used to give a reasonably good approximation if the scale factor is not an integer multiple of 3. The fourfold degeneracy of the ground state in the large λ limit is not reproduced if the scale factor is $b=3l$; the decimation will always yield a ferromagnetic ground state. We have therefore performed the calculations for scale factors $b=2, 4, 5, 7, 8$ and will compare the results as the scale factor increases.

When the cell problem $\mathcal{H}_0$ is solved, the two end-spins of the cell can be in four different configurations. It is easily shown that these four problems are not independent. Let us take both end-spins to be in the $\uparrow$ state and solve this eigenvalue and eigenfunction problem. The eigenvalue problem when the configuration of the end-spins is $(\uparrow\downarrow)$, $(\downarrow\uparrow)$ or $(\downarrow\downarrow)$ is exactly the same and the eigenfunctions in terms of the intermediate spins can be easily obtained by a simple transformation. The eigenfunctions belonging to the $(\uparrow\downarrow)$ end-spin configuration can be obtained from that of the $(\uparrow\uparrow)$ configuration by reversing the spins at the intermediate sites $\alpha=1, 2, 4, 5, 7, 8, \ldots$. The eigenfunctions belonging to the $(\downarrow\uparrow)$ end-spin configuration can be similarly obtained by reversing the spins at sites $\alpha=b-1, b-2, b-4, b-5, b-7, b-8, \ldots$. The eigenfunctions of the $(\downarrow\downarrow)$ configurations are obtained by applying both transformations successively.

Due to the above mentioned transformation properties of the cell functions the renormalised Hamiltonian will have the same structure as the original one, i.e. it will contain a three-spin coupling term and a transverse field, and no new couplings will be generated.

3. Results

If the transverse field strength is rescaled to unity a one-parameter recursion relation is obtained for the coupling λ whose non-trivial fixed point is always at the self-dual point $\lambda = 1$. Linearisation of the recursion relation around $\lambda = 1$ yields the thermal eigenvalue λ_t and the thermal exponent ν. The results for the various scale factors are given in table 1. The table also contains the results for the dynamical exponent z calculated from the rescaling of the transverse field and the values for the specific heat exponent α calculated from the scaling law

$$2-\alpha = (1+z)\nu. \tag{3.1}$$

Furthermore we have studied the behaviour of the model in a longitudinal magnetic field in order to calculate the magnetic eigenvalue λ_m and the magnetic exponent β. It turns out that the inclusion of a longitudinal field will generate during the renormalisation procedure a usual Ising coupling, therefore we have considered the effect of the perturbation

$$\mathcal{H}' = -\lambda_1 \sum_i \sigma_i^z - \lambda_2 \sum_i \sigma_i^z \sigma_{i+1}^z \tag{3.2}$$

in linear order. The magnetic eigenvalue is the largest eigenvalue of the recursion relations in the (λ_1, λ_2) plane at the original fixed point $\lambda = 1$, $\lambda_1 = \lambda_2 = 0$. The results for the magnetic eigenvalue and exponent are also given in table 1.

Table 1. Eigenvalues of the renormalisation group recursion relations and the critical exponents calculated with different scale factors in the decimation.

Scale factor	Eigenvalues		Critical exponents			
	thermal	magnetic				
	λ_t	λ_m	ν	z	β	α
2	3	1.62	0.631	1	0.193	0.738
4	6.85	2.82	0.720	0.645	0.182	0.815
5	9.15	3.38	0.727	0.655	0.177	0.797
7	14.03	4.47	0.737	0.620	0.170	0.806
8	16.67	5.00	0.739	0.621	0.167	0.802

As one can see, instead of the usual odd–even effect we have here an oscillation in z and α depending on whether $b = 3l + 1$ or $b = 3l - 1$.

Plotting the results for the exponents as a function of $1/\ln b$—as suggested by the results on the Ising model—allows a reasonable extrapolation to

$$\nu \sim 0.77. \tag{3.3}$$

Unfortunately a plot against neither $1/\ln b$ nor $1/b$ gives a straight line for β; therefore the estimated value

$$\beta \sim 0.1\text{–}0.13 \tag{3.4}$$

has a big uncertainty.

4. Finite size scaling

The result obtained for ν is somewhat larger than the value suggested by Penson *et al* (1982) from finite size scaling. They have compared the gap for finite systems and calculated ν from the vanishing of the gap. Because of the periodic boundary condition they could use rings containing 3, 6, 9, 12 or 15 sites. Instead of this procedure we have looked at chains with a free boundary condition which allows us to use arbitrary chain length. We went up to $N = 9$ sites because convergence seems to be fast enough.

In the case of a periodic boundary condition the level structure for any finite ring of size $3n$ is such that the lowest level is non-degenerate, while the first excited state is threefold degenerate. In the thermodynamic limit these two levels become degenerate for $\lambda \geqslant \lambda_c$, yielding a fourfold degenerate ground state.

For a free boundary condition the situation is different. The lowest level is again non-degenerate; the next level is, however, twofold degenerate if the number of sites in the chain is $3n$ or $3n+2$, while it is non-degenerate if the number of sites is $3n+1$. On the other hand the third level is non-degenerate or twofold degenerate for the two cases, respectively.

These three levels will become degenerate in the thermodynamic limit. Due to this fact two gaps Δ_1 and Δ_2 can be defined for finite chains.

In the finite size scaling for quantum systems (Hamer and Barber 1981) the relation

$$N\Delta(\lambda_c, N) = (N+1)\Delta(\lambda_c, N+1) \tag{4.1}$$

is used to locate the fixed point, where $\Delta(\lambda, N)$ is the gap calculated for a chain with N sites. In the present case, when for any finite N two gaps are obtained, the fixed point can be calculated from any of them since in the $N \to \infty$ limit the gaps will coincide. Since the boundary condition influences the various gaps differently, it seemed natural to average over the critical couplings and exponents obtained for the individual gaps. In table 2 we give this average of the fixed point couplings calculated from the comparison of different cells. Similarly the ν exponent, given in table 2 and obtained from the β function of Roomany and Wyld (1980), is an average value.

Table 2. The critical coupling λ_c and the critical exponent ν obtained from comparison of finite cells with N and $N+1$ sites. The values given are averages as described in the text.

Cell size	λ_c	ν
3, 4	1.382	0.687
4, 5	1.199	0.722
5, 6	1.123	0.745
6, 7	1.089	0.758
7, 8	1.064	0.765
8, 9	1.049	0.767

Both quantities $\lambda_c(N, N+1)$ and ν converge faster than $1/N$. In fact λ_c seems to converge as $1/N(N+1)$ to the self-dual value $\lambda_c = 1$ and ν converges as $\exp(-N)$ to

$$\nu = 0.77 \tag{4.2}$$

confirming our earlier results obtained by the renormalisation group treatment.

5. Discussion

In this paper we have studied the critical behaviour of a quantum spin system with three spin couplings. The decimation transformation is ideally suited to treat this model by the renormalisation group method since the self-duality of the model is preserved and no new couplings are generated. Taking different scale factors up to $b = 8$, the critical exponents have been calculated yielding the values given in equations (3.3) and (3.4). The value obtained for ν is higher than the one obtained by Penson *et al* (1982) from finite size scaling. Our modified finite size scaling procedure is, however, in agreement with the results of the renormalisation group calculation. Thus this model is not in the same universality class as the four-state Potts model, as one could have guessed from the degeneracy structure of the low lying levels.

The renormalisation group procedure cannot be extended simply to the other m values and therefore it is not suitable for studying when the first-order behaviour will occur. Finite size scaling, however, can be used and we plan to return to this problem later.

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