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1983 J. Phys. A: Math. Gen. 16 829

(http://iopscience.iop.org/0305-4470/16/4/019)

J. Phys. A: Math. Gen. **16** (1983) 829–838. Printed in Great Britain

Approximation schemes for finite lattices

A C Irving and C J Hamer†

Department of Applied Mathematics and Theoretical Physics, University of Liverpool, PO Box 147, Liverpool, L69 3BX, UK

Received 6 August 1982

Abstract. Two algorithms are formulated for systematically truncating the set of basis states required in lattice Hamiltonian calculations, thus allowing larger lattice sizes to be treated. They are tested for the case of the $(1+1)$-dimensional Ising model. It is shown that smoothly convergent finite lattice sequences are obtained, which can successfully be extrapolated to the bulk limit. We point out the relevance of the technique for lattice calculations in higher dimensions.

1. Introduction

Finite-size scaling techniques may be used to explore the spectrum and phase structure of models in lattice field theory and statistical mechanics (Hamer and Barber 1981a, b, hereafter denoted I and II, Roomany and Wyld 1980, Nightingale 1976). One calculates an eigenvalue of the Hamiltonian or transfer matrix on a sequence of lattices of increasing size, and then uses sequence extrapolation algorithms (II, Barber and Hamer 1982) to estimate the bulk limit for an infinite lattice. For two-dimensional models, these procedures equal or surpass in accuracy any other general technique (II, Blöte *et al* 1981, Blöte and Nightingale 1982).

In three or four dimensions, however, the value of this technique is much less obvious. One needs a sequence of four or five different lattice sizes for the extrapolation method to work well; but the extremely rapid proliferation of basis states forbids one from calculating exact eigenvalues for the larger lattices (Roomany and Wyld 1980, Irving and Thomas 1982). In the Hamiltonian field theory formalism (Kogut and Susskind 1975), for instance, one can solve the 5×5-site lattice for the $(2+1)$-dimensional Ising model (Hamer 1982), but for any model more complicated than that, even the 4×4 lattice will be out of reach.

We are forced, therefore, to consider the use of systematic approximation schemes for the larger lattice sizes. The object of this brief report is to investigate two such approximation schemes in detail, and to try them out on a simple, soluble model, namely the $(1+1)$-dimensional Ising model, in order to check whether the hypotheses of finite-size scaling (Fisher 1971, Fisher and Barber 1972, I) are still obeyed, and whether the sequence extrapolation algorithms can still be applied to the approximate finite-lattice sequences.

† Permanent address: Department of Theoretical Physics, Institute of Advanced Studies, Australian National University, Canberra 2600, Australia.

There are several different approximations which might be employed. Each involves a truncation of the set of basis states, which reduces the size of the matrix Hamiltonian whose eigenvalues are to be calculated. They are:

(1) *Truncation* of the single-site spectrum. An example is the work of Barber and Richardson (1981), who considered a truncated O(2) model in $(1+1)$ dimensions, in which the spectrum of spin values allowed at each site was reduced from the integers $[-\infty, +\infty]$ down to $[-1, +1]$. This restriction is similar in spirit to replacing the original continuous O(2) symmetry group by a discrete analogue, a device which has also been used in Monte Carlo calculations (e.g. Rebbi 1980, Petcher and Weingarten 1980). Since we intend here to stick with the original model, we shall not consider this option any further.

(2) *Order N cut-off.* This approximation is associated with a perturbation theory framework, in which one breaks up the Hamiltonian into two pieces $H = H_0 + xV$, where x is the perturbative coupling constant. The eigenstates of H_0 are used as basis states for the calculation. Then in calculating, say, the ground-state energy, one can choose to throw away all basis states except those which can be reached from the ground state of H_0 by application of the perturbation operator V up to N times. If one then increases N in proportion to the lattice size M, as discussed in the text, one may obtain a sequence of approximate finite-lattice eigenvalues which will converge to the correct bulk limit—at least in the region where the perturbation series in x converges. A cut-off of this sort has been used, for example, by Crewther and Hamer (1980).

(3) *E_0 cut-off.* This approximation is also related to the perturbation theory framework, and consists in throwing away all those basis states whose unperturbed energy (eigenvalue of H_0) is above a given cut-off E_0. Again, if one increases the cut-off E_0 in proportion to the lattice size M, a sequence converging to the correct bulk limit should be obtained. This is a rather mild cut-off, and is unlikely to be very useful in three or four dimensions. But it may come in useful for the treatment of two-dimensional models with a continuous symmetry group.

The N cut-off and E_0 cut-off schemes are tested on the $(1+1)$-dimensional Ising model in the remainder of this paper. The qualitative conclusions, which we conjecture will hold in the general case, are as follows:

(a) The E_0 cut-off sequence converges to the *exact* finite-lattice sequence, at *all* couplings, as the lattice size M increases. Thus all the hypotheses and techniques of finite-size scaling may be safely applied in this approximation.

(b) The N cut-off sequence converges 'linearly' (i.e. exponentially fast in M) provided the coupling lies below the critical point. The rate of convergence is the same as for the exact finite-lattice sequence, and thus appears to be controlled by the same physical parameter, the correlation length (Fisher 1971, Au-Yang and Fisher 1975). At the critical point the N cut-off sequence still appears to converge logarithmically, but it is unlikely that the usual finite-size scaling techniques for obtaining critical parameters can be applied. Beyond the critical point, the N cut-off sequence is virtually useless.

It is our hope that the N cut-off approximation scheme will be useful in treating lattice gauge theories in three and four dimensions. Our results here indicate that the N cut-off sequence may be reliably extrapolated to the bulk limit, provided the system does not undergo a phase transition. It remains to be seen whether such a technique can challenge the standard Monte Carlo methods (Binder 1976, Creutz *et al* 1979), which involve a (stochastic) approximation scheme applied to a relatively

large finite lattice. It is our belief that systematic approximation schemes of the present sort will eventually prove more reliable and effective.

2. Formulation

The field theory version of the Ising model in $(1+1)$ dimensions has the simple Hamiltonian (Fradkin and Susskind 1978, Hamer *et al* 1979)

$$H = (g/2a) \sum_{m=1}^{M} [1-\sigma_3(m)-x\sigma_1(m)\sigma_1(m+1)]. \tag{2.1}$$

Here the index m labels sites on a one-dimensional spatial lattice, with periodic boundary conditions, while the time variable is taken to be continuous. The σ_i are Pauli matrices acting on a two-state spin variable at each site, g is a dimensionless coupling constant, a is the lattice spacing, M is the total number of sites and $x = 2/g^2$.

It is usually convenient to deal with the reduced, dimensionless Hamiltonian

$$W = (2a/g)H. \tag{2.2}$$

We shall also work in the 'high-temperature' representation

$$W = W_0 - xV, \tag{2.3}$$

where

$$W_0 = \sum_{m=1}^{M} (1-\sigma_3(m)), \qquad V = \sum_{m=1}^{M} \sigma_1(m)\sigma_1(m+1). \tag{2.4}$$

Then in this representation $\sigma_3(m)$ is diagonal, and x is the perturbation coupling constant.

This model is of course exactly soluble. In the thermodynamic limit $M \to \infty$, the eigenvalues of W were found by Pfeuty (1970): the ground-state energy per site is

$$\omega_0/M = 1-(2/\pi)(1+x)E[4x/(1+x)^2] \tag{2.5}$$

where $E(m)$ is the complete elliptic integral of the second kind. The mass gap is

$$F(x) = \omega_1 - \omega_0 = 2(1-x) \qquad (x \leqslant 1). \tag{2.6}$$

Thus the model exhibits a phase transition at $x = 1$ with critical exponent $\nu = 1$.

The eigenvalues for finite M can also be evaluated analytically (Schultz *et al* 1964). It has been verified (I) that they converge to the bulk limits (2.5) and (2.6) in the manner predicted by finite-size scaling theory. For purposes of reference, we display some of these exact finite-lattice eigenvalues in figure 1. It can be seen that the limiting mass gap is given by (2.6) for $x \leqslant 1$, and is *zero* for $x > 1$, corresponding to the presence of two degenerate ground states in the low-temperature phase.

To compute the finite-lattice eigenvalues numerically (I), we work in a basis of high-temperature eigenstates: that is, eigenstates of W_0, or the spin $\sigma_3(m)$. Starting from the ground state of W_0, which has all spins up, one may build up a complete

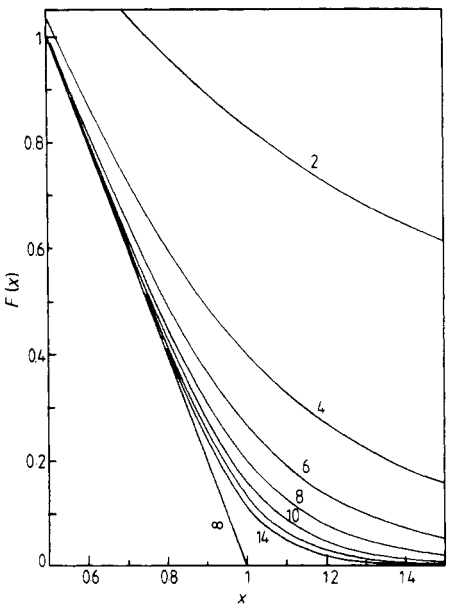

Figure 1. The mass gap $F(x, M) \equiv \omega_1 - \omega_0$ for the finite lattice Ising model in $(1+1)$ dimensions illustrating convergence to the bulk limit which is $F(x) = 2(1-x)$ for $x \leqslant x_c = 1$. The numbers label the lattice size M. For clarity, odd values of M are omitted.

list of the translation-invariant basis states, and of the matrix elements of V connecting them, by iterative applications of the perturbation operator V. Since this operator flips two spins at a time, a total of $N = [M/2]$ applications of V is sufficient to generate the complete set of basis states for W on the finite lattice†. The lowest eigenvalue may now be calculated by standard methods for large sparse matrices: we used a Lanczos algorithm for this purpose. The eigenvalues of interest were calculated accurate to at least seven significant figures.

Our object here is to discuss the effects of two approximation schemes, each involving a truncation of the set of basis states. The first scheme is the 'N cut-off': that is, an approximation in which one halts the iterative process referred to above after a selected number N of applications of V, so that the list of basis states is not completed. There is in fact a 'natural' choice of N corresponding to each lattice size M (the linear dimension), namely $N = [(M-1)/2]$, because this corresponds to the maximal order of perturbation theory in which the finite-lattice results correctly match the bulk limit for ω_0 and ω_1. Beyond that order, the effects of the lattice boundaries become evident in the perturbation series: in diagrammatic terms, one starts to get diagrams which 'wrap around' the periodic lattice.

The second approximation scheme we shall refer to as the 'E_0 cut-off'. This consists of throwing away those basis states whose unperturbed energy E_0 (eigenvalue of W_0) is greater than some maximum $E_0^{\max}$. The 'natural' choice of cut-off here is $E_0^{\max} = 2M \times (2M-2)$ for M odd (even) which again corresponds to the maximal order of perturbation theory in which the finite-lattice results match the bulk limit.

† As a matter of fact, there are two disjoint sectors of states, namely those with even and odd numbers of flipped spins. The lowest eigenvalue in each sector is ω_0 and ω_1, respectively.

In $(1+1)$ dimensions, and for this model in particular, both these cut-offs are very mild in that the saving in basis states is rather small. In fact, for odd site lattices these cut-offs eliminate no basis states at all! But for more complicated models with a continuous symmetry group, or in higher dimensions, the corresponding cut-offs will be much more effective. To study their qualitative effects on the eigenvalues, we have actually chosen cut-offs $N = [M/2] - 1$ and $E_0^{\max} = 2(M-1)$, but have also considered more severe cut-offs.

The application of these cut-offs should affect the low-lying eigenvalues very little. This is illustrated in figure 2, which shows the relative contribution to the vacuum from the basis states as a function of order N and unperturbed energy E_0 at the critical coupling $x = 1$, and for lattice size $M = 14$. The weights of the individual basis states fall off rapidly, in a roughly exponential fashion with E_0, over six orders of magnitude; and decrease in a similar fashion with N, though at a slower rate. Similar behaviour is found at other couplings, for other lattice sizes and for the eigenvalue ω_1.

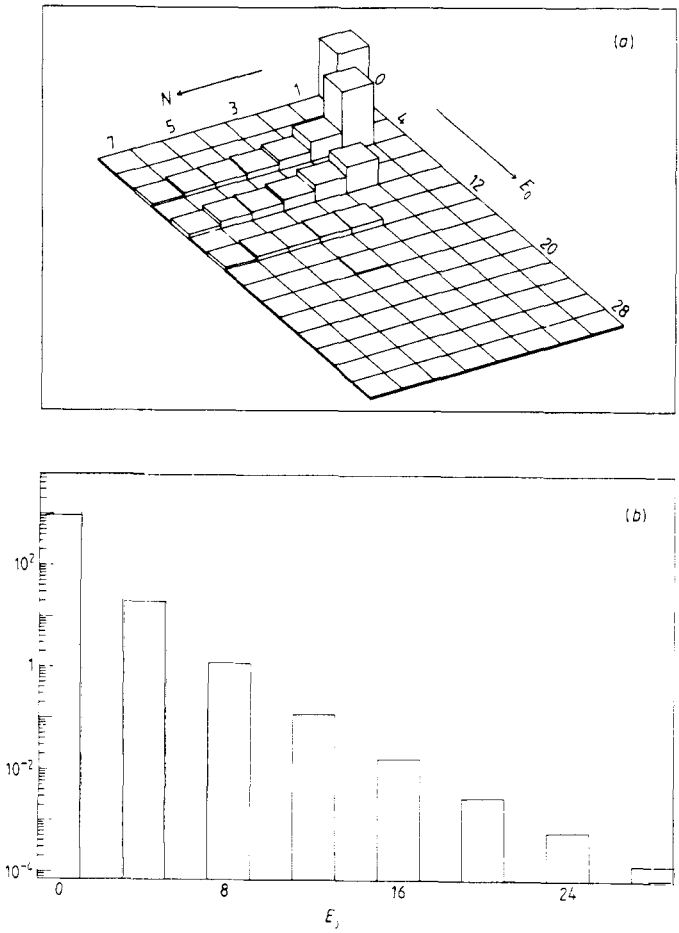

Figure 2. The contribution (amplitude squared) of the basis states to the vacuum state of a 14-site lattice at $x = 1$. In (a) are shown the total contributions (on an arbitrary linear scale) from states of a given E_0 and order of perturbation N. In (b) the average contribution per configuration state is plotted logarithmically (arbitrary scale) against E_0.

3. Results

We shall test the convergence of our two approximation schemes at three different coupling values, namely $x = 0.6$, before the critical point; $x = 1.0$, the critical point; and $x = 1.3$, beyond the critical point.

3.1. $x = 0.6$

Since this coupling is within the radius of convergence of the power series, and both approximation schemes get the perturbation series correct up to order $N \simeq M$, we expect both schemes to converge 'linearly' (i.e. with error $O(e^{-\text{constant} \times M})$) to the bulk limit as $M \to \infty$. This is confirmed in figure 3(a), which shows a semi-log plot of the deviations from the bulk limit against lattice size M for the vacuum state, for the exact finite-lattice sequence, the 'N cut-off' sequence, and the 'E_0 cut-off' sequence. All three sequences exhibit rapid linear convergence to the bulk limit; and furthermore, all three seem to converge at the same rate (i.e. with the same asymptotic slope on the semi-log plot). This can readily be understood. The rate of convergence of the exact finite-lattice sequence is controlled by the correlation length†, which determines the size of the boundary effects: and it is natural to suppose that the same physical parameter should control the convergence of the cut-off sequences as well. Finally, it appears that the E_0 cut-off sequence rapidly converges on the *exact* finite-lattice sequence. The basis states with high E_0 have negligible weight, as shown already in figure 2, and can apparently be thrown away with impunity. We have

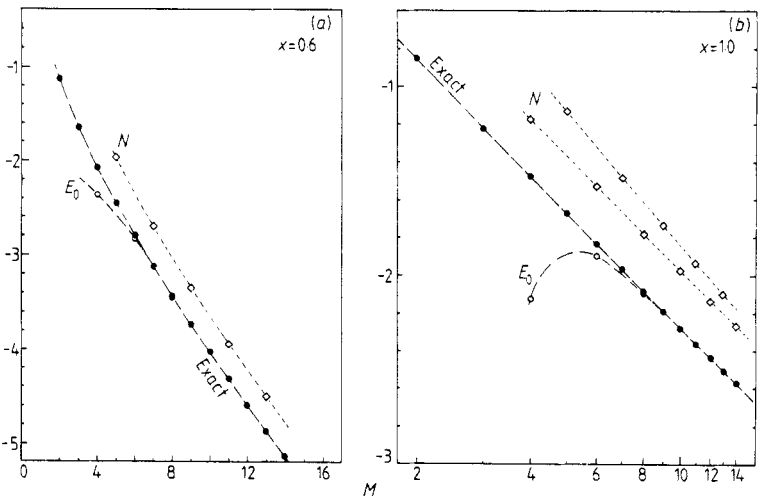

Figure 3. The quantity $\log_{10}|\omega_0/M - (\omega_0/M)_\infty|$ which is the logarithm of the finite-lattice deviation from the bulk limit of the Ising model vacuum energy. In (a) linear convergence is seen to obtain at $x = 0.6$, whereas at the critical point $x = 1$, shown in (b), logarithmic convergence obtains. The results for the exact (●), E_0 cut-off (○) and N cut-off (◇) sequences are shown. The E_0 cut-off values for odd M are the same as the exact ones (see text) and, at $x = 0.6$, the N cut-off values for even M happen to be approximately the same as the exact ones, although the difference has opposite sign.

† We are indebted to Professor R J Baxter for this remark.

confirmed that the same qualitative behaviour holds for more severe cut-offs, $N = [M/2]-2$, and $E_0^{\max} = 2(M-2)$, and for the mass gap† as well as the vacuum energy.

A sequence which is converging linearly may be extrapolated using an iterated Aitken algorithm (II). Unfortunately, the cut-off sequences are 'staggered' between odd and even M values, as may be seen in figure 3. This halves the effective length of the sequence, since Aitken's algorithm does not cope with a staggered sequence at all well, and we are forced to deal with odd and even M values separately‡.

Table 1 shows, as an example, the Aitken tables for the exact, N cut-off and E_0 cut-off sequences for the vacuum energy ω_0/M at $x = 0.6$ using even lattice sizes M. Using all available lattice sizes $(2, 3, 4, \ldots, 14)$, the exact sequence extrapolation gives the vacuum energy and mass gap to at least seven significant figures, which represents an improvement of three to four figures over the $M = 14$ results alone. The shorter even-site exact sequence presented in table 1 is almost as accurate at better than six significant figure accuracy. The order N cut-off sequence rivals this with six§ figure accuracy and the E_0 cut-off is almost as successful with five figure

Table 1. Aitken tables for the vacuum energy (ω_0/M) sequences of finite lattice results at $x = 0.6$ using lattice sizes M, where M is even and $2 \leq M \leq 14$. Results are shown for exact and cut-off sequences. The entries in brackets make use of the $M = 2$ results which might be regarded as special in the cut-off sequences.

0.166 1904			Exact
0.100 6422	0.093 0443		
0.093 8335	0.092 3335	0.092 2435	
0.092 6043	0.092 2536	0.092 2392	0.092 2386
0.092 3315	0.092 2414	0.092 2387	
0.092 2638	0.092 2392		
0.092 2457			
(0.000 0000)			$N \leq [M/2-1]$
0.083 0950	(0.091 3370)		
0.090 5933	0.092 1288	(0.092 2336)	
0.091 8678	0.092 2214	0.092 2379	(0.092 2386)
0.092 1446	0.092 2354	0.092 2385	
0.092 2130	0.092 2379		
0.092 2313			
(0.000 0000)			$E_0 \leq 2(M-1)$
0.096 5279	(0.093 8075)		
0.093 7286	0.091 8425	(0.092 1773)	
0.092 6018	0.092 2461	0.092 2412	(0.092 2380)
0.092 3314	0.092 2412	0.092 2378	
0.092 2638	0.092 2392		
0.092 2457			

† In the high-temperature representation the 'N cut-off' results for the mass gap are peculiar, in that they are already almost exactly equal to the bulk limit. This is because the exact result (2.6) is itself a linear function of x. Using a low-temperature representation (V diagonal rather than H_0), one obtains precisely the same results for the exact finite-lattice eigenvalues, but the effect of truncation is quite different and in practice provides a less useful tool.

‡ This 'staggering' should not occur for lattice gauge models.

§ This particular result is unusually good. Neighbouring couplings show five figure accuracy is more typical.

accuracy. For each cut-off the sequence extrapolation allows a gain of 1–2 extra figures of accuracy over the $M = 14$ result.

A summary of these results is contained in table 2.

Table 2. The accuracy, i.e. $|F(M) - F(\infty)|$, achieved using the exact finite-lattice sequence and the cut-off sequences. The bulk lattice exact results for ω_0/M are given by equation (2.5).

		Exact	N cut-off	E_0 cut-off
$x = 0.6$	ω_0/M	2×10^{-8}	1×10^{-7}	1×10^{-6}
	F	6×10^{-8}	8×10^{-6}	2×10^{-5}
$x = 1$	ω_0/M	5×10^{-8}	8×10^{-6}	7×10^{-6}
	F	4×10^{-4}	2×10^{-3}	1×10^{-1}
$x = 1.3$	ω_0/M	2×10^{-7}	2×10^{-2}	1×10^{-6}
	F	2×10^{-6}	—	8×10^{-5}
Length of sequence		13	6	6

3.2. $x = 1.0$

This is the critical point coupling. According to finite-size scaling theory (Fisher 1971, Fisher and Barber 1972, I), the exact finite-lattice eigenvalues at this point are expected to converge 'logarithmically' (i.e. with error $O(M^{-y})$, where for the mass gap $y = 1$) to the bulk limit $M \to \infty$. This is confirmed† in figure 3(*b*), which shows a log–log plot of the deviations from the bulk limit against lattice size M for the vacuum energy as an example. Again, all these sequences show similar behaviour, and appear to have the same asymptotic slope (corresponding to $y = 2$ for the vacuum state). And again, the E_0 cut-off sequence rapidly converges to the exact sequence. Similar conclusions apply for more severe cuts, and for the mass gap as well as the vacuum energy (though the N cut-off results for the mass gap exhibit the same peculiarity described in the footnote to § 3.1).

A sequence which is converging logarithmically may be extrapolated using a 'modified VBS' algorithm (Vanden Broeck and Schwartz 1979, II, Barber and Hamer 1982). The accuracies achieved are summarised in table 2. For the vacuum energy the overall accuracy is only slightly worse than that achieved for linear convergence (§ 3.1). Again, much of the reduction in accuracy in the cut-off sequences is attributable to the shorter sequence lengths.

3.3. $x = 1.3$

This coupling lies beyond the critical point. Now the exact finite-lattice sequence is once more expected to converge linearly to the bulk limit since we have moved away from the critical region again. This behaviour is illustrated graphically in figure 1. It turns out that the E_0 cut-off sequence converges to the exact one as before, and therefore exhibits the same scaling behaviour. But the N cut-off sequence behaves badly beyond the critical point, as one might expect. The sequence for the vacuum energy does seem to converge to the correct bulk limit, but only in a slow (possibly

† In I, the finite-size scaling hypothesis for the mass gap was analytically proved to be correct, for the exact sequence.

logarithmic) fashion. The sequence for the mass gap appears to converge towards a value -0.6, i.e. a continuation of the straight line $2(1-x)$, which is only valid at high temperature ($x \leqslant 1$). The E_0 cut-off sequence may be extrapolated using the Aitken algorithm with reasonable success, and results are summarised in table 2.

3.4. Critical point parameters

It has been shown in II that by the use of finite-size scaling hypotheses combined with the modified VBS sequence extrapolation algorithm, one may extract highly accurate numerical estimates of the critical parameters from the exact finite-lattice sequence. In the present case, one may quite easily extract a value for the critical coupling x_c accurate to six significant figures, and one for the exponent ν accurate to five significant figures; but we shall not exhibit the results in detail. Since the E_0 cut-off sequence converges to the exact one, it is clearly possible to apply the same hypotheses and methods again. We find that this application is successful, but because the cut-off sequence is 'staggered' (effectively, halved in length), one only obtains an accuracy of four figures for x_c, and two figures for ν. The N cut-off results for the mass gap happen to lie extremely close to the bulk limiting curve $2(1-x)$, as mentioned previously, and hence one could also estimate the critical parameters with good accuracy from these results (for example, a 14-site lattice gives x_c and ν to four and five significant figures respectively). But this situation is peculiar to the Ising model. In general, one cannot expect to apply the scaling hypotheses with any success to the N cut-off sequence near a critical point.

4. Conclusions

For the 'E_0 cut-off' approximation scheme, we have found that the E_0 cut-off sequence rapidly approaches the exact finite-lattice sequence at all coupling values (although presumably the convergence slows as x gets large). It follows automatically that all the standard finite-size scaling methods may be applied, giving accurate values for the eigenvalues and critical parameters in the bulk or thermodynamic limit.

For the 'N cut-off' scheme, it was found that below the critical coupling $x_c = 1$, and within the radius of convergence of the high-temperature power series expansions, the N cut-off sequence converges linearly like the exact sequence. Furthermore, the rate of convergence is the same, and is presumably determined by the same physical parameter, namely the correlation length. It follows that standard extrapolation schemes such as the iterated Aitken algorithm may be applied to obtain accurate estimates of the bulk eigenvalues. Unfortunately, it is not possible in this model to test whether the same conclusions apply in a situation where one is *beyond* the radius of convergence of the power series, but still short of any physical critical point. Our experience (Hamer *et al* 1982) suggests that they do apply.

At the critical coupling $x_c = 1$, the N cut-off sequences appear to converge logarithmically like the exact ones; but because of the peculiarities of the Ising model, we are not able to draw any general conclusions about the estimation of critical parameters in the N cut-off scheme. Beyond the critical point, these results are essentially useless.

Where will these approximation schemes be of use? There is little to be gained in their application to models with a discrete symmetry group in two dimensions,

because the saving in basis states is relatively small, and the only effect will be to reduce the effective length of the finite-lattice sequence due to the 'staggering' discussed in § 3. But for two-dimensional models with a continuous symmetry group some sort of cut-off is essential: and we would suggest that the E_0 cut-off scheme is a natural one to use in these cases. So far as we know, it has not yet been tried in the systematic form discussed here.

In higher dimensions, one is essentially forced into some sort of approximation scheme by the rapid proliferation of states, as was outlined in the introduction. The E_0 cut-off scheme is too mild to be of much use here: it will not eliminate enough states. But we expect some useful results to be obtainable using the N cut-off scheme. To obtain a complete set of states for a discrete model on an M^d lattice requires $O(M^d)$ orders of perturbation. A restriction to states of order $N < M$ therefore provides an enormous saving. For example, for a Z(2) pure gauge theory in $(2+1)$ dimensions, a cut-off at order $M-1$ on a 5×5 lattice allows one to handle 1000 rather than 160 000 states. The savings for more complicated groups are even more spectacular. We are currently investigating the use of these techniques in $2+1$ dimensions.

Acknowledgments

CJH would like to thank the SERC for financial support, and Professor C Michael and the University of Liverpool for their hospitality while this work was carried out.

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