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Mean-field-like variational and renormalisation group studies of (1 + 1)-dimensional spin models

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Abstract. Two recently proposed methods, the variational cluster wavefunction approximation and the mean-field-like renormalisation group transformation, are used to describe the phase transitions in the Hamiltonian version of the two-dimensional $Z(q)$ symmetric spin models. The convergence of the two schemes to the known results is analysed. It is shown that in their usual form neither of these methods can reproduce fine details of the phase diagram, although the renormalisation group method gives in general better convergence.

1. Introduction

Mean-field theory is the oldest and simplest approximation describing phase transitions. Since the advent of sophisticated renormalisation group (RG) procedures a great variety of RG transformations has been proposed, suitable in different situations (cf renormalisation in momentum or real space for classical or quantum variables, etc). An interesting procedure based on a mean-field-like approximation has been proposed by Indekeu *et al* (1982). They suggested an RG transformation based on rescaling clusters treated in a mean-field approximation (MFRG).

Extended mean-field-like approximations have been revived in a different context when Horn (1981) proposed a variational treatment of Hamiltonian lattice theories, a procedure that is similar in spirit to the Bethe–Peierls or extended mean-field approximation.

In both cases the Ising model in a transverse field served as a reference to show that the procedures give a reasonable description of the phase transition. Later on the MFRG was applied to random systems (Droz *et al* 1982, Plascak 1984a, Droz and Pekalski 1985) and to geometrical phase transitions (De'Bell 1983). It has also been generalised to study dynamic critical phenomena (Indekeu *et al* 1984, Plascak 1984b). The variational calculation was used to describe phase transitions in the $Z(q)$ model (Jengo *et al* 1982) and the one-dimensional Heisenberg chain (Sólyom 1985). Except for the last calculation, usually only small clusters have been considered and the convergence of the method as the cluster size increases is not well known.

In this paper we attempt to study the convergence of the two procedures mentioned above by analysing the results for the $Z(q)$ model for as large clusters as could be treated with reasonable effort. The model, which was chosen for its non-trivial phase

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diagram, and the two approximation schemes are described in § 2. The details of the results of the variational calculation are given in § 3, while those of the mean-field-like RG transformation are described in § 4. The comparison of the efficiency of the two procedures as well as the conclusions are given in § 5.

2. The model and the approximation schemes

In the present paper we will study the behaviour of the one-dimensional Hamiltonian version of the two-dimensional classical $Z(q)$ symmetric spin model with cosine interaction between nearest neighbours. The classical model is defined by assigning to each lattice site i a classical spin vector, which, however, can point in one of only q possible directions characterised by the angle $\theta_i = (2\pi/q)l_i$, $l_i = 0, 1, 2, \ldots, (q-1)$. The energy of the system depends on the configuration of the spin directions

$$E = -\sum_{i,j} V(\theta_i - \theta_j). \tag{2.1}$$

In a simplest case the interaction is between first neighbours only and is of the form $V(x) = \cos x$.

The one-dimensional Hamiltonian version of the model (Elitzur *et al* 1979) has the form

$$H(\lambda) = -\sum_{i=1}^{N} [\tfrac{1}{2}(R_i + R_i^+) + \lambda \cos(\theta_i - \theta_{i+1})] \tag{2.2}$$

where R_i^+ and R_i are the raising and lowering operators for the angle θ_i:

$$R_i^+|\theta_i\rangle = |\theta_i + 2\pi/q\rangle$$
$$R_i|\theta_i\rangle = |\theta_i - 2\pi/q\rangle. \tag{2.3}$$

The spin vector still points in one of the q possible directions. However, the R_i operators induce transitions between neighbouring orientations.

As was pointed out by Elitzur *et al* (1979) this model is self-dual and the ground-state energy satisfies the duality relationship

$$E_0(\lambda) = \lambda E_0(1/\lambda). \tag{2.4}$$

Duality does not necessarily hold for the excited states and also the degeneracy of the ground state can be different in the original and dual models. As seen from (2.2), for $\lambda \gg 1$ the spins line up parallel to each other. However, the q possible orientations of the spin are equivalent and therefore the ground state will be q-fold degenerate. In the opposite limit, $\lambda \ll 1$, it is more convenient to work in a different basis defined by

$$|n_i\rangle = \frac{1}{\sqrt{q}} \sum_{\theta_i} e^{in\theta_i} |\theta_i\rangle \qquad n = 1, 2, \ldots, q \tag{2.5}$$

where the summation goes over the possible values of the angle θ_i. In this basis the first part of the Hamiltonian is diagonal, while the second part can be expressed in terms of raising and lowering operators as

$$H = -\sum_{i=1}^{N} \left[\cos\left(\frac{2\pi}{q} n_i\right) + \tfrac{1}{2}\lambda (R_i R_{i+1}^+ + R_i^+ R_{i+1}) \right] \tag{2.6}$$

where

$$R_i^+|n_i\rangle=|(n_i+1) \bmod q\rangle$$
$$R_i|n_i\rangle=|(n_i-1) \bmod q\rangle. \tag{2.7}$$

Clearly, for $\lambda \ll 1$ it is energetically favourable to have $n_i=0$ at most sites and the ground state is non-degenerate.

For $q=2$, 3 and 4, corresponding to the Ising model, the three-state Potts model and the symmetric Ashkin-Teller model, respectively, there is a usual second-order phase transition between the two phases found above for $\lambda \gg 1$ and $\lambda \ll 1$, occurring at $\lambda=1$, as imposed by the self-duality. For larger q values there is strong evidence (Elitzur *et al* 1979, Hamer and Kogut 1980, Einhorn *et al* 1980, Alcaraz and Köberle 1980) for two successive phase transitions with a Kosterlitz-Thouless-like massless phase for intermediate couplings λ, although the phase diagram in the case $q=5$ is not yet clear (Ruján *et al* 1981, Patkós and Ruján 1985).

In the following we study how these transitions are described, on the one hand, by the variational calculation and, on the other hand, by the mean-field-like RG approach.

Our variational calculation is, in fact, an extended mean-field calculation using large clusters. The system is divided into clusters containing M atoms each. The wavefunction of the system is chosen as a product of identical cluster wavefunctions, which, in turn, are linear combinations with arbitrary coefficients of all the q^M possible configurations of the states of the M atoms inside the cluster. The ground-state energy is obtained by minimising the expectation value

$$E=\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{2.8}$$

with respect to the q^M coefficients of the trial wavefunction, corresponding to the different configurations.

Using the Hamiltonian written in the form of (2.6) this procedure turns out to be equivalent to an extended mean-field method in which a cluster of M spins is embedded into an effective medium acting on the two end spins. The Hamiltonian of the finite cluster is

$$H_c=-\sum_{i=1}^{M}\cos\left(\frac{2\pi}{q}n_i\right)-\tfrac{1}{2}\lambda\sum_{i=1}^{M-1}(R_i^+R_{i+1}+R_iR_{i+1}^+)-h(R_1+R_M)-h^*(R_1^++R_M^+) \tag{2.9}$$

where h is a complex effective field. The ground state of the finite system can be calculated exactly for arbitrary h and then h can be fixed by minimising the ground-state energy with respect to it.

For small λ the minimum will appear for $h=0$, giving rise to a unique ground state. In the wavefunction representation many configurations will appear with zero weight and all coefficients are real. For large λ, however, all coefficients will be finite and complex. The relative phase between the various coefficients will give rise to the q-fold degeneracy of the ground state. In terms of the effective field this will mean a finite complex value for h.

It is expected that the ground-state energy obtained in this way converges to the exact ground state of the infinite chain when larger and larger clusters are taken. At the same time the location of the phase transition should also converge to its value in the infinite system. This convergence will be studied in the next section.

An alternative approach to locate phase transition points using mean-field clusters was proposed by Indekeu *et al* (1982). This method is based on performing a RG transformation on finite clusters by mapping a cluster of M spins on a cluster with a smaller number of spins M'.

Let us consider a cluster of M spins with a symmetry-breaking field applied at the two ends as given by (2.9). The order parameter defined as

$$O_M(\lambda, h) = \frac{1}{M} \sum_{i=1}^{M} \tfrac{1}{2}(\langle R_i \rangle + \langle R_i^+ \rangle) \tag{2.10}$$

will have a finite complex value, its modulus being, for small h, proportional to h. If a similar calculation is performed for a cluster with M' spins in an external field h', the order parameter will be $O_{M'}(\lambda, h')$. Since the order parameter is proportional to the external field, a scaling relation can be defined by requiring

$$\left.\frac{\partial O_{M'}(\lambda', h')}{\partial h'}\right|_{h'=0} = \left.\frac{\partial O_M(\lambda, h)}{\partial h}\right|_{h=0}. \tag{2.11}$$

This gives a well defined scaling relationship between λ and λ'. The fixed-point coupling λ^* gives the location of the phase transition between the ordered and disordered phases, while linearisation of the scaling relation around the fixed point value gives in the usual way the critical exponent ν

$$\lambda' - \lambda^* = (M/M')^{1/\nu}(\lambda - \lambda^*). \tag{2.12}$$

Both the location of the transition and the value of the critical exponent depend on the number of sites in the cluster. In § 4, we will study how the exact results are approached as larger and larger clusters are considered.

3. Cluster variational calculation

For this method an ansatz for the wavefunction is necessary. A trial wavefunction will be constructed by dividing the infinite lattice into clusters of M sites and labelling the sites by a cluster index $\alpha (\alpha = 1, 2, \ldots, \infty)$ and an intracluster index $j = 1, 2, \ldots, M$. The state at the site (α, j) can be characterised by $n_{\alpha,j}$ using the basis given in (2.5). Allowing for all possible configurations $|\{n_{\alpha,j}\}\rangle$ of the spin vectors inside a cluster, the cluster wavefunction is written as a linear combination of them with arbitrary coefficients $a(\{n_{\alpha,j}\})$

$$\psi^{\alpha}_{\text{cluster}} = \sum_{\{n_{\alpha,j}\}} a(\{n_{\alpha,j}\}) |\{n_{\alpha,j}\}\rangle. \tag{3.1}$$

The wavefunction of the infinite chain is chosen as a product of the cluster wavefunctions

$$\psi = \prod_{\alpha} \psi^{\alpha}_{\text{cluster}}. \tag{3.2}$$

We will assume, in what follows, that the clusters are identical in the sense that the coefficients $a(\{n_{\alpha,j}\})$ do not depend on the cluster index. Still, since the spin vector can point in q possible directions, there are q^M possible configurations for a cluster

and therefore q^M arbitrary coefficients in the wavefunction. The minimalisation procedure was performed for $q = 2, 3, \ldots, 8$ and for clusters as large as could be reasonably treated numerically.

For $q = 2$, which is the Ising model, and for which this type of calculation was done by Horn (1981) using clusters up to three sites, our calculation was carried up to 14 sites. The results are given in tables 1 and 2. Below a certain λ_c the ground state is non-degenerate and disordered, while above λ_c a finite magnetisation appears continuously, as shown in figure 1. In order to analyse the series obtained for λ_c, the convergence accelerating procedure by Vanden Broeck and Schwartz (1979) (VBS)

Table 1. VBS table for the critical coupling of the $Z(2)$ model. The first column contains the results of the variational calculation for clusters with up to 14 sites.

M							
1	0.5						
2	0.585 089	0.688 580					
3	0.631 785	0.715 573	0.747 594				
4	0.661 770	0.730 219	0.749 645	0.749 906			
5	0.682 621	0.738 570	0.749 876	0.749 726	0.749 866		
6	0.697 811	0.743 373	0.749 449	0.750 352	0.749 893	0.749 866	
7	0.709 203	0.746 055	0.748 636	0.748 625	0.748 636	0.748 625	0.748 637
8	0.717 905	0.747 371	0.748 625	0.748 636	0.748 625	0.748 637	0.748 625
9	0.724 623	0.748 013	0.748 332	0.748 106	0.748 202	0.748 209	
10	0.729 842	0.748 226	0.748 205	0.748 224	0.748 209		
11	0.733 907	0.748 202	0.748 227	0.748 207			
12	0.737 072	0.747 499	0.747 995				
13	0.739 526	0.749 177					
14	0.741 441						

Table 2. The ground-state energy and the change in its slope at $\lambda = 1$ using site- and bond-cluster calculations, as well as the order parameter O_M for the $Z(2)$ model.

M	$E_0(\lambda = 1)$	$\left.\frac{\partial E_0}{\partial \lambda}\right\|_{\lambda = 1-\epsilon} - \left.\frac{\partial E_0}{\partial \lambda}\right\|_{\lambda = 1+\epsilon}$	$O_M(\lambda = 1)$
1	−1.25	0.250 00	0.866 025
2	−1.256 986	0.203 92	0.842 733
3	−1.260 561	0.177 04	0.826 483
4	−1.262 797	0.158 41	0.813 703
5	−1.264 343	0.144 35	0.803 046
6	−1.265 482	0.133 18	0.793 846
7	−1.266 358	0.124 01	0.785 724
8	−1.267 055	0.116 29	0.778 438
9	−1.267 622	0.109 68	0.771 822
10	−1.268 093	0.103 93	0.765 759
11	−1.268 490	0.098 87	0.760 160
12	−1.268 830	0.094 37	0.754 957
13	−1.269 125	0.090 33	0.750 097
14	−1.269 382	0.086 68	0.745 538
VBS approximant	−1.272	0.03	0.65
Exact	−1.273 240	0	0

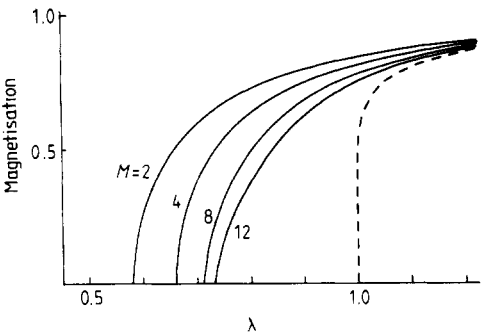

Figure 1. Magnetisation in the Ising model in a transverse field ($Z(2)$ model) obtained in the variational calculation for increasing cluster sizes M. The broken curve shows the exact result.

was applied. The subsequent approximants in column $L+1$ are generated from those in column L and $L-1$ by the relation

$$\frac{1}{[M, L+1]-[M, L]}+\frac{\alpha_L}{[M, L-1]-[M, L]}=\frac{1}{[M+1, L]-[M, L]}+\frac{1}{[M-1, L]-[M, L]}. \tag{3.3}$$

The series to be analysed is put into the first column, while $[M, 0]=\infty$. The parameters α_L are not uniquely defined. From the several suggested choices, the results of only one corresponding to

$$\alpha_L=-[1-(-1)^L]/2 \tag{3.4}$$

are reproduced in the tables. As is seen, unfortunately the results do not converge to $\lambda_c=1$, the exactly known transition point. Other choices of α_L do not give better results. This indicates that this variational calculation is notoriously slowly convergent.

It is interesting to realise that a similar calculation can be performed in the dual model, where instead of a cluster of sites a cluster of bonds is taken. Figure 2 shows the variational ground-state energy for $q=2$ and $M=1$ using site or bond clusters, respectively. As is seen, the dual model gives lower energy for $\lambda<1$, while for $\lambda>1$ the original model gives better results. If in each regime the lower energy state is

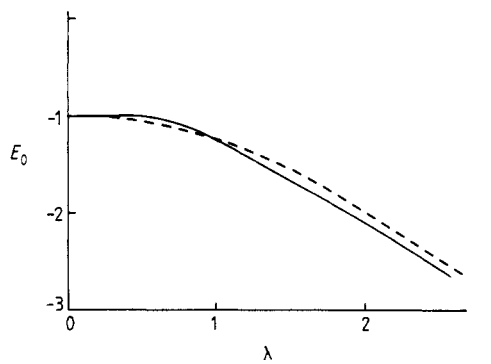

Figure 2. Ground-state energy of the $Z(2)$ model in a site mean-field approximation (full curve) and in a bond mean-field approximation (broken curve).

taken, the transition to the ordered phase occurs at $\lambda=1$, but is of first order. The jump in the slope of the energy at $\lambda=1$ decreases as the cluster size increases, as given in table 2, and eventually the second-order transition is recovered.

The results of the site-cluster calculation for $q=3$ are shown in table 3. In contrast to the $q=2$ case the transition to the ordered phase is of first order for any cluster size, as observed already by Horn (1981) for short clusters. In our calculation we took clusters with maximum $M=8$ sites. The discontinuity of the slope decreases with increasing cluster size and in the limit $M\to\infty$ a second-order transition should be recovered. Here, too, the convergence of the critical coupling to $\lambda_c=1$ is extremely slow. When the dual model is also considered in a bond-cluster approximation, the situation turns out to be the same as for $q=2$. The bond-cluster approximation gives lower energy for $\lambda<1$ without any transition while the site-cluster approximation is better for $\lambda>1$ and the first-order transition from the disordered to the ordered phase takes place at $\lambda_c=1$. This discontinuity weakens as the cluster size increases, yielding after all a continuous transition.

For $q=4$, the behaviour is exactly the same as for $q=2$.

When $q>4$, it is expected that two transitions will take place at dual values of λ with an extended critical (Kosterlitz-Thouless-like) phase between the disordered and ordered phases. Unfortunately, this variational calculation, using site clusters, shows no indication of this behaviour. The results obtained for $q=5$, 6, 7 and 8 with clusters containing up to five or six sites are presented in table 4, together with the VBS

Table 3. Critical coupling λ_c and the jump in the ground-state energy at λ_c for the $Z(3)$ model for increasing cluster sizes.

M	λ_c	$\left.\frac{\partial E_0}{\partial\lambda}\right\|_{\lambda=\lambda_c-\epsilon} - \left.\frac{\partial E_0}{\partial\lambda}\right\|_{\lambda=\lambda_c+\epsilon}$
1	0.666 666	0.2500
2	0.743 815	0.1914
3	0.783 820	0.1608
4	0.808 937	0.1405
5	0.826 342	0.1253
6	0.839 158	0.1132
7	0.848 988	0.1031
8	0.856 748	0.0942
VBS approximant	0.89	0.08
Exact	1	0

Table 4. Critical coupling λ_c of the $Z(q)$ model for increasing cluster sizes.

M	$q=5$	$q=6$	$q=7$	$q=8$
1	0.345 49	0.250 00	0.188 26	0.146 45
2	0.410 16	0.298 04	0.224 91	0.175 19
3	0.446 70	0.325 30	0.245 75	0.191 54
4	0.470 56	0.343 16	0.259 4	0.202 2
5	0.487 27	0.355 7	0.268 9	0.209 8
6	0.499 4			
VBS approximant	0.54	0.39	0.29	0.24

approximants for the critical coupling. The site cluster gives a transition to an ordered phase far below $\lambda = 1$, contrary to the expectation. The region around $\lambda = 1$ should in fact be in the Kosterlitz-Thouless phase and the ordering should occur for $\lambda > \lambda_c > 1$ only.

Considering again the dual model with the bond-cluster approximation, it is found, as for other q values, that for $\lambda < 1$ the bond-cluster method gives lower energy, while for $\lambda > 1$ the site-cluster approach is better. For $\lambda \geq 1$ the lowest energy solution of the cluster variational method gives an ordered state and only one transition is found.

We will return to the analysis of these results in § 5.

4. Mean-field-like RG transformation

In this section we will describe the results obtained when the mean-field-like RG method is applied to the $Z(q)$ model. First of all, it is found that the best results are obtained when M and M', the numbers of sites in the clusters to be compared, are close enough, because then in each step of renormalisation only a smaller fraction of the degrees of freedom is eliminated.

Choosing $M' = M - 1$, the results for the fixed point coupling λ^* and the critical exponent ν are given in table 5 for $q = 2$. Comparison with the results of the earlier variational calculation shows immediately that this RG transformation on the mean-field clusters enhances the convergence and a much better result is achieved.

Table 5. Fixed-pointing coupling λ^* of the mean-field-like RG transformation for the $Z(q)$ model and the critical exponent ν for increasing cell sizes. Mapping is always from M sites to $M-1$ sites.

	$q=2$		$q=3$		$q=5$	
M	λ^*	ν	λ^*	ν	λ^*	ν
2	0.7832	1.48	0.9122	1.28	0.5837	1.65
3	0.8436	1.32	0.9402	1.12	0.6465	1.51
4	0.8771	1.26	0.9548	1.06	0.6846	1.48
5	0.8986	1.23	0.9638	1.02	0.7108	1.46
6	0.9136	1.20	0.9699	1.00	0.730	1.45
7	0.9247	1.19	0.9744	0.99		
8	0.9332	1.18				

A similar conclusion can be drawn from the results for $q = 3$. The fixed point coupling and the exponent ν are also shown in table 5. For both $q = 2$ and $q = 3$ the VBS procedure gives an extrapolated critical coupling which is very close to $\lambda_c = 1$. However, the different choices of the α_L parameter in (3.3) give results which differ by a few per cent, so better accuracy cannot be achieved.

The convergence of the exponent ν is, on the other hand, very slow, their exact values being $\nu = 1$ for $q = 2$ and $\nu = 0.833$ for $q = 3$.

For $q = 5$, where two transitions are expected, the mean-field-like RG transformation gives a single usual second-order transition. The critical couplings and critical exponents obtained for different cluster sizes are listed in table 5. The critical coupling

seems to converge to a value of the order $\lambda^* \sim 0.8$, which is certainly too low compared to other estimates.

The situation is the same for larger values of q. The scaling relation (2.11) has always only one non-trivial fixed point and therefore strictly speaking only one transition is found. We can recognise, however, that a similar problem occurs when the $Z(q)$ model is studied by finite-size scaling (Patkós and Ruján 1985). In finite-size scaling the critical coupling is defined by requiring that the scaled mass gap be identical when two finite chains of different length are compared. In other words, the scaled mass gap ratio should be unity at the critical coupling. This same quantity should be smaller than unity in a disordered phase and larger than unity in an ordered phase. In the $Z(q)$ model, where there should be an extended critical Kosterlitz–Thouless-like phase, the scaled mass gap ratio should be unity over a finite range of couplings. Instead of that one finds that the scaled mass gap ratio is close to unity over a finite range and then deviates on both sides. Similarly, we can expect that the quantity analogous to the scaled mass gap ratio, which is here

$$\left.\frac{\partial O_M(\lambda, h)}{\partial h}\right|_{h=0} \left(\left.\frac{\partial O_{M'}(\lambda, h)}{\partial h}\right|_{h=0}\right)^{-1} \tag{4.1}$$

will tend to unity in the coupling region corresponding to the critical massless phase. This ratio is shown in figure 3 for $q=7$, $M=5$, $M'=4$ and $M=4$, $M'=3$. There is a slight indication that the ratio (4.1) tends to unity in a region around $\lambda = 1$, although from the present cluster sizes no definite conclusions can be drawn.

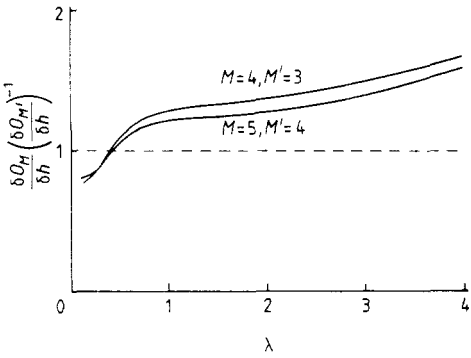

Figure 3. The ratio of $\partial O_M(\lambda, h)/\partial h|_{h=0}$ and $\partial O_{M'}(\lambda, h)/\partial h|_{h=0}$ for the $Z(7)$ model comparing clusters with $M=4$ to $M'=3$ and $M=5$ to $M'=4$.

5. Discussion and conclusions

In earlier works, when the cluster variational approach and the mean-field-like RG transformation were proposed to study the phase transition in spin chains, usually only short clusters were considered. In the present paper we extended these calculations to large clusters in order to study the convergence of the methods as a function of increasing cluster sizes. It was found that the cluster variational approach for the critical coupling of the $Z(q)$ model gives such a slowly converging series that even from the largest available cluster sizes the extrapolated value of the critical coupling for $q=2$ is about 25% off the correct value. This means that, for models where the

critical coupling is not known, this method cannot be used to locate it with good precision.

The method, in its present form, namely assuming identical cluster wavefunctions, which makes it equivalent to a mean-field-like calculation, does not give a Kosterlitz-Thouless-like phase for large q for intermediate couplings λ. In the framework of a variational calculation one can choose other forms for the wavefunction which, e.g., do not break the translational invariance in such a drastic way as the cluster calculation and thereby correlations can be better built into the ansatz (Horn and Weinstein 1984, Duncan and Roskies 1985, Dagotto and Moreo 1985, Virosztek 1985). It is not clear whether such improved variational calculations can reproduce the Kosterlitz-Thouless phase (Jengo *et al* 1982).

The mean-field-like RG method gives a better result for the critical coupling for small q than the variational calculation, although convergence as a function of the cell size is still slow. As has been pointed out recently by Indekeu *et al* (1987), this can be due to an improper choice of the scaling relation. Since the effective field acts on the spins at the boundary only, while the order parameter is the bulk magnetisation, their scaling dimensions can be different and the quantity $\partial O_M/\partial h$ should not be scale invariant. They propose an RG transformation where three clusters of sizes M, M' and M'' are compared. Alternatively one can keep a simple scaling relationship if, instead of the bulk magnetisation given in (2.10), the surface magnetisation

$$O_{SM} = \tfrac{1}{4}(\langle R_1\rangle + \langle R_1^+\rangle + \langle R_M\rangle + \langle R_M^+\rangle) \tag{5.1}$$

is used in (2.11). Whether this procedure gives a better convergence and clearer indication of a Kosterlitz-Thouless phase for large q will be the subject of further investigations.

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