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1977 J. Phys. A: Math. Gen. 10 L253

(http://iopscience.iop.org/0305-4470/10/12/009)

J. Phys. A: Math. Gen., Vol. 10, No. 12, 1977. Printed in Great Britain.

LETTER TO THE EDITOR

Kadanoff renormalisation for the s-state Potts model in three dimensions

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Received 10 October 1977

Abstract. A lower bound transformation of the type introduced by Kadanoff is applied to the discrete s-state Potts model in $d=3$ dimensions. For all values of $s=2, 3, 4, 5, 6$ the transformation predicts a continuous transition.

The discrete s-state Potts model (Potts 1952) has the Hamiltonian

$$\mathscr{H} = -J\sum_{\langle ij\rangle}\delta_{\sigma_i\sigma_j} - \sum_{i\alpha}\xi_\alpha\delta_{\sigma_i\alpha} \tag{1}$$

where i denotes a lattice site and where the spins σ_i can take s discrete values $\sigma_i = 1, 2, \ldots, S$. The index α runs over these s states and ξ_α represents a symmetry breaking field favouring the state α. The interaction energy between nearest-neighbour pairs is $-J$ if they are in the same state and zero otherwise in contrast to a general spin Ising model. However $s=2$ obviously corresponds to the spin-$\frac{1}{2}$ Ising model.

The s-state Potts model has s degenerate ferromagnetic ($J>0$) ground states in the absence of any fields. Landau mean-field theory (Mittag and Stephen 1971) predicts a first-order transition in all dimensions for $S>2$, essentially due to the presence of a coupling trilinear in the magnetisation. Baxter (1973) has shown that the discrete s-state Potts model on a $d=2$ square lattice has a first-order transition for $s>4$ and a higher-order transition for $s\leqslant 4$. However, the critical behaviour of the s-state Potts model in three dimensions has been the subject of much dispute. Since $s=4$ is the dividing point between second- and first-order transitions in two dimensions and mean-field theory is thought to be more meaningful in higher dimensions, one might expect that the dividing point in three dimensions is somewhere between $s=2$ and $s=4$.

Series expansions for the discrete three-state Potts model in three dimensions have not been very conclusive about the order of the transition (Ditzian and Oitmaa 1974, Straley 1974, Enting 1974, Kim and Joseph 1975). Renormalisation group studies using a continuum generalisation of the $s=3$ Potts model at $d=3$ (Golner 1973) and in $d=4-\epsilon$ dimensions (Rudnick 1975) predict a first-order transition, but real space renormalisation group calculations on the discrete three-state Potts model suggest a second-order transition (Burkhardt *et al* 1976). The discrepancy between these results raises the question of whether there is a basic difference between the continuous and discrete Potts models. Experimentally, there are realisations of the continuous three-state Potts model (Aharony *et al* 1977, Barbara *et al* 1977) and in both cases a first-order transition is observed.

Real space renormalisation group methods have been applied to the $d=2$ s-state Potts model by Dasgupta (1977) and den Nijs and Knops (1977). These authors used a lower bound renormalisation transformation (LBRT) of the type developed by Kadanoff (1975). For $s=3$ and $s=4$, the transformation correctly predicts a continuous phase transition. However the transformation fails to detect the first-order transition that is known to occur for $s>4$. One possible reason for this failure is that the basic cluster of spins in $d=2$ is too small. A cluster containing four sites cannot properly represent an interaction energy involving five or more different states. For this reason we shall consider the discrete s-state Potts model in three dimensions on a cubic lattice where the basic cluster contains eight sites. In this case we should be able to examine the model for values of s up to eight before encountering the difficulties of the finite cluster size and test the Kadanoff method to see if it predicts a first-order transition for some value of s in this range.

The Hamiltonian is written in the form

$$\mathscr{H}(\sigma)=-\sum_{\text{cubes}}\sum_{l}K_l S_l(\sigma) \tag{2}$$

where the set $S_l(\sigma)$ includes all possible invariants which satisfy the point group symmetry of the cube (see Dasgupta 1977 for examples of the corresponding invariants on a square). Following Kadanoff (1975) we shall work in an invariant subspace of the constants K_l for which $\mathscr{H}(\sigma)$ is symmetric under a permutation of spin positions. This invariant subspace can be reached from the initial Hamiltonian in equation (1) by first performing an exact decimation transformation (Kadanoff and Houghton 1975) on a BCC lattice. In the absence of a field all s-states are equivalent and there are 22 different invariants $S_l(\sigma)$ for the cube. However for values of $s<8$, not all of these interactions are linearly independent. The number of independent invariants for each value of s is given in table 1. In real space renormalisation transformations a first-order transition is associated with a discontinuity fixed point (Nienhuis and Nauenberg 1975) with a magnetic exponent $y=d$ for each eigenoperator conjugate to a discontinuous order parameter. In addition, a thermal exponent $y=d$ would imply $\alpha=1$ and hence a latent heat at the transition.

We have applied the Kadanoff LBRT within the restricted subspace of interactions described above and the results for $s=2, 3, 4, 5, 6$ are given in table 1. The results for $s=2$ and $s=3$ have been obtained previously by Kadanoff (1975) and Burkhardt *et al* (1976) respectively but those for $s=4, 5, 6$ are new. From the table it is easily seen that $y<d$ for both the thermal and magnetic exponents in all cases and the transition is predicted to be continuous rather than first order. We have not been able to

Table 1. s-state Potts model in $d=3$. Critical exponents obtained using LBRT. n_e and n_o are the number of independent invariants of even and odd symmetry respectively. P^* is the value of the variational parameter obtained using the Kadanoff criterion and J/T_c is the corresponding critical temperature.

S	n_e	n_o	y_T	y_H	α	δ	P^*	J/T_c
2	5	4	1·5898	2·4646	0·1130	4·6037	0·8069	0·324
3	10	15	2·0709	2·5107	0·5514	5·1308	0·9055	0·401
4	15	26	2·3524	2·6124	0·7247	6·7399	0·9469	0·459
5	18	35	2·5055	2·6927	0·8026	8·7628	0·9803	0·505
6	20	40	2·5992		0·8458		1·0115	0·543

complete the table with the magnetic exponents for $s=6$, 7, 8 and the thermal exponents for $s=7$, 8 due to the amounts of computational time required to generate the weight function describing the coupling of the 'old' spins to the 'new' spins in the LBRT. However a plot of the leading exponents as a function of s does not show any indication that y will approach 3 for $s<8$.

The reasons why the Kadanoff LBRT does not predict a first-order transition for some value of $s<8$ are not clear. The criterion proposed by Kadanoff (1975) for selecting the 'best' fixed point out of the set allowed by the approximate recursion relations has been recently examined by Knops (1977) and Barber (1977). A true minimisation of the free energy requires the variational parameter p to be adjusted at each iteration of the LBRT and hence a calculation of p as a function of the coupling constants K_l at each iteration. The optimum bound to the exact free energy thus involves a multi-dimensional optimisation over many parameters, one for each iteration, and evaluation of the exponents requires a calculation of $\mathrm{d}p/\mathrm{d}K_l$. However it is doubtful that such a true optimisation calculation would improve the results reported here since it has been recently suggested by van Leeuwen (private communication from M Barber) that $p(K_l)$ may contain an irregular part with an exponent $1-\alpha$, leading to a divergent $\mathrm{d}p/\mathrm{d}K_l$ when $\alpha>0$. One possible explanation for the failure of the Kadanoff method is that the change from continuous behaviour to first-order behaviour at the transition is associated with the appearance of a fixed point where the interactions are of infinite range. Perhaps the effective range of interaction changes as s is increased from two. Above some critical value of s the range may become essentially infinite and mean-field theory would presumably be correct for values of s above this critical value. If this suggestion is correct then the present finite cluster calculation would not detect such a change in behaviour.

The author would like to thank Dr T W Burkhardt for many stimulating discussions and the use of the variational computer programs, and Dr M P M den Nijs for sending a preprint of his work prior to publication. A useful conversation with Dr A P Young is also acknowledged.

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