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Improved mean-field-like renormalisation group approach for $Z(q)$ symmetric spin models

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Abstract. Various modifications of the mean-field renormalisation group method are analysed to study the convergence of the critical coupling and critical exponents to their exact values as the cluster size increases. Appropriate choice of the length scaling factor or of the scaling quantity can give appreciable improvement over the conventional procedure for short clusters. The best values are achieved when both the bulk and surface critical behaviour are explicitly taken into account.

1. Introduction

In a previous paper (Niebur and Sólyom 1987, hereafter referred to as I) we have analysed the convergence of the mean-field-like variational and renormalisation group approaches. In both cases the method is based on performing calculations on finite clusters. The results obtained in a variational scheme with cluster wavefunctions should converge to the exact result as the size of the clusters goes to infinity. It was shown in I that the convergence is in fact rather slow. Better results are obtained if a mean-field renormalisation group (MFRG) transformation (Indekeu *et al* 1982) is performed on the finite clusters. In fact MFRG gives quite good results for the critical couplings of the $Z(q)$ model for $q=2$, 3 and 4, where the transition is of second order, although the values for the critical exponent ν are rather poor. For larger q values, $q \geqslant 5$, where a Kosterlitz-Thouless phase is expected between the ordered and disordered phases, MFRG gives only slight indications for this behaviour. Moreover the cluster calculation could not give a good estimate for the point where the order parameter vanishes, although there was some indication that this happens at the self-dual point for any q, as suggested by Zittartz (unpublished).

Several attempts have been made to improve upon the results of the MFRG method. Slotte (1987) showed that for two- and three-dimensional Ising models considerable improvement can be achieved if the length scaling factor is determined from the number of bonds and not from the number of sites. On the other hand, in I we argued that the quantity that scales in the same way as the effective field is not necessarily the average magnetisation of the cluster and proposed new scaling equations by assuming that the scaling quantity is the magnetisation in specific points of the finite cluster.

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A more elaborate scheme was suggested by Indekeu *et al* (1987). It is based on separating the surface and bulk terms in the magnetisation and performing the renormalisation in two steps, comparing three different clusters.

In the present paper we will consider these new methods to study how they improve the results obtained in I for the $Z(q)$ model. In § 2 the reader is reminded of the model studied and of the main ideas of MFRG. The results obtained with the use of the modified length scaling factor are given here. In § 3 we show how the results change if the quantity to be scaled is not the average magnetisation. The renormalisation using three clusters and surface as well as bulk fields is described in § 4. Finally, § 5 contains a discussion of the results.

2. MFRG with modified length scaling factor

In the $Z(q)$ symmetric spin model the spin vector at site i can be oriented in the directions given by the polar angle $\theta_i = 2\pi n_i/q$ where $n_i = 0, 1, 2, \ldots, (q-1)$ and the spin state is characterised by the set of numbers n_i. In the Hamiltonian version of the model raising, R_i^+, and lowering, R_i, operators are introduced with the definition

$$\begin{aligned} R_i^+|n_i\rangle &= |(n_i+1) \bmod q\rangle \\ R_i|n_i\rangle &= |(n_i-1) \bmod q\rangle. \end{aligned} \tag{2.1}$$

Assuming a simple $\cos(\theta_i - \theta_{i+1})$ coupling between nearest-neighbour spins, the Hamiltonian of the system can be written (Elitzur *et al* 1979) as

$$H = -\sum_i \cos\left(\frac{2\pi n_i}{q}\right) - \tfrac{1}{2}\lambda \sum_i (R_i^+ R_{i+1} + R_i R_{i+1}^+) \tag{2.2}$$

where λ is the coupling constant.

In a mean-field treatment of this model, a finite cluster with M sites is taken and a complex effective field, h_s, acting on the boundary spin replaces the action of the spins outside the cluster. The Hamiltonian to be considered is then

$$\begin{aligned} H_M = -\sum_{i=1}^{M} \cos\left(\frac{2\pi n_i}{q}\right) - \tfrac{1}{2}\lambda \sum_{i=1}^{M-1} (R_i^+ R_{i+1} + R_i R_{i+1}^+) \\ - h_s(R_1 + R_M) - h_s^+(R_1^+ + R_M^+) \end{aligned} \tag{2.3}$$

where h_s^+ is the complex conjugate of h_s. This notation is used to avoid confusion with the fixed-point value of h_s for which the notation h_s^* will be used.

The MFRG transformation is defined, as usual, by comparing a cluster with M sites to a cluster with $M' < M$ sites. The basic assumption is that the order parameter $O(\lambda, h_s)$, which is the average magnetisation of the cluster for fixed effective field h_s

$$O(\lambda, h_s) = \frac{1}{M} \sum_{i=1}^{M} \tfrac{1}{2}(\langle R_i\rangle + \langle R_i^+\rangle) \tag{2.4}$$

scales in the same way as the effective field itself, i.e. under a length scaling transformation around the fixed point λ^* and $h_s^* = 0$,

$$\begin{aligned} \lambda' - \lambda^* &= L^{1/\nu}(\lambda - \lambda^*) \\ h_s' &= L^{\alpha} h_s \end{aligned} \tag{2.5}$$

$O_M(\lambda, h_s)$ satisfies

$$O_{M'}(\lambda', h_s') = L^{\alpha} O_M(\lambda, h_s). \tag{2.6}$$

A natural assumption was that the length scale is proportional to the number of sites in the cluster, i.e. when the renormalisation group transformation is performed from M sites to M' sites one takes $L = M/M'$. The results obtained with this assumption for the $Z(q)$ symmetric $(1+1)$-dimensional spin model were given in I. It was shown that the critical exponents converge rather slowly as M increases.

Slotte (1987) pointed out that a different definition of the length scaling factor is possible. In mean-field theory the coupling to external sites is taken into account, therefore a cluster with M sites embedded in a mean field simulates a somewhat larger cluster with free ends. Slotte suggests that a better definition of the length scale is obtained by counting the number of bonds instead of the number of sites. In the case of a chain this leads to a new scale factor

$$L = (M+1)/(M'+1). \tag{2.7}$$

The value of the fixed-point coupling is unchanged, but for the critical exponent ν new estimates are obtained. Table 1 contains the old and new estimates of ν for $q = 2$ and 3, as obtained for different cluster sizes. Everywhere we have taken $M' = M - 1$.

Table 1. New estimates of the critical exponent ν for the $Z(q)$ model.

	$\nu(q=2)$		$\nu(q=3)$	
M	Old	New	Old	New
2	1.48	0.87	1.28	0.75
3	1.32	0.94	1.12	0.80
4	1.26	0.97	1.06	0.82
5	1.22	1.00	1.02	0.83
6	1.20	1.02	1.00	0.85
7	1.19	1.03	0.99	0.86
8	1.18	1.04		

It is seen that in fact for short clusters the results seem to converge much faster to the exactly known exponents, $\nu = 1$ for $q = 2$ and $\nu = 0.8333\ldots$ for $q = 3$, than in the case of the earlier estimates. However, for clusters with $M > 6$ the values go above the exact result and will settle to the known result for very large chains only.

3. MFRG with different choices of the scaling quantity

As mentioned in the previous section, the basic assumption of the MFRG method is that the average magnetisation of the cluster scales in the same way as the effective field. For a finite system, where boundary effects are important and the magnetisation is not homogeneous inside the cluster, this assumption is not *a priori* true, and this may be one of the reasons why MFRG converges so slowly. We suggested in I that, instead of the average magnetisation, perhaps the magnetisation on the surface,

$$O_{SM} = \tfrac{1}{4}(\langle R_1 \rangle + \langle R_1^{+} \rangle + \langle R_M \rangle + \langle R_M^{+} \rangle) \tag{3.1}$$

Table 2. Fixed-point coupling λ^* and critical exponent ν for $q=2$ and 3. Scaling is assumed for the magnetisation of the boundary spins.

	$q=2$		$q=3$	
M	λ^*	ν	λ^*	ν
2	0.7832	1.48	0.9122	1.28
3	0.8550	1.51	0.9453	1.31
4	0.8905	1.53	0.9605	1.33
5	0.9119	1.51	0.9694	1.39
6	0.9262	1.56		
7	0.9365	1.57		
8	0.9442	1.54		
9	0.9430	1.50		

Table 3. Fixed-point coupling λ^* and critical exponent ν for $q=2$ and 3. Scaling is assumed for the magnetisation at the centre of the clusters of M and $M-1$ spins. ν_1 is determined with a length scaling factor $L=M/(M-1)$, while ν_2 with $L=(M+1)/M$.

	$q=2$			$q=3$		
M	λ^*	ν_1	ν_2	λ^*	ν_1	ν_2
2	0.7832	1.48	0.87	0.9122	1.27	0.74
3	0.8290	1.05	0.74	0.9338	0.88	0.63
4	0.8817	1.21	0.94	0.9569	1.05	0.82
5	0.8966	1.04	0.85	0.9632	0.87	0.71
6	0.9185	1.17	0.99	0.9720	0.99	0.84
7	0.9259	1.04	0.90	0.9751	0.84	0.73
8	0.9379	1.13	1.00			
9	0.9422	1.04	0.93			
10	0.949	1.09	0.99			

Table 4. The same as table 3, except that mapping is from clusters with spin M to that with spin $M-2$, the length scaling factor for ν_1 is $L=M/(M-2)$, while for ν_2 $L=(M+1)/(M-1)$.

	$q=2$			$q=3$		
M	λ^*	ν_1	ν_2	λ^*	ν_1	ν_2
3	0.8085	1.27	0.80	0.9247	1.09	0.69
4	0.8525	1.13	0.83	0.9444	0.95	0.70
5	0.8896	1.14	0.90	0.9602	0.97	0.77
6	0.9069	1.11	0.92	0.9673	0.91	0.76
7	0.9224	1.12	0.96	0.9736	0.92	0.79
8	0.9316	1.10	0.96			
9	0.9401	1.09	0.97			
10	0.9458	1.08	0.97			

should be considered in the scaling relation (2.6). The idea was that, since the effective field acts on the boundary spins, the magnetisation on the boundary might scale in the same way as the effective field itself. The results obtained for the fixed-point coupling λ^* and the thermal exponent ν for $q=2$ and 3 are given in table 2.

Contrary to expectation, the results are worse than those obtained in I using the average magnetisation. The critical couplings are somewhat better, but the results for the exponent ν are, however, much worse. They do not show any tendency of convergence to the known results. This shows clearly that the assumption according to which the effective field and the magnetisation on the surface scale in the same way is not correct. On the other hand, one can argue that the mean field acting on the cluster should, in fact, reflect the properties of the infinite embedding medium and should, therefore, be proportional to the bulk magnetisation. Since the bulk magnetisation is best approximated on sites deep in the cluster, we will assume now that the quantity that scales like the effective field is the magnetisation in the centre of the cluster,

$$O_c = \tfrac{1}{2}(\langle R_c\rangle + \langle R_c^+\rangle) \tag{3.2}$$

where the site c is $M/2$ for M even or $(M+1)/2$ for M odd. The results obtained by using this quantity in the scaling equations (2.5) and (2.6) with $L = M/M'$, $M' = M-1$, are given in table 3. Apart from an oscillation in the exponent ν due to the even–odd effect, the values of ν seem to converge much better than with the usual method, although not as well as in table 1 when the modified length scaling factor is used. The proposal of Slotte (1987) to choose the length scaling factor as $L = (M+1)/M$ does not improve the results appreciably because of the even–odd oscillations.

The even–odd oscillation can be eliminated or decreased if an even cluster is mapped to an even one and an odd cluster to an odd one. Choosing $M' = M-2$, the results for the critical coupling and the critical exponent ν are given in table 4, showing reasonable convergence to the known values.

4. MFRG for bulk and surface critical behaviour

As seen in the previous section, one problem with the usual MFRG method can be that the average magnetisation and the effective field do not scale in the same way. Following a suggestion by Droz *et al* (1985) on how to study surface critical phenomena in finite-size scaling, Indekeu *et al* (1987) proposed a modified version of MFRG based on using both bulk and surface terms. In addition to the effective field h_s which acts on the surface spins only, they introduce a bulk field h acting homogeneously on all spins. The Hamiltonian of the $Z(q)$ model takes the form

$$H = -\sum_{i=1}^{M}\cos\left(\frac{2\pi n_i}{q}\right) - \tfrac{1}{2}\lambda\sum_{i=1}^{M-1}(R_i^+R_{i+1} + R_iR_{i+1}^+)$$
$$-\sum_{i=1}^{M}(hR_i + h^+R_i^+) - h_s(R_1 + R_M) - h_s^+(R_1^+ + R_M^+). \tag{4.1}$$

Indekeu *et al* assume that the bulk and surface fields are scaled as

$$h' = L^{y_H}h \qquad h_s' = L^{y_{H_s}}h_s \tag{4.2}$$

when the length scale is changed, i.e. the model with M sites is mapped on a model with M' sites. They assume $L = M/M'$. More important, they assume that the average magnetisation of the cluster scales like the bulk magnetisation, i.e.

$$O_{M'}(\lambda', h', h'_s) = L^{d-y_H} O_M(\lambda, h, h_s) \tag{4.3}$$

where d is the dimension of the system. In classical statistical mechanics d is the spatial dimension. When going from classical statistical mechanics to a quantum problem by the transfer matrix, the dimension should be replaced by $d_s + z$, where d_s is the spatial dimension of the quantum problem and z is the dynamical exponent describing the scaling in the temporal direction (Jullien *et al* 1978). We will choose $z = 1$, corresponding to scaling the energies in the same way as the length. For the $q = 2$ Ising and $q = 3$ Potts models at least, this value is known to be exact.

In order to be able to determine the fixed-point coupling λ^* and the critical exponents ν, y_H and y_{H_s} separately, one has to perform two successive scalings, first from M to $M' = M - 1$ and then from M' to $M'' = M - 2$, using the equations

$$\begin{aligned} &O_{M'}(\lambda', h', h'_s) = (M/M')^{d-y_H} O_M(\lambda, h, h_s) \\ &h'_s = (M/M')^{y_{H_s}} h_s \qquad h' = (M/M')^{y_H} h \\ &\lambda' - \lambda^* = (M/M')^{1/\nu}(\lambda - \lambda^*) \end{aligned} \tag{4.4a}$$

and

$$\begin{aligned} &O_{M''}(\lambda'', h'', h''_s) = (M'/M'')^{d-y_H} O_{M'}(\lambda', h', h'_s) \\ &h''_s = (M'/M'')^{y_{H_s}} h'_s \qquad h'' = (M'/M'')^{y_H} h' \\ &\lambda'' - \lambda^* = (M'/M'')^{1/\nu}(\lambda' - \lambda^*). \end{aligned} \tag{4.4b}$$

These equations allow a unique determination of λ^* and of the combination $d - y_H - y_{H_s}$. For the exponents ν, y_H and y_{H_s}, however, somewhat different results are obtained depending on whether the first or second set of equations (4.4a) or (4.4b) is used, although the variations are not large.

Our results for $q = 2$ and 3 are listed in tables 5 and 6, respectively. Comparing with the other methods this procedure has the merit of giving very good estimates for the critical couplings y_H and y_{H_s}. It should be noted that y_H and y_{H_s} vary linearly with $1/M$ and the extrapolated values were obtained from such a fit. The results agree well with the known values of the critical exponents. The value for ν is not so good and depends on the scaling equation used.

Table 5. Fixed-point coupling λ^* and critical exponents ν, y_H and y_{H_s} for the $Z(2)$ model.

M	λ^*	$\nu^{MM'}$	$\nu^{M'M''}$	$y_H^{MM'}$	$y_H^{M'M''}$	$y_{H_s}^{MM'}$	$y_{H_s}^{M'M''}$
3	0.9424	1.227	1.350	1.651	1.585	0.517	0.585
4	0.9684	1.157	1.207	1.705	1.673	0.508	0.541
5	0.9797	1.119	1.148	1.736	1.717	0.504	0.523
6	0.9856	1.098	1.116	1.757	1.745	0.501	0.514
7	0.9893	1.081	1.096	1.773	1.764	0.501	0.508
8	0.9917	1.071	1.081	1.784	1.780	0.502	0.505
9	0.9933	1.056	1.071	1.793	1.788	0.502	0.503
10	0.9945	1.049	1.065	1.799	1.797	0.501	0.501
Extrapolated	1.00	0.97	0.92	1.86	1.87	0.500	0.500
Exact	1	1	1	1.875	1.875	0.5	0.5

Table 6. Fixed-point coupling λ^* and critical exponents ν, y_H and y_{H_s} for the $Z(3)$ model.

M	λ^*	$\nu^{MM'}$	$\nu^{M'M''}$	$y_H^{MM'}$	$y_H^{M'M''}$	$y_{H_s}^{MM'}$	$y_{H_s}^{M'M''}$
3	0.9768	1.088	1.226	1.612	1.537	0.461	0.536
4	0.9871	1.018	1.076	1.662	1.623	0.432	0.471
5	0.9916	0.984	1.014	1.693	1.669	0.414	0.438
6	0.9941	0.962	0.977	1.716	1.698	0.401	0.419
7	0.9955	0.948	0.954	1.733	1.720	0.391	0.404
8	0.9967	0.924	0.931	1.747	1.737	0.384	0.394
9	0.9972	0.922	0.922	1.759	1.747	0.376	0.388
Extrapolated	1.00	0.83	0.76	1.85	1.85	0.34	0.34
Exact	1	0.833	0.833	1.867	1.867	0.33	0.33

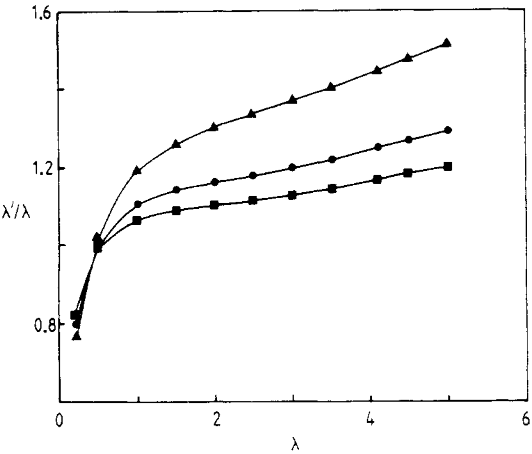

Figure 1. λ'/λ against λ for the $Z(7)$ model for different cluster sizes. ▲, $M = 3$; ●, $M = 4$; ■, $M = 5$.

Similar results are obtained if the scale factors M/M' and M'/M'' in equations (4.4*a*) and (4.4*b*) are replaced by $(M+1)/(M'+1)$ and $(M'+1)/(M''+1)$, respectively, as suggested by Slotte (1987). The exponents obtained this way go to the same limit, but approach it from the other side.

Until now we considered the cases $q = 2$ and 3 only, where the transition is of second order. We have seen in I that for $q \geq 5$, where a Kosterlitz–Thouless phase is expected, the MFRG gave just a hint for its existence but no definite conclusion could be drawn. Using the present method we have calculated λ' using (4.4*a*) for $q = 7$, $M = 3$, 4 and 5. Everywhere $M' = M - 1$, $M'' = M - 2$. In figure 1 we plot λ'/λ as a function of λ. If there is a Kosterlitz–Thouless phase around $\lambda = 1$, λ'/λ should approach unity in an extended region, deviating from it in the disordered and ordered phases. From the present results it is difficult to make any statement about the extent of the Kosterlitz–Thouless phase.

5. Discussion

In the present paper we have considered various improvements to the usual MFRG method. In the conventional definition of the MFRG transformation there are three points where modifications can be made. The first is the choice of the length scaling factor, namely whether the length should be taken to be proportional to the number of sites or, as suggested by Slotte (1987), to the number of interactions considered. The second point is the choice of the quantity that satisfies scaling, that is whether it is the average magnetisation or the magnetisation in the middle of the cluster, where boundary effects are less important. Finally, there is some arbitrariness as to whether the effective field acting on the cluster should scale in the same way as the bulk magnetisation, or whether bulk and surface fields have to be distinguished, as suggested by Indekeu *et al* (1987).

We have seen that there is no ideal choice that would give best estimates for both the critical coupling and the critical exponents. The best critical coupling is obtained with the method in which the bulk and surface contributions are treated simultaneously. This has the advantage of yielding both bulk and surface critical exponents, but the values for ν are not very good. Even in this case the method is good for second-order transitions only. For $q > 5$, where a Kosterlitz–Thouless phase is expected, the method is not very reliable to detect this phase.

Considerable improvement is found in the value of ν if the length scaling factor is chosen from the number of bonds and not from the number of sites, although the values do not converge monotonically to their exact values. Reasonably good values are obtained also if the magnetisation in the centre of the cluster is taken as a scaling quantity.

It would be interesting to see whether this tendency is valid in other models as well, to see what the best procedure is when critical couplings or exponents are to be determined.

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