Z. Physik B 33, 381–384 (1979)

Zeitschrift
für Physik B

Renormalization Group Calculation for Cells with Inequivalent Spins

H. Falomir* and H.O. Mártin**
Laboratorio de Física Teórica, Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata, República Argentina

Received December 4, 1978

We have considered a real-space renormalization group transformation for a bidimensional Ising model, carrying out approximate calculations for cells where site spins do not play the same role. The dependence on the ratio between the number of intercell and intracell nearest-neighbour interactions has also been discussed.

I. Introduction

The possibility of studying the properties of an Ising model near its critical point with a renormalization group transformation (R.G.T.) has been extensively investigated [1].
If we divide the lattice of spins into cells, we can define a specific R.G.T. by taking cell spins as the new variables for the Hamiltonian, cell spins being defined through a mapping of internal configuration of cells onto global ones.
An approximate way of implementing these transformations is the so called cumulant expansion, first introduced in this context by Neimeijer and van Leeuwen [2].
As the choice of the size and shape of the considered cells is arbitrary, it is possible to find inequivalent sites, i.e. different spins in a given cell do not play the same role because they interact whith a different number of spins of the neighbour's cells. Furthermore, for a particular choice of cells different mappings into global state define different R.G.T. This should not have consequences in an exact calculation of critical exponents characterizing the phase transition; but as an approximate method is needed, the results do depend on those choices [6, 3].
The main purpose of the present work is to investigate the consequences of choosing cells with inequivalent spins and to find the best assignement of the cell spin according to some optimization criteria. The simplest cell that presents this feature is the triangular one, shown in Fig. 1, and we deal with it in detail. We have used a mapping that depends on some free parameters, and we have fixed their value with a criterion like those introduced by Kadanoff and Houghton [3, 6], and Bell and Wilson [4, 6].
In Sect. II we present a summary of the formalism that is used in Sect. III for the study of the cell of Fig. 1. In Sect. III we also discuss the effect that the ratio between the number of intercell and intracell interactions has on the first order cumulant expansion results. In Sect. IV we state our conclusions.

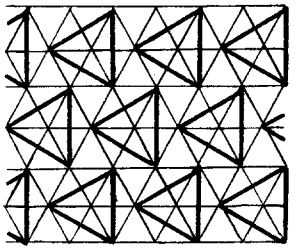

Fig. 1. The Chosen cell

II. Brief Review of the Formalism

The R.G.T. is defined through

$$\exp[H'(\mu)] = \sum_{\sigma} \prod_{a} P(\{\sigma_a^i\}, \mu_a) \exp[H(\sigma)] \qquad (1)$$

* Fellow of the Consejo Nacional de Investigaciones Científicas y Técnicas de Argentina.
** Fellow of the Comisión de Investigaciones Científicas de la Provincia de Buenos Aires, Argentina.

0340-224X/79/0033/0381/$01.00

$H(\sigma)$ is the Hamiltonian in terms of the site spins $\sigma^i = \pm 1$) and coupling constants K_i (K_1 for first neighbours, K_2 for second neighbours, etc.). $H'(\mu)$ is the transformed Hamiltonian with cell spin variables ($\mu_a = \pm 1$) coupled in the same way as in $H(\sigma)$, but with renormalized coupling constants K_i'. The index "a" refers to the a-th cell, and $P(\{\sigma_a^i\}, \mu_a)$ is the coefficient that weighs the individual configuration building the collective state with cell spin μ_a.

The R.G.T. implies the following relations:

$$K_n' = R_n(K_m) \tag{2}$$

between original and renormalized coupling constants. When (2) is expanded around the critical point, K_m^*, the thermal (Y_T) and magnetic (Y_H^A) scaling indices are obtained [6].

Several requirements must be satisfied: the partition function must remain invariant under R.G.T., $H'(\mu)$ must be real and the mapping between internal and global states must remain invariant under the simultaneous reversal of σ and μ spins [1]. Thus we demand:

$$P(\{\sigma_a^i\}, 1) + P(\{\sigma_a^i\}, -1) = 1 \tag{3}$$

$$P(\{\sigma_a^i\}, \mu_a) \geqq 0 \tag{4}$$

$$P(\{-\sigma_a^i\}, -\mu_a) = P(\{\sigma_a^i\}, \mu_a)$$

and therefore,

$$P(\{-\sigma_a^i\}, \mu_a) = 1 - P(\{\sigma_a^i\}, \mu_a). \tag{5}$$

The weights P can even be functions of a set of free parameters, q_i; $i = 1, \ldots, n$. As a result of this parametrization, the cumulant expansion [1] calculations of $R_n(K_m)$ give the fixed point K_m^* and the scaling indices as function of the q_i. Then the parameters can be fixed through an optimizing criterion.

Bell and Wilson [4, 6] have suggested considering those q_i values that make the scaling indices essentially constant in a range of q_i as the "best" q_i values.

Another criterion, originally introduced by Kadanoff and Houghton [3, 6] consists of accepting as the "best" q_i values those for which the difference of the results obtained from the computation of some quantity by two independent ways is a minimum.

Neither the first criterion nor the second one are based on the comparison of the results obtained with the exact values (from Houtappel's solution for the triangular lattice [5]).

III. Cells with Inequivalent Spins

A lattice with 2×2 square cells has been studied in [3, 6] using:

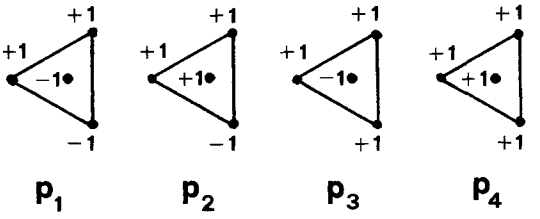

Fig. 2. The independent configuration weights

$$P(\{\sigma_a^i\}, \mu_a) = (1/2)\{1 + \mu_a \operatorname{tgh}[q \sum_{i \in a} \sigma_a^i]\} \tag{6}$$

where q is a free parameter.

When

$$\sum_{i \in a} \sigma_a^i = 0 \tag{7}$$

$P = 1/2$ for any value of q, as it should be according to the symmetry of the cell and the condition (5). On the other hand, when spins are inequivalent there is no reason to force that value on the P weighting configurations satisfying (7).

We have chosen the cell shown in Fig. 1 to investigate the effect of having an inequivalent spin, i.e. the central one. Owing to our choice of the cell and to conditions (3) and (5) there are only four independent P. They are called $p_S (S = 1, \ldots, 4)$, and they weigh the contribution of each configuration to the cell state with spin $\mu = 1$, as shown in Fig. 2. The p_S themselves will be taken as the free parameters. Note that p_1 refers to the critical configuration satisfying (7).

We have carried out the calculation of K_I^* (critical coupling constant of the equivalent Ising model), Y_H^A and Y_T by using the cumulant expansion in first and second order. We have also computed the magnetic scaling index from the properties of the correlation function for "eigenoperators" as in [3], getting the value Y_H^C. This allows us to apply the criterion of Kadanoff and Houghton to the difference between Y_H^A and Y_H^C.

We must mention that the values of p_S which best approximate the exact values of K_I^*, Y_H and Y_T are quite different.

On the other hand, we have found out that the scaling indices do not remain essentially constant in any allowed region of the p_S.

Therefore, neither the criterion of considering as the optimum p_S values those which best approximate the exact results nor the Bell and Wilson criterion can be applied.

We shall refer now to the Kadanoff and Houghton criterion. Since in the first order calculations Y_H^C is independent of p_1, we have applied this criterion to

Table 1. The K_I^*, Y_H^A and Y_T values obtained with $p_S=1$, $S=1,\ldots,4$

Approximation	K_I^*	Y_H^A	Y_T
First order	0.4222	2.121	0.738
Second order	0.2985	1.830	0.813
Exact	0.2747	1.875	1.0

Table 2. The ratio N_v/N_{H_0} and the first order calculations of K_I^* for different cells. ((*): This is the best value obtained by varying the independent configuration weights for this cell)

CELL	N_V/N_{H_0}	K_I^*	EXACT K_I^*
	1.0	0.4222	0.2747 (TRIANGULAR LATTICE)
	0.67	0.3356 [2]	
	0.25	0.3003 [7]	
	0.75	0.5931 (*)	0.4407 (SQUARE LATTICE)
	0.50	0.5186 [6]	
	0.25	0.4697 [6]	

the second order results, obtaining as the best p_S values

$$p_S=1, \quad S=1,\ldots,4$$

with the minimum difference

$$Y_H^A - Y_H^C = 0.415.$$

With these values of the parameters we have also obtained the best approximation to the exact value of K_I^* in both the second and first order calculations.
The above mentioned results are summarized in Table 1.
The fact that the results obtained differ from the exact ones more than those shown in previous calculations with different cells can be understood on the basis of the relation between the number of first order interactions between two neighbour cells N_v and the number of first order interactions inside a cell N_{H_0}. In our case this relation is $N_v/N_{H_0}=1$. In Table 2 it is shown that the results for both the triangular and the square lattice become better when this ratio decreases. This effect has already been mentioned in [7, 8]. This is due to the fact that in the cumulant expansion approximation the interaction among cells is considered as a small perturbation added to the Hamiltonian which describes the interactions inside the cells.

IV. Conclusion

We should like to comment on our results for the most critical configuration, i.e. the first one shown in Fig. 1. The results indicate $p_1=1$ as the "best" value, showing up the effects of the inequivalency of the spins in our cell. Note the difference with the case of square 2×2 cells, where the configuration with vanishing total spin contributes with weight 1/2 to the global state with spin ± 1.
In other words, the lower orders of the cumulant expansion calculation show an inequivalent role played by different spins in the chosen cell. This inequivalence can be understood clearly if first neighbour interactions are considered, since the spin at a vertex of a cell interacts with five spins of the neighbour cells, whereas the central one interacts with only three. Moreover, when higher order interactions are taken into account, our conclusion related to the values of p_1 remains unchanged because the additional coupling constants are small compared with the first order coupling constant.
We have found that the value of the ratio N_v/N_{H_0} could explain the differences between our results and the exact ones. We expect the above conclusions to remain true for calculations involving cells with a more favourable ratio N_v/N_{H_0}.

We would like to thank J. Alessandrini, L. Epele, H. Fanchiotti, R. Gamboa Saraví, C. Carcía Canal, J.A. Martínez and H. Vucetich for useful discussions.

References

1. Neimeijer, Th., van Leeuwen, J.M.J.: Phase Transitions and Critical Phenomena. Vol. 6, Chap. 7 (Renormalization Theory for Ising-like Spin Systems) Domb, C., Green, M.S. (eds.). London, NewYork: Acad. Press 1972
Barber, M.N.: Phys. Reports **29** C, 1 (1977)
Van Leeuwen, J.M.J.: Fundamental Problems in Statistical Mechanics. Vol. 3 (Renormalization Theory for Spin Systems) Cohen (ed.). Amsterdam: North Holland Publishing Company 1975

2. Neimeijer, Th., van Leeuwen, J.M.J.: Physica **71**, 17 (1974)
Neimeijer, Th., van Leeuwen, J.M.J.: Phys. Rev. Lett. **31**, 1411 (1973)
3. Kadanoff, L.P., Hougton, A.: Phys. Rev. B **11**, 377 (1975)
4. Bell, T., Wilson, K.: Phys. Rev. B **11**, 3431 (1975)
5. Houtappel, R.M.F.: Physica **16**, 425 (1950)
6. Hsu, S., Gunton, J.D.: Phys. Rev. B **15**, 2688 (1977)
7. Jan, N., Glazer, A.M.: Phys. Lett. **59** A, 3 (1976)
8. Hsu, S., Neimeijer, Th., Gunton, J.D.: Phys. Rev. B **11**, 2699 (1975)

H. Falomir
H.O. Mártin
Laboratorio de Fisica Teórica
Departamento de Física
Facultad de Ciencias Exactas
Universidad Nacional de La Plata
Calle 115 esq. 49, C.C. N° 67
1900 La Plata
Argentina