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The weight function and optimal transformations

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Abstract. A class of optimal transformations is defined through the weight function which, when implemented into simple approximations of the renormalisation group, predicts values for the thermal exponent, y_T, and the magnetic field exponent, y_H, which are in better agreement with the exact results than those obtained with the majority sign rule. Specifically, we find that for the ferromagnetic triangular Ising lattice $y_T = 0.914$ and $y_H = 1.908$ (using the same approximation, the majority sign rule predicts $y_T = 0.736$ and $y_H = 1.669$). This weight function is used to calculate the properties of the ferromagnetic and antiferromagnetic square Ising lattice with a two-cell cluster and a one-hypercube approximation. The weight function is the first stage in the development of a real-space renormalisation group transformation free of the 'peculiarities' observed by Griffiths.

1. Introduction

The renormalisation group (RG) (Domb and Green 1976), as a technique for evaluating the partition functions of systems which undergo phase transitions, was developed by Wilson (1971a, b) and was formulated as a calculational tool by Wilson and Fisher (1972), who transformed the Ising model from real into momentum space (MSRG) and summed an infinite series of partial traces to evaluate the partition function. They limited the integration to short wavelengths, thereby excluding from the RG transformation the singularities associated with the critical point, which is an essential feature for the transformation to be analytic. Niemeijer and Van Leeuwen (Domb and Green 1976) were able to apply the ideas of Wilson directly to a lattice in real space via the introduction of a weight function, an operator which maps the state of the spins in a Kadanoff cell onto a renormalised spin state. Their particular realisation of the weight function is the majority sign rule (MSR) in which the state of the majority of spins in the Kadanoff cell determines the state of the renormalised spin. The MSR has been used in the analysis of many two- and three-dimensional systems but the results obtained do not show the same accuracy as those obtained from high-temperature series expansion.

Recently, Griffiths and Pearce (1978) and Griffiths (1981) have shown that a certain class of real-space renormalisation group (RSRG) is not regular: the parameters of the renormalised Hamiltonians are not smoothly dependent on the interaction parameters of the original Hamiltonian. It is also possible that, in the thermodynamic limit, the renormalised Hamiltonians are non-existent and the transformation is, therefore, mathematically meaningless. The RSRG equation is given by

$$e^{H'(\mu)} = \sum_{\{\sigma\}} P(\mu, \sigma)\, e^{H(\sigma)} \tag{1}$$

where H' (H) refers to the renormalised (original) Hamiltonian, μ (σ) is the renormalised (original) spin variables and $P(\mu, \sigma)$ is the weight function. The transformation is expected to be smooth if the weight function modulates the terms of the partition function in such a manner that the singularities are suppressed. The necessary conditions for the weight function are

$$\sum_{\{\mu\}} P(\mu, \sigma) = 1 \tag{2a}$$

$$\sum_{\{\sigma\}} P(\mu, \sigma)\, e^{H(\sigma)} \geq 0 \tag{2b}$$

where (a) ensures the invariance of the free energy and (b) limits the transformation to the space of real Hamiltonians. Equation (2b) is guaranteed if we have the stronger condition $1 \geq P(\mu, \sigma) \geq 0$. The right-hand side of equation (1) may be expressed in terms of a modified Hamiltonian

$$H(\mu, \sigma) = H(\sigma) + \ln P(\mu, \sigma). \tag{3}$$

Griffiths (1981) notes that in all instances of 'peculiarities' in RSRG transformations, the modified partition function, that is $\Sigma_{\{\sigma\}} e^{H(\mu,\sigma)}$, undergoes a phase transition. The singularities observed in these transformations are those present in the system $H(\sigma)$ and are related to the long-wavelength fluctuations which are specifically left unsummed in MSRG through the momentum cut-off procedure. Hence, the presence of a phase transition in the modified system indicates that the counterpart of the momentum cut-off is not, in general, present in RSRG. Thus, an additional and essential feature of the weight function is required, namely that the long-wavelength fluctuations of the partition function of $H(\sigma)$ should be excluded from the modified partition function.

In this work we report results obtained with a weight function which, for ferromagnetic systems only, is of the same form as the one used by Kadanoff (1975). In the present case, however, the free parameter of the weight function is related to the nearest-neighbour interaction. This has the effect of decoupling the lattice and thus making it impossible for long-wavelength fluctuations to develop. The transformation is applied to the one-dimensional ferromagnetic lattice and to the two-dimensional square ferromagnetic and antiferromagnetic Ising model. The results, in all cases, show an improvement over those obtained with the MSR.

If we allow the relationship between the weight function and the strength of the nearest-neighbour interaction to be treated as an adjustable parameter, we find good agreement between y_T, y_H and K_C (the critical coupling) and their exact values. This part of our work complements the optimal transformations considered by Witten and Prentis (1981). They considered deviations of the weight function from the majority sign rule and obtained good agreement between K_C and y_H with their exact values. In certain instances, however, there was a discrepancy between the calculated and exact thermal exponent. A similar discrepancy in the thermal exponent has appeared also in the variational cumulant expansion (Shenker *et al* 1979) and in a consistent analysis of the lower-bound one-hypercube approximation (van Saarloos *et al* 1978, Knops 1977).

In § 2 we describe our weight function and apply it to the one-dimensional ferromagnetic Ising model. The weight function is extended to allow for the analysis of two-dimensional models and the results of the calculations are presented in § 3. We also incorporate this weight function within the one-hypercube approximation and the results for the two-dimensional square ferromagnetic Ising model are presented in § 4. We point out a method of extending this approach in § 5 where we also look at general methods of ensuring regular RSRG transformations.

2. The weight function

The models we look at are Ising spins defined on one- and two-dimensional lattices. The Hamiltonian consists of a set of reduced interactions K_{ni} where n denotes the number of spins involved in the interactions and i labels the type, for example K_{21} (nearest neighbour), K_{22} (next nearest neighbour). The one-dimensional reduced Hamiltonian is given by

$$H(\sigma) = -\mathscr{H}/k_B T = K_{21} \sum_{ij} \sigma_i \sigma_j + K_{11} \sum_i \sigma_i + K_{00}. \tag{4}$$

The one-dimensional lattice is blocked into two spin cells (see figure 1) separated by a distance l and with a renormalised spin variable μ associated with each cell. The necessary conditions are not sufficient to define a unique weight function. Consider the weight function for the ith cell:

$$P(\mu, \sigma) = [\exp(\mu_i p(\sigma_i + \sigma_{i+1}))]/[2 \cosh p(\sigma_i + \sigma_{i+1})]. \tag{5}$$

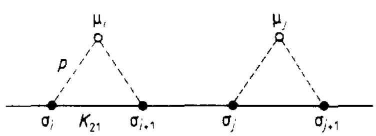

Figure 1. A segment of the one-dimensional Ising chain showing the blocking into Kadanoff cells labelled i and j. μ_i and μ_j are the renormalised spins, and the original spin variables are σ_i, σ_{i+1}, and σ_j and σ_{j+1}. p is the interaction between the two systems and K_{21} is the nearest-neighbour interaction between the σ spins.

This is of the same general form as the one used by Nelson and Fisher (1975) and Kadanoff (1975). However, in order to prevent the development of long-wavelength fluctuations in the modified Hamiltonian, p is defined through the equation

$$\Delta 2 \cosh p(\sigma_i + \sigma_{i+1}) = \exp(K_{21}\sigma_i\sigma_{i+1}). \tag{6}$$

Thus

$$p = \tfrac{1}{2} \ln[e^{2K_{21}} + (e^{4K_{21}} - 1)^{1/2}]. \tag{7}$$

The modified Hamiltonian written in terms of this weight function is

$$H(\mu, \sigma) = K_{21} \sum_{nn} \sigma\sigma_{nn} + p \sum_i \mu_i(\sigma_i + \sigma_{i+1}) - K_{21} \sum_i \sigma_i\sigma_{i+1}. \tag{8}$$

The renormalised spins are not dynamical variables and hence the modified system consists of nearest-neighbour interaction between σ spins belonging to different cells, but no resultant interactions between the spins in a cell. It is straightforward to calculate the renormalised couplings K'_{21} and K'_{00} which in zero magnetic field are

$$K'_{00} = \tfrac{1}{2}\ln(4\cosh 2K_{21}) \tag{9a}$$

$$K'_{21} = \tfrac{1}{2}\ln(2\cosh 2K_{21}). \tag{9b}$$

In figure 2 we show the variation of p and the weight function with K_{21} and in figure 3 the variation of the weight function with p. There are several features worth noting:

(i) The requirements on the weight function as expressed in equation (2) are satisfied for all values of p.

(ii) $\cosh 2p = e^{2K_{21}}$—if the system is in a ground state with energy E_0 then the normalising part of the weight function cancels $\exp(E_0)$.

(iii) For a given configuration of the renormalised system, the summation of the infinite number of configurations of the σ spins factorises into a number of independent sections, thus making it impossible for long-wavelength fluctuations to develop in the modified partition function.

(iv) In the strong coupling limit, that is as $T \to 0$, the weight function becomes the majority sign rule and at the weak coupling limit the weight function is $\tfrac{1}{2}$ for all states of the spins in the cell.

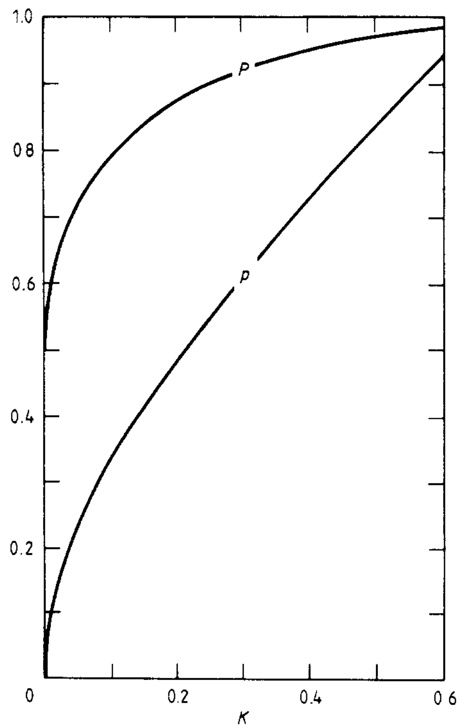

Figure 2. Variations of the weight function P and the coupling parameter p with nearest-neighbour interaction K. In the strong coupling limit ($K_{21} \to \infty$) P tends to the majority sign rule.

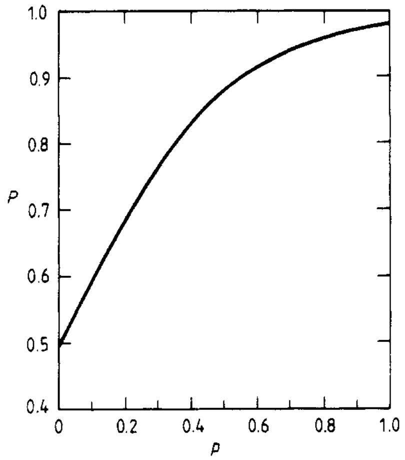

Figure 3. Variation of the weight function P (for the case where all spins in the Kadanoff cell, that is μ_i, and σ_i and σ_{i+1} are aligned) against the coupling parameter p.

(v) The contributions to the modified partition function are the same for all equivalent σ configurations, which is quite unlike the majority sign rule where the contributions to the modified partition function depend on the blocking of the cells.

A surprising feature of the weight function described by equations (5) and (7) is the close relationship between the values of p at the critical couplings for the two- and three-dimensional systems and those obtained by Kadanoff *et al* (1976) from their optimising procedure. At $K_C = 0.4407$ ($2d$) and $K_C = 0.158$ ($3d$) the values of p from equation (6) are 0.764 and 0.418 whilst the values obtained by Kadanoff *et al* (1976) from optimising the free energy are 0.766 and 0.403. We postulate that, in general, weight functions associated with analytic transformations should display the properties noted above for the one-dimensional ferromagnetic Ising system.

3. The two-dimensional lattice

We now consider a two-cell cluster for the square Ising ferromagnet with each cell consisting of four spins and, in addition, we impose periodic boundary conditions. The weight function is

$$P(\mu, \sigma) = \left[\exp\left(\mu_i p \sum_{l \in i} \sigma_l\right)\right]\left(2 \cosh p \sum_{l \in i} \sigma_l\right)^{-1}. \tag{10}$$

It is impossible to decouple the lattice with a single value of p as we were able to do for the one-dimensional ferromagnet due to the connectivity of the lattice. We satisfy condition (ii), that is the normalising factor cancels the contribution of the ground-state energy in the modified partition function

$$\cosh 4p = e^{8K_{21}} = e^{2rK_{21}}. \tag{11a}$$

Thus

$$p = \tfrac{1}{4} \ln[e^{2rK_{21}} + (e^{4rK_{21}} - 1)^{1/2}]. \tag{11b}$$

The resulting system is described by the modified Hamiltonian

$$H(\mu,\sigma)=K_{21}\sum_{ij}\sigma_i\sigma_j+\sum_i\left(p\mu_i\sum_{l\in i}\sigma_l-\ln 2\cosh p\sum_{l\in i}\sigma_l\right). \tag{12}$$

The ground state of this system consists only of fields (i.e. either $+p$ or $-p$) acting on the σ variables. A consistent treatment requires that p be dependent on the configurational energies such that this condition is always satisfied. This would lead to the removal of the 'peculiarities' observed by Griffiths (1981). However, in this work we stay within the one-parameter subspace and look for conditions for selecting an optimum value for p.

The fixed point (K_{21}^{C}), y_{T} and y_{H} are given for the two-cell cluster in table 1 and for comparison we have included the results obtained from a two-cell cluster and four-cell cluster (Nauenberg and Nienhuis 1974) using the MSR. The above results are free of adjustable parameters, that is $r=4$. If r is treated as an adjustable parameter then at $r=2$ the correct critical temperature is obtained and there is also close agreement with the known critical exponents. The variation of the relevant properties of the transformation with r are shown in figure 4.

Table 1. Results for the ferromagnetic and antiferromagnetic square Ising model, two-cell cluster with periodic boundary conditions and modified weight function.

	Present work		Previous work		
Parameter	Ferromagnet two cell	Antiferromagnet two cell	Two-cell cluster with majority sign rule	Four-cell cluster with majority sign rule	Exact results
K_{C}	0.399	0.399	0.392	0.418	0.4407
y_{T}	0.939	0.939	0.883	0.929	1.000
y_{H}	1.776	<0	1.765	1.822	1.875
$y_{\mathrm{H}}^{\mathrm{st}}$	<0	1.776	<0	<0	

In order to analyse the critical properties of the square Ising antiferromagnet, it is only necessary to modify the weight function in such a manner that the symmetries of the system are preserved. That is

$$P(\mu,\sigma)=\frac{[\exp(\mu_i p(\sigma_i-\sigma_{i+1}+\sigma_{i+2}-\sigma_{i+3}))]}{[2\cosh p(\sigma_i-\sigma_{i+1}+\sigma_{i+2}-\sigma_{i+3})]}. \tag{13}$$

The fixed-point and critical exponents fulfil the expected symmetry requirements (van Leeuwen 1975). If r is treated as a variable we find that at $r=2$ there is close agreement between the calculated and exact critical properties. The critical curve for the antiferromagnet in a uniform field is also calculated using the two-cell cluster and this curve together with the conjectured curve of Müller-Hartmann and Zittartz (1977), which is known to be accurate but not exact, are shown in figure 5.

We have also investigated he properties of the triangular lattice using a two- and three-cell cluster with periodic boundary conditions. The weight function for this

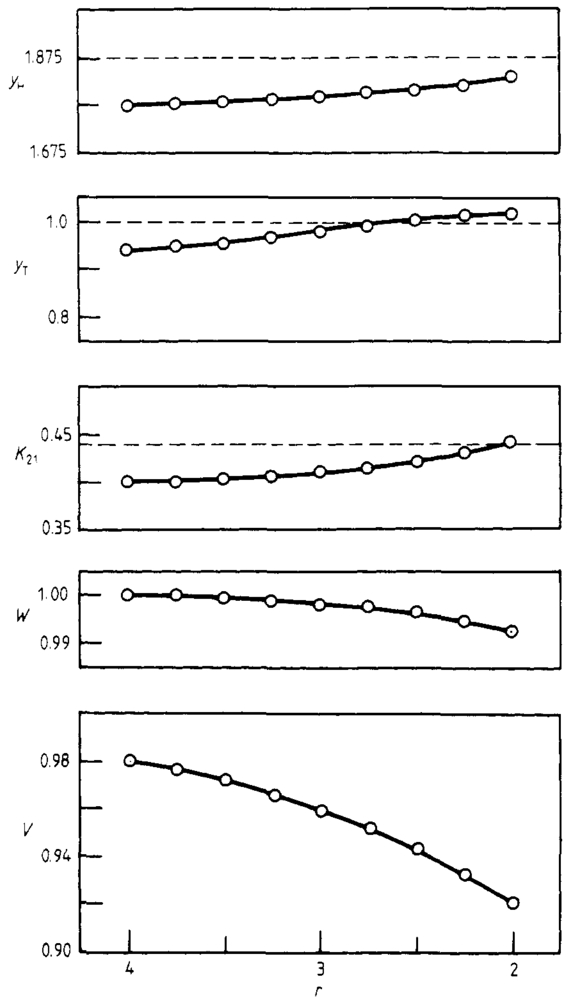

Figure 4. The variation of properties of the RG transformation for the two-cell cluster with r (see equation (9)). y_H and y_T are the magnetic and thermal exponents respectively and K_{21} the nearest-neighbour interaction for the two-dimensional square Ising lattice. W and V are values of the weight function: W is the case where all spins in the Kadanoff cell are aligned and V is the case where all but one of the σ spins are aligned.

model is

$$P(\mu, \sigma) = \left[\exp\left(\mu_i p \sum_{l \in i} \sigma_l\right)\right] \Big/ \left(2 \cosh p \sum_{l \in i} \sigma_l\right) \tag{14}$$

where $p = \frac{1}{3} \ln[e^{3rK_{21}} + (e^{6rK_{21}} - 1)^{1/2}]$ and r is 3 for the triangular lattice. The results are shown in figure 6 for the two-cell cluster and in figure 7 for the three-cell cluster and also in table 2. Again we note that at the critical temperature there is good agreement with the known critical exponents, unlike the results of Witten and Prentis (1981). The general features observed for the square lattice are also observed for this model and we draw attention to the systematic improvement on the results obtained with the MSR.

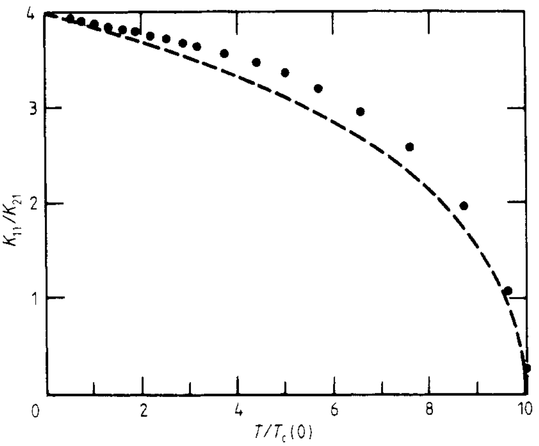

Figure 5. Phase diagram of an antiferromagnet in a uniform field. The broken curve is the conjecture of Müller-Hartmann and Zittartz (1977) and the full circles are the results from the two-cell cluster and the modified weight function.

4. The one-hypercube approximation

The lower-bound one-hypercube approximation is a simple and reliable method for obtaining critical exponents and it has been applied to a variety of models. We refer the reader to Kadanoff *et al* (1976) for details of the method. There is, however, a serious flaw in that the weight function is dependent on the free energy and, as van Saarloos *et al* (1978) were able to show, the singularities in the free energy are now present in the RG transformation. It is possible to implement the weight function described by equations (10) and (11) into the approximation, thus removing from the transformation the inherent non-analytic features introduced in the original application. Griffiths (1981) notes that the one-hypercube has an attractive feature—the potential moving scheme factorises the modified partition function, thus preventing the development of the long-wavelength fluctuations. The RG equations are identical to those described by Knops (1977) but the parameter p is determined by equation (12) with $r = 4$. The fixed-point and critical exponents are shown in column 2 of table 3. The thermal exponent is close to the value obtained through a consistent treatment of the lower-bound method (van Saarloos *et al* 1978; see column 5 of table 3). There is, however, a marginal eigenvalue, y_T^m, associated with the transformation. We may satisfy other conditions by varying r: for example, at $r = 3.81$ the free energy is an extremum and the relevant exponents are shown in column 3 of table 3. In an exact calculation, the eigenvector associated with the thermal exponent is perpendicular to the critical surface and this condition is satisfied at $r = 3.95$. The results are shown in column 4 and show remarkable agreement with the exact values.

5. Conclusion

Griffiths and Pearce (1978) and Griffiths (1981) have drawn attention to the fact that RSRG have no inbuilt mechanism to prevent the summation of long-wavelength fluctuations which are present in the partition function. An essential property of the

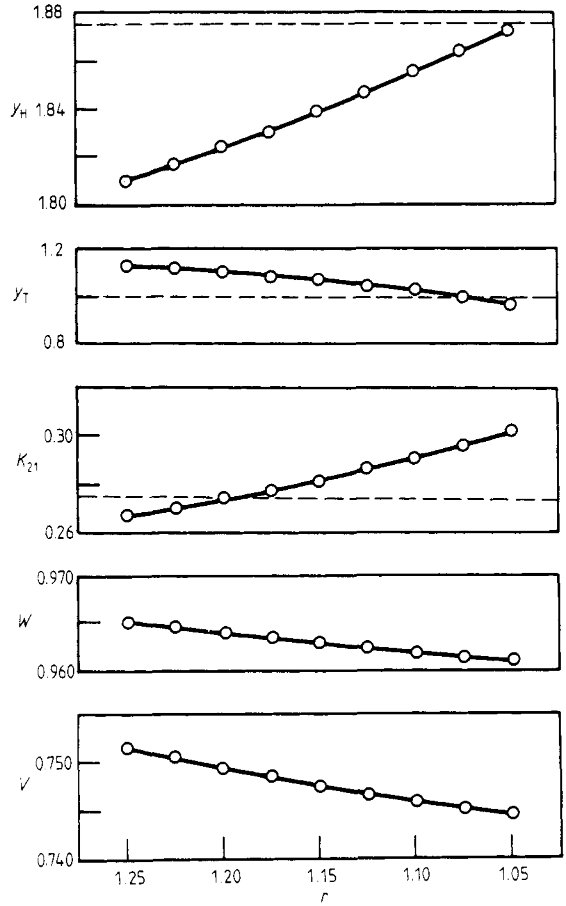

Figure 6. The variation of the properties of the RG transformation for the two-cell cluster (three-spin triangular cells) with r (see equation (13)). y_H and y_T are the magnetic and thermal exponents and K_{21} is the nearest-neighbour interaction for the two-dimensional triangular lattice. W and V are values of the weight function (a) for all spins in the Kadanoff cell aligned and (b) with one σ spin opposite to the other spins in the Kadanoff cell.

weight function must be the removal of these fluctuations from the modified partition function. We have shown how the weight function may be used to achieve the equivalent of the momentum cut-off for the one-dimensional Ising model. The differential RSRG of Hilhorst *et al* (1978) can be viewed in this light—the normalising factor of this weight function cancels all the nearest-neighbour interactions in the triangular lattice. The summation of the modified Hamiltonian is thus reduced to a set of fields $\{p(r_i)\}$ acting on spins $\sigma(r_i)$; this is a system without a phase transition and the RG transformation is free of non-analytic features.

We were unable to define a weight function with all the proposed properties for the two-dimensional systems, although by satisfying some conditions improved results were obtained. We were able to demonstrate that, within the two-and three-cell cluster and the one-hypercube approximation, the feature of linking the weight function to the strength of the nearest-neighbour interactions leads to a consistent

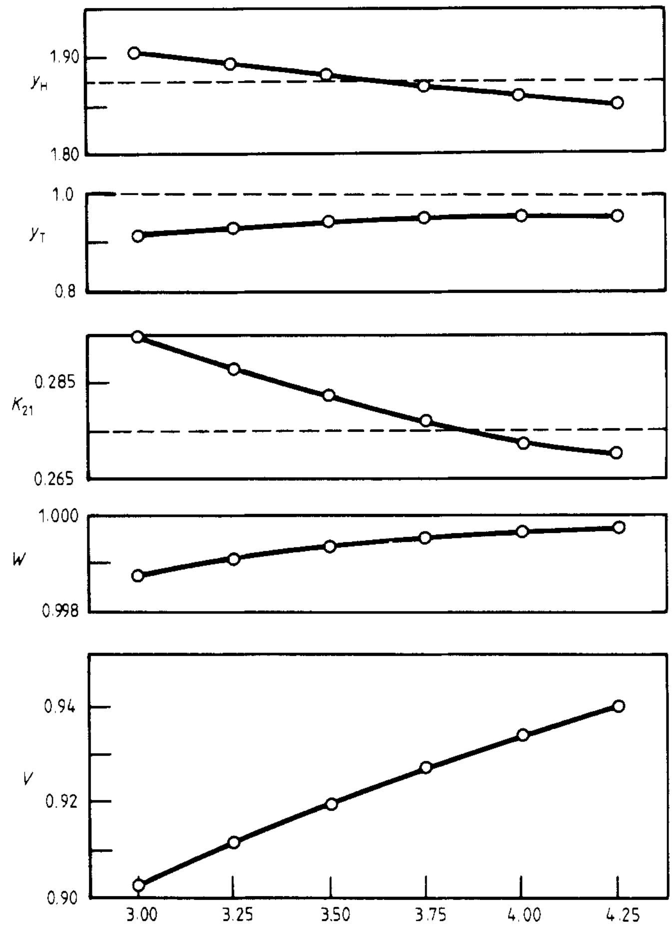

Figure 7. The variation of the properties of the RG transformation for the three-cell cluster (three-spin triangular cells) with r. y_H and y_T are the magnetic and thermal exponents and K_{21} the nearest-neighbour interaction for the triangular lattice. W and V are the values of the weight function (a) for all spins in the Kadanoff cell aligned and (b) with one σ spin opposite to other spins in the Kadanoff cell.

Table 2. Results from the ferromagnetic triangular Ising model. Two-cell and three-cell cluster with periodic boundary conditions and modified weight function.

	Present work		Previous work		
Parameter	Ferromagnet cell	Three-cell cluster	Two-cell cluster†	Three-cell cluster†	Exact
K_c	0.188	0.295	0.365	0.255	0.2747
y_T	1.185	0.914	0.791	0.739	1.000
y_H	1.575	1.908	2.022	1.669	1.875

† Domb and Green (1976).

Table 3. Results from the square Ising ferromagnet using the lower-bound (LB) one-hypercube approximation.

Parameter	One-hypercube $r=4$	$r=3.80$ optimal free energy	$r=3.95$ y_T normal to critical surface	van Saarloos *et al* (1978)
p^*	0.752	0.763	0.756	0.761
y_T	0.943	1.057	0.989	0.926
y_H	1.875	1.878	1.876	1.877
y_T^m	0	0	0	<0

set of critical values. This is in contrast to the results obtained by Witten and Prentis (1981) whose optimal transformations either required unrealistic values for the weight function or led to values of y_T which were lower than expected. It is hoped that improved results for the thermal exponent will be obtained with the lower-bound cumulant expansion (Shenker *et al* 1979) if the weight function described by equations (10) and (11) is used instead of the majority sign rule.

Acknowledgments

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