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The 3-state Potts model in (2+1) dimensions

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Abstract. The 3-state Potts model in (2+1) dimensions is studied using series and Monte Carlo methods. High temperature series for the vacuum energy, mass gap and susceptibility are computed on the square and triangular lattices using linked cluster expansions. Monte Carlo estimates are obtained by the stochastic truncation method. The model is found to undergo a weak first-order transition, as in the Euclidean version of the model.

1. Introduction

The 3-state Potts model in three dimensions is an interesting one, and it is a delicate question to determine whether it undergoes a first-order or a second-order phase transition. The model has been studied in the past using a variety of methods, including series expansions (Straley 1974, Kim and Joseph 1975, Miyashita *et al* 1979), renormalisation group analyses (Nienhuis *et al* 1981, Newman *et al* 1984), and Monte Carlo simulations (Blöte and Swendsen 1979, Knak Jensen and Mouritsen 1979, Herrmann 1979, Wilson and Vause 1987). After some early uncertainty, the consensus was that the phase transition in the model is weakly first order.

Interest in the model was recently rekindled by some studies of SU(3) gauge theory at finite temperature. This theory exhibits a global Z_3 symmetry corresponding to the centre of the SU(3) group, and hence Svetitsky and Yaffe (1982a, b) have predicted that the deconfinement transition in the four-dimensional gauge theory should lie in the same universality class as the Z_3 or 3-state Potts model in three dimensions. The deconfinement transition has been thought hitherto to be first order, in agreement with this prediction; but in a large Monte Carlo simulation, the APE collaboration (Bacilieri *et al* 1988) found a very large correlation length, increasing with lattice size, which would appear to indicate a second-order transition. In another study the Columbia group (Brown *et al* 1988) found that the latent heat is less than had been estimated previously, but that the transition is still first-order. In fact a situation like this is by no means unfamiliar at a weak first-order transition. The 5-state Potts model in two dimensions can be exactly solved at the critical point (Baxter 1973), and it is known to undergo a first-order transition: but its correlation length or inverse mass gap at the transition point, while finite, is exponentially large, and quite inaccessible to approximate numerical methods (Hamer 1981).

The debate over the deconfinement transition has stimulated new studies of the 3-state Potts model, and several Monte Carlo treatments (Fukugita and Okawa 1989, Gavai *et al* 1989, Gupta *et al* 1990) have recently appeared, concentrating particularly on the correlation length. They conclude that the correlation length remains finite,

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though large, and develops a discontinuity at the critical point. Thus the transition is confirmed as being first order.

In the present work we have set out to study the quantum Hamiltonian version of the 3-state Potts model in (2+1) dimensions: this has not been studied before, to our knowledge. We use both series and Monte Carlo methods. Now in fact Monte Carlo techniques are not so well established in the quantum Hamiltonian framework as they are in the Euclidean framework. Several methods of this sort have been proposed in the context of lattice gauge theory (Heys and Stump 1983, Blankenbecler and Sugar 1983, Chin *et al* 1984, DeGrand and Potvin 1985, Barnes *et al* 1986), but there have been very few applications to lattice spin systems, with the notable exception of the studies by Nightingale and Blöte (1986, 1988). The method we use here is a variant technique called 'stochastic truncation' (Allton *et al* 1989), which is in fact quite close to that used by Nightingale and Blöte.

The methods we use are briefly reviewed in section 2. Our results are presented in section 3, beginning with some 'high-temperature' series, and proceeding to the Monte Carlo estimates. Our conclusions are summarised in section 4. The transition does indeed appear to be weakly first order, with a finite spontaneous magnetisation at the critical point, and a mass gap which drops discontinuously to zero. The accuracy and efficiency of the stochastic truncation method appear quite good.

2. Methods

The cluster expansion methods which we have used to calculate the high-temperature series were reviewed in another recent paper (He *et al* 1990), so we will not go into detail here. Suffice it to say that, for instance, the ground state energy per site can be written as a sum of contributions from all the linked clusters with different topologies which can be embedded on the lattice, each weighted by its appropriate lattice constant. The main stages in the calculation are: first, the generation of a list of linked clusters, each with its lattice constant and a list of all the sub-clusters which can be embedded in it; second, calculation of a series for the ground-state energy of each cluster, from which all the sub-cluster terms are subtracted, to leave the intrinsic or 'cumulant' cluster energy. These are then combined to give the bulk result. The first stage is model independent, but the second obviously depends on the particular model. It involves constructing a Hamiltonian matrix for each given cluster, from which the perturbation series is calculated. The size of the matrix is proportional to 3^{n_v} for a cluster of n_v sites or vertices in the 3-state Potts model, and this is the limiting factor in the calculation. The longest calculation was that of the mass gap on the triangular lattice, which involved some 736 clusters, and occupied about 4×10^4 CPU seconds on an IBM3090 machine.

The stochastic truncation method (Allton *et al* 1989) used in the Monte Carlo calculations is a version of the simple power method for finding the dominant eigenvalue and eigenvector of a matrix H. Starting from some arbitrary vector $|\psi^{(0)}\rangle$, the dominant eigenvector is 'projected out' by multiplying with the matrix H many times. Suppose that we are working in some arbitrary basis of vectors $|i\rangle$, and that the dominant eigenvector $|\phi_0\rangle$ can be expanded

$$|\phi_0\rangle = \sum_i c_i^0 |i\rangle \tag{2.1}$$

where for simplicity we assume that the amplitudes c_i^0 are positive real numbers. In

the stochastic truncation scheme, one constructs a sequence of (unnormalised) approximations to $|\phi_0\rangle$:

$$|\psi^{(m)}\rangle = \sum_i n_i^{(m)} |i\rangle \tag{2.2}$$

where the 'occupation numbers' $n_i^{(m)}$ are now integers rather than real numbers. The vector $|\psi^{(m)}\rangle$ is obtained from $|\psi^{(m-1)}\rangle$ by an application of the matrix H, as in the power method, according to the following rules. Define an 'ensemble size'

$$N^{(m)} = \sum_i n_i^{(m)} \tag{2.3}$$

and suppose we begin from some arbitrary initial trial vector $|\psi^{(0)}\rangle$ and 'score' $S^{(0)}$. Then at each succeeding iteration m, a new trial vector $|\psi^{(m)}\rangle$ and score $S^{(m)}$ are generated by the two basic rules:

$$n_k^{(m)} = \sum_i R\left(H_{ki} \frac{n_i^{(m-1)}}{S^{(m-1)}} \right) \tag{2.4}$$

$$S^{(m)} = \frac{N^{(m)}}{N^{(m-1)}} S^{(m-1)}. \tag{2.5}$$

Here $R(x)$ is a 'rounding function', according to which x is rounded either up or down to an integer by a Monte Carlo procedure (Allton *et al* 1989), such that on averaging over many trials

$$\langle R(x) \rangle = x. \tag{2.6}$$

Thus equation (2.4) implements the power method in a stochastic fashion, while equation (2.5) is merely an auxiliary rule designed to equilibrate the ensemble size $N^{(m)}$.

Assume the system reaches an equilibrium after many iterations, where $N^{(m)}$ and $S^{(m)}$ fluctuate around some fixed average values. Then comparing (2.4) with the eigenvalue equation

$$\sum_i H_{ki} c_i^0 = E_0 c_k^0 \tag{2.7}$$

we see that on average

$$\langle n_k \rangle \alpha c_k^0 \tag{2.8}$$

and the eigenvalue is given by

$$\langle S \rangle = E_0 \tag{2.9}$$

providing we ignore correlations between $n_i^{(m)}$ and $S^{(m)}$ (this turns out to be a good approximation in practice). So the trial vectors $|\psi^{(m)}\rangle$ provide discrete, stochastic approximations to the dominant eigenvector $|\phi_0\rangle$, according to (2.8). For basis states with very small amplitudes c_i^0, the occupation numbers $n_i^{(m)}$ will usually be zero, corresponding to an effective truncation of the set of basis states at each iteration.

The quantum Hamiltonian of the 3-state Potts model in two space and one time dimensions can be written (Mittag and Stephen 1971, Solyom 1981)

$$H = 2 \sum_i \left[1 - \cos\left(\frac{2\pi}{3} L_i \right) \right] \qquad -\lambda \sum_{\langle ij \rangle} (R_i^+ R_j^- + R_i^- R_j^+) \tag{2.10}$$

where i labels the sites on a two-dimensional square lattice of M^2 sites, $\langle ij \rangle$ denotes nearest-neighbour pairs of sites, λ is the coupling (corresponding to the inverse

temperature in the Euclidean formulation), and L_i, $R_i^{\pm}$ are operators at each site which in a basis of eigenstates of L_i obey the rules:

$$L_i|l_i\rangle = l_i|l_i\rangle \qquad l_i = 0,\ 1 \text{ or } 2 \tag{2.11}$$

and

$$R_i^{\pm}|l_i\rangle = |(l_i \pm 1) \bmod 3\rangle \tag{2.12}$$

so that $R_i^{\pm}$ are raising and lowering operators for the spin l_i, modulo 3. Periodic boundary conditions are assumed. To ensure that the ground state is the dominant eigenstate, we actually applied the stochastic truncation method to the matrix

$$H' = 3M^2 - H. \tag{2.13}$$

The matrix elements of H' are all either positive or zero. The initial state $|\psi^{(0)}\rangle$ was simply taken as the $\lambda = 0$ ground state, with $l_i = 0$ on every site.

The efficiency and accuracy of the method depend crucially on the way in which equation (2.4) is implemented. One does not want to waste time generating a final state $|k\rangle$ at the mth iteration if its occupation number $n_k^{(m)}$ is going to be rounded to zero. Now for a given initial state $|i\rangle$, the sum of the off-diagonal terms

$$T = \sum_{k \neq i} H'_{ki} \frac{n_i^{(m-1)}}{S^{(m-1)}} \tag{2.14}$$

is known *a priori*: there are $4M^2$ link operators which can act on state $|i\rangle$, and $H'_{ki} = \lambda$ for each one. So we adopt the technique of rounding T to an integer $\bar{T}$ initially, and choosing $\bar{T}$ of the $4M^2$ link operators at random to generate final states $|k\rangle$, each with occupation number $n_k^{(m)} = 1$ (Hamer and Court 1990).

We chose to 'symmetrise' (Irving and Thomas 1982) our basis states under lattice translations, rotations and reflections. This involves performing these lattice symmetry operations on each new state, counting how many times the resulting configurations are degenerate, and choosing a standard representative from among them. The sector of states possessing these symmetries is much smaller than the full basis set, and thus one achieves higher accuracy; but the time required to symmetrise the states is expensive, and would not be worthwhile for lattices larger than those we have considered here. The states were also gathered together into a master file by a hash-sorting algorithm as they were generated.

Some form of variational guidance is necessary to help the approach to equilibrium and increase the accuracy of the Monte Carlo estimates (Chin *et al* 1984, Hamer and Court 1990). One way of implementing this is to perform a similarity transformation

$$|\psi'\rangle = U|\psi\rangle \tag{2.15}$$

$$H' = UHU^{-1} \tag{2.16}$$

where

$$U_{ij} = \langle i|\chi_0\rangle \delta_{ij} \tag{2.17}$$

and $|\chi_0\rangle$ is some approximation to the true ground-state eigenvector. The eigenvalues are unchanged, and the algorithm is applied as before to $|\psi'\rangle$ and H'; but the accuracy may be much improved. We have chosen to apply an exponential cut-off on the 'unperturbed' energy, with

$$\langle i|\chi_0\rangle = \exp(-cE_i^0) \tag{2.18}$$

where c is some constant, and E_i^0 is the eigenvalue of

$$H_0 = 2\sum_i \left[1 - \cos\left(\frac{2\pi}{3} L_i\right)\right] \tag{2.19}$$

corresponding to basis state $|i\rangle$. The constant c is varied until the estimated error in the average score reaches a minimum.

Ground state expectation values can be computed from the expression

$$\langle\phi_0|Q|\phi_0\rangle \simeq \frac{\langle\psi'^{(m)}|Q|\psi^{(m)}\rangle}{\langle\psi'^{(m)}|\psi^{(m)}\rangle} \tag{2.20}$$

where Q is the operator whose expectation value is wanted, and $|\psi^{(m)}\rangle$, $|\psi'^{(m)}\rangle$ are two *independently* evolved ensembles. We cannot use the same ensemble $|\psi^{(m)}\rangle$ on both sides, because although $\langle n_k\rangle \alpha c_k^0$ from equation (2.8), it does not follow that $\langle n_k^2\rangle \alpha (c_k^0)^2$. We have used this method to estimate the derivative of E_0 with respect to λ. If

$$H = H_0 - \lambda V \tag{2.21}$$

then by the Feynman–Hellmann theorem

$$\frac{dE_0}{d\lambda} = \frac{E_0 - \langle H_0\rangle_0}{\lambda} \tag{2.22}$$

so the required derivative can be deduced from the ground-state expectation value of H_0.

3. Results

3.1. Series

Using the linked cluster expansion method, 'high temperature' series in λ have been calculated for the ground-state energy, the mass gap, and the susceptibility of the model for both square and triangular lattices. The magnetic field term to be added to the Hamiltonian (2.10) was taken as

$$H_M = h\sum_i (R_i^+ + R_i^-) \tag{3.1}$$

and the susceptibility is defined as

$$\chi = -\frac{1}{M^2}\frac{\partial^2 E_0}{\partial h^2}\bigg|_{h=0} \tag{3.2}$$

The series coefficients are listed in table 1. We have performed a standard *D*log Padé analysis (Guttmann 1989) of the series for the mass gap and the susceptibility, as for a model with a second-order phase transition. The results are exhibited in table 2. The critical parameters deduced from this analysis are†

$$\text{mass gap:} \qquad \lambda_c^{(s)} = 0.388(3) \qquad \nu = 0.54(2) \tag{3.3}$$

$$\text{susceptibility:} \qquad \lambda_c^{(s)} = 0.388(2) \qquad \gamma = 0.97(2). \tag{3.4}$$

† A superscript (s) is added to the series estimate, to distinguish it from what follows.

Table 1. High temperature series in λ for the ground-state energy per site E_0/M^2, the susceptibility χ and the mass gap F. Coefficients of λ^n are listed for the square and triangular lattices.

n	E_0/M^2	χ	F
Square lattice			
0	0	1.333 333 333 33	3.000 000 000 00
1	0	3.555 555 555 56	−4.000 000 000 00
2	−0.666 666 666 667	9.185 185 185 19	−3.333 333 333 33
3	−0.111 111 111 111	23.111 111 111 11	−0.555 555 555 555
4	−0.314 814 814 815	59.684 499 314 1	−11.697 530 864 2
5	−0.290 466 392 318	151.820 098 562	9.675 582 990 40
6	−0.526 034 522 176	390.632 163 601	−68.068 110 806 3
7	−0.776 812 477 773	999.968 952 092	112.475 516 097
8	−1.463 119 284 70	2 572.682 391 01	−505.227 530 390
Triangular lattice			
0	0	1.333 333 333 33	3.000 000 000 00
1	0	5.333 333 333 33	−6.000 000 000 00
2	−1.000 000 000 000	20.888 888 888 9	−7.000 000 000 00
3	−0.833 333 333 333	82.222 222 222 2	−11.166 666 666 7
4	−1.416 666 666 67	324.008 230 453	−30.212 962 963 0
5	−2.765 946 502 06	1 279.477 747 29	−76.442 386 831 3
6	−6.475 723 022 41	5 061.705 359 73	−251.101 566 072
7	−16.440 536 408 3	20 057.179 177 2	−736.072 480 059
8	−45.012 324 962 2	79 586.694 175 1	−2 581.293 256 92

Table 2. *D*log Padé approximants to the mass gap and susceptibility on the square lattice. An asterisk denotes a defective approximant.

	$[N/N-1]$		$[N/N]$		$[N/N+1]$	
N	Pole	Residue	Pole	Residue	Pole	Residue
(Mass gap)						
2	0.2447	(0.108)	0.3852	(0.522)	0.3887	(0.539)
3	0.3903	(0.549)	0.3886	(0.538)	0.3887	(0.539)*
4	0.3871	(0.526)				
(Susceptibility)						
2	0.3552	(−0.710)	0.3864	(−0.955)	0.3889	(−0.979)
3	0.3896	(−0.987)	0.3883	(−0.972)	—	
4	0.3869	(−0.951)				

The critical points deduced from the two series are in perfect agreement with each other. The question to be settled, of course, is whether a first-order transition supervenes before this putative second-order critical point is reached.

3.2. Monte Carlo

The stochastic truncation method discussed in section 2 has been used to calculate the lowest energy eigenvalues in both the spin-0 and spin-1 sectors of the Hamiltonian (2.10), together with their derivatives, for lattice sizes $M = 2$ up to 5. The results are

Table 3. Table of values for the ground state energy per site, E_0/M^2, as a function of coupling λ and lattice size M. Also listed are the resulting estimates for the bulk limit, $M \to \infty$; and estimates from the [4/4] Padé approximant to the high temperature series of table 1.

λ	$M=2$	3	4	5	∞ (estimated)	Series
0.05	−0.033 396 (1)	−0.001 712 (1)	−0.001 683 (1)	−0.001 682 (3)	−0.001 682 (3)	−0.001 682 6
0.10	−0.013 897 (1)	−0.007 061 (1)	−0.006 823 (2)	−0.006 815 (7)	−0.006 815 (7)	−0.006 812 8 (3)
0.15	−0.032 165 (1)	−0.016 472 (1)	−0.015 626 (3)	−0.015 57 (2)	−0.015 55 (2)	−0.015 564 (3)
0.20	−0.059 194 (1)	−0.030 605 (2)	−0.028 44 (3)	−0.028 23 (3)	−0.028 20 (3)	−0.028 20 (2)
0.25	−0.096 417 (1)	−0.050 591 (2)	−0.045 86 (4)	−0.045 24 (4)	−0.045 1 (1)	−0.045 13 (10)
0.30	−0.145 766 (1)	−0.078 609 (2)	−0.069 17 (6)	−0.067 8 (3)	−0.067 0 (5)	−0.067 0 (4)
0.35	−0.209 563 (1)	−0.119 397 (2)	−0.102 04 (5)	−0.097 5 (3)	−0.094 (1)	−0.094 9 (12)
0.40	−0.290 079 (1)	−0.182 996 (3)	−0.159 4 (4)	−0.152 4 (6)	−0.147 (2)	−0.131 (4)
0.45	−0.388 757 (1)	−0.281 455 (3)	−0.266 7 (4)	−0.264 8 (7)	−0.264 0 (7)	−0.180 (11)
0.50	−0.505 479 (1)	−0.412 373 (4)	−0.405 6 (5)	−0.406 (1)	−0.405 6 (5)	−0.26 (4)

Table 4. Values for the derivative of the ground-state energy per site, $(1/M^2)(\partial E_0/\partial\lambda)$, as a function of coupling λ and lattice size M. Also shown are the estimated bulk limit, $M \to \infty$; and the slope of the [4/4] Padé approximant to the series of table 1.

λ	$M=2$	3	4	5	∞ (estimated)	Series
0.05	−0.137 221 (4)	−0.069 443 (7)	−0.067 72 (2)	−0.067 66 (6)	−0.067 66 (6)	−0.067 668 (1)
0.10	−0.285 008 (2)	−0.014 591 1 (9)	−0.138 55 (2)	−0.138 17 (7)	−0.138 1 (1)	−0.138 11 (2)
0.15	−0.448 980 (2)	−0.232 702 (7)	−0.214 67 (2)	−0.213 05 (9)	−0.212 5 (2)	−0.212 8 (1)
0.20	−0.636 908 (2)	−0.336 251 (8)	−0.299 9 (2)	−0.294 9 (2)	−0.292 (1)	−0.294 0 (7)
0.25	−0.858 475 (2)	−0.469 99 (1)	−0.401 4 (2)	−0.388 7 (2)	−0.380 (2)	−0.385 (3)
0.30	−1.123 372 (3)	−0.665 45 (2)	−0.541 6 (3)	−0.510 2 (9)	−0.490 (5)	−0.493 (9)
0.35	−1.436 339 (3)	−0.999 32 (2)	−0.811 2 (3)	−0.720 (1)	—	−0.63 (3)
0.40	−1.789 388 (3)	−1.593 92 (5)	−1.616 (3)	−1.64 (2)	—	−0.83 (8)
0.45	−2.157 354 (3)	−2.333 02 (4)	−2.560 (4)	—	—	−1.2 (3)
0.50	−2.505 476 (2)	−2.856 43 (3)	−2.961 (3)	—	—	−2.0 (8)

Table 5. Values for the mass gap F as a function of coupling λ and lattice size M. Also listed are estimates of the bulk limit, $M \to \infty$, and values from the [4/4] Padé approximant to the mass gap series of table 1.

λ	$M=2$	3	4	5	∞ (estimated)	Series
0.05	2.790 353 (2)	2.791 325 (7)	2.791 51 (3)	2.7915 (4)	2.791 51 (3)	2.791 5
0.10	2.561 989 (1)	2.563 37 (2)	2.564 77 (7)	2.5664 (8)	2.566 4 (8)	2.565 0
0.15	2.314 861 (1)	2.311 51 (2)	2.315 9 (5)	2.3172 (7)	2.317 2 (7)	2.317 3 (1)
0.20	2.049 704 (1)	2.027 85 (3)	2.037 6 (7)	2.042 (2)	2.043 (2)	2.043 (1)
0.25	1.770 447 (2)	1.700 23 (4)	1.715 (1)	1.725 (2)	1.73 (1)	1.732 (4)
0.30	1.485 826 (2)	1.315 90 (4)	1.317 (2)	1.346 (8)	1.37 (2)	1.37 (1)
0.35	1.209 127 (2)	0.881 77 (5)	0.790 (5)	0.79 (2)	0.9 (1)	0.91 (5)
0.40	0.955 503 (2)	0.468 53 (6)	0.239 (9)	0.10 (2)		
0.45	0.737 536 (3)	0.196 10 (8)	0.026 (9)	0.02 (3)		
0.50	0.561 297 (3)	0.075 66 (9)	0.01 (2)	−0.01 (4)		

Table 6. Values for the derivative of the mass gap $\partial F/\partial\lambda$ as a function of coupling λ and lattice size M. Also shown are some estimates of the bulk limit, $M \to \infty$, and the slope of the [4/4] Padé approximant to the series of table 1.

λ	$M=2$	3	4	5	∞ (estimated)	Series
0.05	−4.381 20 (3)	−4.355 2 (2)	−4.48 (3)	−4.53 (3)	−4.60 (5)	−4.343 2 (1)
0.10	−4.754 45 (2)	−4.778 0 (2)	−4.765 (8)	−4.78 (2)	−4.78 (2)	−4.729 (1)
0.15	−5.129 16 (2)	−5.322 0 (3)	−5.243 (4)	−5.216 (7)	−5.18 (3)	−5.198 (7)
0.20	−5.464 65 (1)	−6.066 0 (2)	−5.941 (5)	−5.850 (6)	−5.8 (1)	−5.81 (2)
0.25	−5.676 38 (2)	−7.086 8 (4)	−7.073 (7)	−6.886 (9)	−6.8 (2)	−6.68 (12)
0.30	−5.663 15 (2)	−8.280 0 (5)	−9.05 (1)	−8.87 (4)	—	−8.0 (3)
0.35	−5.352 73 (2)	−8.859 3 (6)	−11.84 (5)	−13.1 (2)	—	—
0.40	−4.748 93 (2)	−7.184 9 (8)	−8.15 (9)	−5.9 (4)	—	—
0.45	−3.949 26 (2)	−3.698 8 (9)	−1.1 (2)	0.3 (4)	—	—
0.50	−3.105 50 (1)	−1.425 4 (8)	—	—	—	—

given in tables 3-6. For each data point, 2000 iterations were carried out, of which the first 500 were discarded, to ensure that the system had reached equilibrium. The remaining scores were averaged over bins of up to 256 iterations, and then the bin averages were treated as statistically independent data points in estimating the statistical error (Binder 1976). In this way the effect of correlations between successive scores was minimised. The initial ensemble size varied, but for the $M = 5$ lattice at $\lambda = 0.40$, for instance, it was $N^{(0)} = 10^4$, this calculation required 3000 CPU seconds on a Fujitsu VP100 machine, or 0.15 ms per state per iteration.

The results for the ground-state energy per site are listed in table 3 and graphed in figure 1. The convergence of the finite-lattice results is quite rapid, and by crudely plotting them against $1/M^2$ (Privman and Fisher 1983) reasonable estimates of the bulk limit $M \to \infty$ can be obtained, as given in table 3. Also shown are some series estimates, obtained from the [4/4] Padé approximant to the ground-state energy series. The agreement between the two methods is very good, up to $\lambda = 0.35$; beyond that, the finite-lattice estimates swing away from the series line, indicating a phase transition between $\lambda = 0.35$ and 0.40.

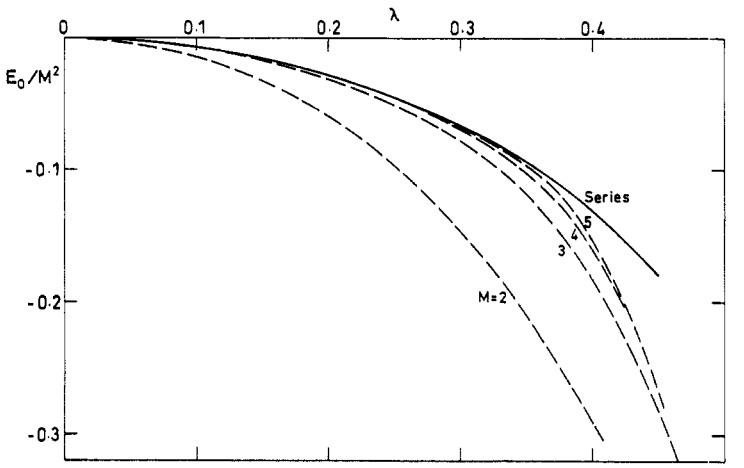

Figure 1. Graph of the ground-state energy per site, E_0/M^2, as a function of coupling λ. The finite-lattice Monte Carlo results are shown as broken curves, while the full curve is the [4/4] Padé approximant to the series of table 1.

Table 4 and figure 2 show results for the derivative of the ground-state energy. For the $M = 5$ lattice the results became unreliable beyond the critical region, due to a very small overlap between the two independent ensembles used in equation (2.20), so no values are listed there. In any case, it is clear that a sharp change in the slope is developing at the phase transition. Whether the change is discontinuous, as at a first-order transition, or smooth as at a second-order transition, cannot really be decided on the basis of this data. The total change in slope over the transition region is about 1.4 ± 0.3.

Table 5 and figure 3 show results for the mass gap between the spin-1 sector and the spin-0 sector. Once again, the agreement between the Monte Carlo and series estimates is excellent, out to $\lambda = 0.35$. The convergence of the finite-lattice results to the bulk limit is not monotonic, in contrast to the usual behaviour for a second-order

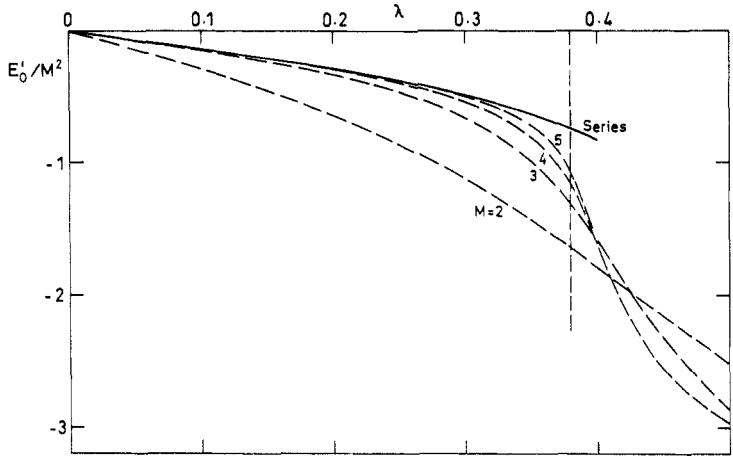

Figure 2. Derivative of the energy per site, $(1/M^2)(\partial E_0/\partial\lambda)$, as a function of coupling λ. The broken curves are the Monte Carlo results for lattice size M, while the full curve is the derivative of the [4/4] series approximant. The broken vertical line marks the estimated position of the phase transition.

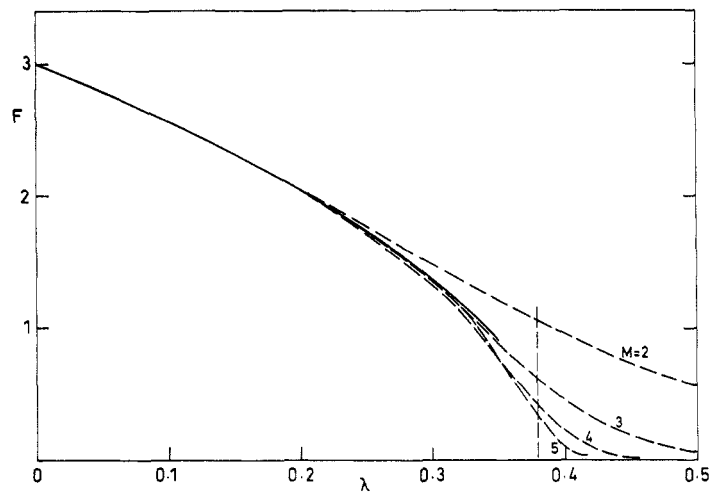

Figure 3. The mass gap F as a function of coupling λ. The broken curves are Monte Carlo results, the full curve is the [4/4] Padé approximant to the series of table 1, and the broken vertical line marks the expected phase transition.

transition; and a distinct step-like structure appears to be developing around $\lambda = 0.38$ for the larger lattices. Beyond that the mass gap is clearly converging rapidly to zero. This behaviour seems to indicate a first-order transition, albeit with a rather small discontinuity in the mass gap.

Table 6 and figure 4 show the derivative of the mass gap. A peak is clearly seen, getting higher and sharper as the lattice size increases. This behaviour could be consistent with either a first-order or a second-order transition.

In order to tie down the phase transition more precisely, we have carried out a search for the 'pseudo-critical points', given in finite-size scaling theory as follows.

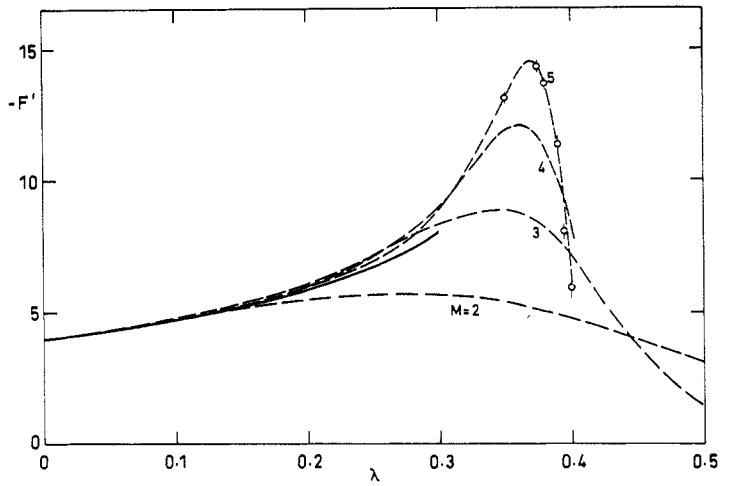

Figure 4. Derivative of the mass gap, $-\partial F/\partial\lambda$, as a function of coupling λ. The broken curves are Monte Carlo results, and the full curve the slope of the [4/4] approximant to the mass gap.

Define the 'scaled mass gap ratio'

$$R_M(\lambda) = \frac{MF_M(\lambda)}{(M-1)F_{M-1}(\lambda)} \tag{3.5}$$

where $F_M(\lambda)$ is the mass gap for lattice size M, then the pseudo-critical point λ_M^* for lattice size M is taken as (Hamer and Barber 1981) the point such that

$$R_M(\lambda_M^*) = 1$$

consistent with the hypothesis that $F_M(\lambda)$ scales like $1/M$ at the critical point. The sequence of λ_M^* values actually converges to the critical point λ_c as $M \to \infty$, no matter whether the transition is second-order or first-order (Hamer 1983). Table 7 lists the values λ_M^* obtained for $M = 2$ to 5. They converge quite rapidly, and a plot against $1/M^2$ leads to a bulk limit of $\lambda_c = 0.379(3)$. This lies short of the series value $\lambda_c^{(s)}$, although only by 2% or so, and thus indicates that the transition is indeed first-order. Taking $\lambda_c = 0.379$, we estimate from the mass-gap data discussed above that the discontinuity in the mass-gap at the transition is 0.4 ± 0.07, or $15 \pm 2\%$ of its maximum value.

Table 7. Table of pseudo-critical points λ_M^* and finite-lattice estimates of the spontaneous magnetisation M_M as a function of lattice size M, together with their estimated bulk limits.

M	λ_M^*	M_M
2	0.2975 (1)	1.1612
3	0.3644 (1)	1.0440 (2)
4	0.376 (1)	0.953 (4)
5	0.377 (3)	0.91 (4)
∞ (estimated)	0.379 (3)	0.64 (10)

A finite-size scaling estimate can also be obtained for the spontaneous magnetisation at the transition. As discussed by Uzelac (1980) and Hamer (1982), the best results are given by an indirect technique, involving matrix elements of the magnetic field operator. In the low-temperature regime, we expect three degenerate ground states $|\phi_0\rangle$, $|\phi_1\rangle$, $|\phi_2\rangle$ in this model, belonging to the three spin sectors $L=0$, 1 and 2 respectively, where $L=\Sigma_i l_i$ is the total spin. Considering the 3×3 sub-matrix of the Hamiltonian spanned by these three states alone, one finds that the spontaneous magnetisation is given by

$$M_0 = \lim_{\substack{M\to\infty \\ h\to 0}} \left(\frac{1}{M^2} \quad \frac{\partial E_0}{\partial h} \right) = \lim_{M\to\infty} \left(\frac{1}{M^2} \sqrt{\alpha_{01}^2 + \alpha_{02}^2 + \alpha_{12}^2} \right) \Bigg|_{h=0} \tag{3.6}$$

where

$$\alpha_{01} = \langle \phi_1 | \sum_i (R_i^+ + R_i^-) | \phi_0 \rangle \tag{3.7}$$

and similarly for α_{02} and α_{12}. Using an approach similar to that outlined in section 2, values were obtained† for these matrix elements at the pseudo-critical points, giving rise to the magnetisation values listed in table 7. A crude plot against $1/M$ extrapolates to a bulk limit $M_0 = 0.64 \pm 0.2$, or $43 \pm 7\%$ of its maximum possible value. This provides very clear evidence of a first-order transition.

4. Conclusions

Using linked cluster expansion methods, high temperature series expansions were calculated for the ground-state energy, the mass gap and the susceptibility of this model. A Padé analysis of the square lattice series indicates a putative or incipient second-order critical point at coupling $\lambda_c^{(s)} = 0.388(2)$, with indices $\gamma = 0.97(2)$, $\nu = 0.54(2)$.

A finite-size scaling analysis of our Monte Carlo data shows that actually a first-order transition occurs just 2% short of this incipient second-order point, at $\lambda_c = 0.379(3)$. The second-order critical point indicated by the series analysis may then be interpreted as a spinodal pseudo-transition, such as those discussed in previous series analyses by Ditzian and Kadanoff (1979), and Privman and Schulman (1982), for example.

The clearest evidence of the first-order transition comes from the spontaneous magnetisation estimates, which approach a finite bulk limit of 0.64 ± 0.1, or $43 \pm 7\%$ of the maximum possible value. This is in good accord with Euclidean Monte Carlo studies (Knak Jensen and Mouritsen 1979, Wilson and Vause 1987, Gavai *et al* 1989), which find a discontinuity of about 40% in the order parameter at the transition point. Thus it appears that the relative size of the discontinuity may even be a universal parameter, although we know of no theoretical reason for this at a first-order transition in three dimensions.

The mass gap also shows signs of a first-order transition, with a finite step developing at the transition point. Combining series and Monte Carlo information, we estimate the discontinuity as 0.44 ± 0.07, or $15 \pm 2\%$ of its maximum value. Finally, the derivative of the ground-state energy changes by 1.4 ± 0.3 in total over the transition region, but it is impossible to tell whether this is due to a smooth transition, or an actual

† These estimates required the evolution of six independent ensembles, two for each spin sector.

discontinuity, i.e. a 'latent heat'. The Euclidean Monte Carlo studies (Knak Jensen and Mouritsen 1979, Wilson and Vause 1987, Gavai *et al* 1989), show a rather small discontinuity embedded within a larger, smooth variation.

The emerging picture is that of a weak first-order transition, as found in the Euclidean model. To provide further confirmation of this, it would be useful to have some low-temperature series to add to our high-temperature series: we hope to compute these in future work. As regards the Monte Carlo work, our strategy has been to try and compute accurate eigenvalues for small lattices, and use finite-size scaling to estimate the bulk limiting behaviour. For a first-order transition such as this, finite-size scaling is not such a powerful tool (Privman and Fisher 1983), and so it would be useful to have some data for larger lattices as well. In fact, Peczak and Landau (1989) have observed that for a very weak first-order transition (5-state Potts in two dimensions) one may even observe a *crossover* in finite-size scaling from apparent second-order behaviour on small lattices to first-order behaviour on large lattices.

In any case, the good agreement between the series and Monte Carlo estimates in the high-temperature regime is sufficient to show that the stochastic truncation approach provides an accurate and efficient Monte Carlo technique. We hope this will encourage further applications of the method.

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