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Stochastic truncation for the (2+1)D Ising model

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Abstract. The method of 'symmetrized' stochastic truncation is applied to the (2+1)-dimensional Ising model, to calculate the ground-state energy, mass gap, magnetization and susceptibility on lattices of sizes up to 6×6 sites. The method is shown to be a powerful and accurate Monte Carlo technique, provided the lattice size is not too large, and the model is suitably 'convergent'. Finite-size scaling estimates of the critical indices are $\nu=0.627(2)$, $\alpha=0.12(2)$, $\beta=0.324(3)$, and $\gamma=1.23(1)$. An estimate of the combination $\gamma/\nu+2\beta/\nu=3.000(1)$ is obtained, in outstanding agreement with the expected hyperscaling relation.

1. Introduction

Finite-size scaling theory (Fisher 1971, Barber 1984) has proved to be a very powerful tool for the exploration of critical behaviour in lattice models. There are two alternative strategies one may adopt. The first one (Nightingale 1976, Hamer and Barber 1980, 1981) is to compute the properties of a sequence of small, finite lattice systems exactly, using a method such as the Lanczos algorithm, and then extrapolate to the properties of the bulk lattice using the theory of finite-size scaling. The second strategy (e.g. Bhanot *et al* 1987, Alves *et al* 1990) is to perform approximate calculations for much larger lattices, using a Monte Carlo technique, and thus approach the bulk limit directly.

For simple two-dimensional models, the first strategy has been very successful, and is capable of great precision. For three-dimensional models, however, the number of basis states proliferates so fast that one is limited to only very small lattice sizes, and the finite-lattice sequence is too short to do a very accurate extrapolation to the bulk limit. For the (2+1)-dimensional Ising model on a triangular lattice, for instance, the largest system which has been solved exactly to date (Hamer and Johnson 1986, hereafter referred to as I; Henkel 1989) is the 5×5 lattice, which already involves 116K basis states. The 6×6 lattice would involve around 160 M basis states, which puts it beyond the reach of exact calculations at the present time; although by a *tour de force* Lin (1990) has recently managed to obtain exact Lanczos eigenvalues for the Heisenberg spin model on a lattice of 32 sites. Several attempts have been made (Irving and Hamer 1983, Patkos and Rujan 1985) to find a way of cutting off the less important basis states so as to make a 6×6 calculation feasible, but to date they have tended to give unacceptable systematic errors.

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The method we discuss here, namely 'symmetrized stochastic truncation' (Allton *et al.* 1989, Hamer and Court 1990, Hamer *et al* 1990), represents something of a halfway house between the two strategies outlined above. It is a Monte Carlo method which is slow, but very accurate, and capable of giving essentially exact results for small lattices. It is not suitable for lattices of huge size, but should be capable of extending the reach of the Lanczos technique to somewhat larger lattices, providing sufficiently good results to allow an accurate extrapolation to the bulk limit.

Our aim in the present work was to use stochastic truncation to calculate various thermodynamic quantities for the (2+1)-dimensional Ising model on a 6×6 lattice, with an accuracy sufficient to allow improved estimates of the critical indices of the model, via finite-size scaling. In the event, we have fallen somewhat short of this aim. Improved estimates of the critical parameters have been obtained, but these are due mainly to more careful extrapolation procedures, and more complete results for the 5×5 lattice. The results for the 6×6 lattice are good, but not quite good enough: they would need to be approximately one order of magnitude more accurate to allow improved finite-size scaling extrapolations. This ought to be possible in the near future. Enough has certainly been done to establish the feasibility of the method.

In section 2 of the paper we discuss the stochastic method and its advantages and limitations. The numerical results are presented in section 3, and our conclusions are summarized in section 4.

2. Method

The quantum Hamiltonian of the (2+1)-dimensional Ising model on a triangular lattice may be written (Fradkin and Susskind 1978) in the dimensionless form

$$H=\sum_m(1-\sigma_3(m))-x\sum_{m,\hat{\mu}}\sigma_1(m)\sigma_1(m+\hat{\mu})-h\sum_m\sigma_1(m) \tag{2.1}$$

where m labels sites, and $\hat{\mu}$ labels the three axis vectors of the triangular lattice. The σ_i are Pauli matrices acting on a two-state spin variable at each site, x is the inverse 'temperature' variable, and h is the magnetic field. Periodic boundary conditions are assumed:

$$\sigma_i(m+M\hat{\mu})=\sigma_i(m) \tag{2.2}$$

for the $M\times M$ lattice. In the 'high-temperature' representation, $\sigma_3(m)$ is taken diagonal, and the basis states are taken as eigenstates of $\sigma_3(m)$:

$$\sigma_3(m)=\pm1. \tag{2.3}$$

2.1. *The basic algorithm*

The stochastic truncation method has been discussed in several recent papers (Nightingale and Blöte 1986, Allton *et al* 1989, Hamer and Court 1990, Hamer *et al* 1990). It is a Monte Carlo version of the simple power method for finding the dominant eigenvalue and eigenvector of a matrix H, and simulates the Schrödinger equation, as follows. Suppose the eigenvector $|\psi_0\rangle$ is represented by a superposition of basis states $|i\rangle$:

$$|\psi_0\rangle=\sum_i a_i|i\rangle \tag{2.4}$$

then the amplitudes a_i obey the Schrödinger equation

$$a_k = \frac{1}{E_0} \sum_i H_{ki} a_i \tag{2.5}$$

where E_0 is the corresponding eigenvalue. In the stochastic truncation method, one generates an approximate eigenvector (unnormalized) which at the mth iteration is represented by

$$|\psi^{m)}\rangle = \sum_i n_i^{m)} |i\rangle \tag{2.6}$$

where the amplitudes or 'occupation numbers' $n_i^{m)}$ are integers (in the simplest case). Define also an 'ensemble size'

$$M^{m)} = \sum_i n_i^{m)} \tag{2.7}$$

and a 'score' $S^{m)}$ which approximates the eigenvalue; then the trial vector at the next iteration is defined by the rules

$$n_k^{m+1)} = \sum_i R\left(\frac{H_{ki} n_i^{m)}}{2^{m)}}\right) \tag{2.8}$$

and

$$S^{m+1)} = S^{m)} N^{m+1)} / N^{m)} \tag{2.9}$$

where $R[x]$ is a 'rounding function' which rounds x either up or down to the next integer value by a Monte Carlo process such than on average

$$R[x] = x. \tag{2.10}$$

Each iteration thus corresponds to a further application of the Hamiltonian matrix to the trial vector, following the prescription of von Neumann and Ulam. Equation (2.9) is simply designed to compensate for fluctuations in the ensemble size, and to bring the system into equilibrium. When the system reaches equilibrium, a comparison of equation (2.8) with the eigenvalue equation (2.5) shows that, on average,

$$\langle n_k \rangle \alpha a_k \tag{2.11}$$

and

$$\langle S \rangle = E_0 \tag{2.12}$$

which is the eigenvalue we are interested in.

In practice we work with a matrix H', defined by

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

so that the ground state of H is the dominant eigenstate (with the largest eigenvalue) of H'; and furthermore, the matrix H' has all elements positive semidefinite, so that the amplitudes a_i are all real and positive, as assumed implicitly at equation (2.6).

The efficiency and accuracy of this method depend crucially on the details of implementation of this procedure. In the present case, we have aimed for the maximum possible accuracy, at the expense of increased computing time, as follows:

(i) The 'rounding function' R has been taken as

$$R[x] = \begin{cases} x & \text{if } x \geqslant 1 \\ 1 & \text{if } 1 > x > \varepsilon \\ 0 & \text{if } \varepsilon > x \geqslant 0 \end{cases} \tag{2.14}$$

where ε is a random number between [0, 1] generated by a Monte Carlo routine. Thus for large amplitudes x the exact value is retained (and the occupation numbers are actually taken as real numbers rather than integers), while small amplitudes are stochastically rounded to either zero or one, which effectively truncates the number of basis states involved.

(ii) The individual enetries $H_{ki}n_i^{m)}/S^{m)}$ in equation (2.8) are likely to be small, and would usually be rounded to zero, so one would waste a lot of time in processing each element individually. We take advantage of the fact that if the magnetic field h is zero, the off-diagonal matrix elements are all the same in magnitude (equal to the coupling x). For each given initial state $|i\rangle$, we therefore round the sum $\Sigma_{k\neq i} H_{ki}n_i^{m)}/S^{m)}$ to an integer $\bar{T}$, and choose $\bar{T}$ final states at *random* from the possible states that can be reached via the link operators $\sigma_1(m)\sigma_1(m+\hat{\mu})$, each with occupation number $n_k^{m+1)}=1$. For further details see Hamer and Court (1990).

(iii) We have chosen to 'symmetrize' our basis states under lattice translations, rotations and reflections. These lattice symmetry operations must be performed on each new state, and then a standard representative must be chosen from among the resulting configurations. By identifying states which are degenerate under these symmetry operations, the size of the full basis set is much reduced, which should allow higher accuracy. The final states are then 'gathered', by looking up each state in a master file of spin codes, and adding up the separate contributions to each final state amplitude.

These 'symmetrization' and 'gathering' procedures are very much the same as one would perform in a Lanczos algorithm (Lin 1990). They are very expensive in computer time, and increase the total time by some two orders of magnitude for the 6×6 lattice. If one does not perform these procedures, on the other hand, the ensemble rapidly 'fragments' into a set of N independent random walkers, each with occupation number $n=1$, which all have to be processed independently. One would not be able to handle anything like the ensemble sizes which we have used in what follows.

If the system is a 'convergent' one, dominated by a relatively small number of basis states with large amplitudes, then after symmetrization and gathering the average occupation number $\langle n\rangle$ will be large, and since one is effectively processing $\langle n\rangle$ members of the ensemble all together at each step, one may compensate for the time spent in these extra procedures.

2.2. Variational guidance

Some form of variational guidance is essential in a large system if one is to obtain good accuracy. Suppose that a variational approximation to the ground-state eigenvector is already known, $|\psi_0\rangle \cong \chi_0\rangle$. Then one way of implementing variational guidance (DeGrand and Potvin 1985) 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 then to apply the algorithm as before to $|\psi'\rangle$ and H'. The eigenvalues are unchanged, and so the average score $\langle S\rangle$ still estimates the eigenvalue E_0; but the accuracy of the estimate may be very much improved.

The Ising model in the high-temperature representation is a 'convergent' system, and one finds (Irving and Hamer 1983) that the basis-state amplitudes in the ground state decrease exponentially with the number of 'flipped spins', or with the unperturbed energy E_i^0, where E_i^0 is the eigenvalue of

$$H_0 = \sum_m (1 - \sigma_3(m)). \tag{2.18}$$

Taking this into consideration, and also the fact that flipped spins like to cluster together, we have chosen to use a two-parameter variational wavefunction:

$$\langle i | \chi_0 \rangle = \exp(-c_1 E_i^0 + c_2(2l_i - E_i^0)) \tag{2.19}$$

where c_1, c_2 are variational parameters to be optimized, and l_i is the number of flipped spins which have another flipped spin next-door to them in basis state $|i\rangle$. These variational weighting factors were separately rounded and multiplied in for each chosen final state.

2.3. Calculation of other thermodynamic quantities

In order to calculate critical exponents for the model, we need to know derivatives of the eigenvalues as well as the eigenvalues themselves. Denote the first two eigenvectors of H as $|\psi_0\rangle$ and $|\psi_1\rangle$, with eigenvalues E_0 and E_1, which belong to the even and odd spin-flip sectors respectively; then the quantities of interest to us are (Barber 1984) the mass gap

$$F(x) = E_1(x) - E_0(x) \tag{2.20}$$

the Callan–Symanzik beta function

$$\beta(x) \equiv F(x)/(F(x) - 2xF'(x)) \tag{2.21}$$

the 'specific heat' per site

$$\tilde{C}(x) = \frac{-x^2}{M^2} \frac{\partial^2 E_0}{\partial x^2} \tag{2.22}$$

and the susceptibility per site

$$\chi(x) = \frac{-1}{M^2} \frac{\partial^2 E_0}{\partial h^2}\bigg|_{h=0}. \tag{2.23}$$

The 'thermal' derivatives can be calculated as follows. Set $h = 0$, and consider a small increment Δ in the coupling x; then we can write the Hamiltonian as

$$H = H_0 + (x + \Delta) V \tag{2.24}$$

and perform a Taylor expansion for the eigenvector and eigenvalue:

$$|\psi_0(x+\Delta)\rangle = \sum_i [a_{0i}(x) + a_{1i}(x)\Delta + \tfrac{1}{2}\alpha_{2i}(x)\Delta^2]|i\rangle + O(\Delta^3) \tag{2.25}$$

$$E_0(x+\Delta) = E_0(x) + E_0'(x)\Delta + \tfrac{1}{2}E_0''(x)\Delta^2 + O(\Delta^3). \tag{2.26}$$

Substituting these expressions into the Schrödinger equation and equating coefficients of powers of Δ one obtains the following equations:

$$a_{0k} = \frac{1}{E_0}\left\{E_k^0 a_{0k} + x\sum_i V_{ki} a_{0i}\right\} \tag{2.27a}$$

$$a_{1k} = \frac{1}{E_0}\left\{E_k^0 a_{ik} + \sum_i V_{ki}[x a_{1i} + a_{0i}] - E_0' a_{0k}\right\} \tag{2.27b}$$

$$a_{2k} = \frac{1}{E_0}\left\{E_k^0 a_{2k} + \sum_i V_{ki}[x a_{2i} + 2a_{1i}] - 2E_0' a_{1k} - E_0'' a_{0k}\right\} \tag{2.27c}$$

where the parameter x in the amplitudes has been suppressed for clarity. At the mth. iteration in a stochastic representation of these amplitudes, one may define the corresponding equations:

$$n_{0k}^{m+1)} = R\left(\frac{E_k^0 n_{0k}^{m)}}{E_0^{m)}}\right) + \sum_i R\left(x\frac{V_{ki} n_{0i}^{m)}}{E_0^{m)}}\right) \tag{2.28a}$$

$$E_0^{m+1)} = E_0^{m)} \sum_i n_{0i}^{m+1)} \Big/ \sum_i n_{0i}^{m)} \tag{2.29a}$$

$$n_{1k}^{m+1)} = R\left(\frac{E_k^0 n_{0k}^{m)}}{E_0^{m)}}\right)\left(\frac{n_{1k}^{m)}}{n_{0k}^{m)}}\right) + \sum_i R\left(x\frac{V_{ki} n_{0i}^{m)}}{E_0^{m)}}\right)\left(\frac{n_{1i}^{m)}}{n_{0i}^{m)}} + \frac{1}{x}\right) - \frac{E_0'^{m)}}{E_0^{m)}} \cdot n_{0k}^{m+1)} \tag{2.28b}$$

$$E_0'^{m+1)} = E_0'^{m)} \sum_i n_{1i}^{m+1)} \Big/ \sum_i n_{1i}^{m)} \tag{2.29b}$$

$$n_{2k}^{m+1)} = R\left(\frac{E_k^0 n_{0k}^{m)}}{E_0^{m)}}\right)\left(\frac{n_{2k}^{m)}}{n_{0k}^{m)}}\right) + \sum_i R\left(x\frac{V_{ki} n_{0i}^{m)}}{E_0^{m)}}\right)\left(\frac{n_{2i}^{m)}}{n_{0i}^{m)}} + \frac{2}{x}\frac{n_{1i}^{m)}}{n_{0i}^{m)}}\right) - 2\frac{E_0'^{m)}}{E_0^{m)}} n_{1k}^{m+1)} - \frac{E_0''^{m)}}{E_0^{m)}} \cdot n_{0k}^{m+1)} \tag{2.28c}$$

$$E_0''^{m+1)} = E_0''^{m)} \sum_i n_{2i}^{m+1)} \Big/ \sum_i n_{2i}^{m)}. \tag{2.29c}$$

Equations (2.28a) and (2.29a) merely re-express equations (2.8) and (2.9). At equilibrium, we have $\langle n_{1i}\rangle \alpha a_{1i}$ from equations (2.28), and averaging equations (2.29) gives E_0 and its first two derivatives.

The magnetic field derivatives can be determined in a similar fashion. If we assume h is small, and expand:

$$H = H_0 + xV^1 + hV^2 \tag{2.30}$$

$$|\Psi_0\rangle = \sum_i [\tilde{a}_{0i} + \tilde{a}_{1i}h + \tfrac{1}{2}\tilde{a}_{2i}h^2]|i\rangle + 0(h^3) \tag{2.31}$$

$$E_0(h) = \tilde{E}_0 + \tilde{E}_1 h + \tfrac{1}{2}\tilde{E}_2 h^2 + 0(h^3) \tag{2.32}$$

substitute in the Schrödinger equation and equate powers of h, then

$$\tilde{a}_{0k} = \frac{1}{\tilde{E}_0}\left\{E_k^0 \tilde{a}_{0k} + x\sum_i V_{ki}^1 \tilde{a}_{0i}\right\} \tag{2.33a}$$

$$\tilde{a}_{1k} = \frac{1}{\tilde{E}_0}\left\{E_k^0 \tilde{a}_{1k} + x\sum_i V_{ki}^1 \tilde{a}_{1i} + \sum_i V_{ki}^2 \tilde{a}_{0i} - \tilde{E}_1 \tilde{a}_{0k}\right\} \tag{2.33b}$$

$$\tilde{a}_{2k} = \frac{1}{\tilde{E}_0}\left\{E_k^0 \tilde{a}_{2k} + x\sum_i V_{ki}^1 \tilde{a}_{2i} + 2\sum_i V_{ki}^2 \tilde{a}_{1i} - 2\tilde{E}_1 \tilde{a}_{1k} - \tilde{E}_2 \tilde{a}_{0k}\right\}. \tag{2.33c}$$

Note that since the magnetic operator V^2 flips single spins, and $|\psi_0\rangle$ lies in the even spin-flip sector, it follows that in fact $\tilde{a}_{0k}$, $\tilde{a}_{2k}$ are only non-zero in the even spin sector, $\tilde{a}_{1k}$ is only non-zero in the odd spin sector, and $\tilde{E}_1 = 0$. At the mth stochastic iteration, the corresponding equations are:

$$\tilde{n}_{0k}^{m+1)} = R\left(\frac{E_k^0 \tilde{n}_{0k}^{m)}}{\tilde{E}_0^{m)}}\right) + \sum_i R\left(x \frac{V_{ki}^1 \tilde{n}_{0i}^{m)}}{\tilde{E}_0^{m)}}\right) \qquad \text{(even sector)} \tag{2.34a}$$

$$\tilde{E}_0^{m+1)} = \tilde{E}_0^{m)} \sum_i \tilde{n}_{0i}^{m+1)} \Big/ \sum_i n_{0i}^{m)} \tag{2.35a}$$

$$\tilde{n}_{1k}^{m+1)} = R\left(\frac{E_k^0 \tilde{n}_{1k}^{m)}}{\tilde{E}_0^{m)}}\right) + \sum_i R\left(x \frac{V_{ki}^1 n_{1i}^{m)}}{\tilde{E}_0^{m)}}\right) + \sum_i R\left(\frac{V_{ki}^2 \tilde{n}_{0i}^{m)}}{\tilde{E}_0^{m)}}\right) \qquad \text{(odd sector)} \tag{2.34b}$$

$$\tilde{n}_{2k}^{m+1)} = R\left(\frac{E_k^0 \tilde{n}_{2k}^{m)}}{\tilde{E}_0^{m)}}\right) + \sum_i R\left(x \frac{V_{ki}^1 \tilde{n}_{2i}^{m)}}{\tilde{E}_0^{m)}}\right) + 2\sum_i R\left(\frac{V_{ki}^2 \hat{n}_{1i}^{m)}}{\tilde{E}_0^{m)}}\right) - \frac{\tilde{E}_2^{m)}}{\tilde{E}_0^{m)}} \tilde{n}_{0k}^{m+1)} \qquad \text{(even sector)} \tag{2.34c}$$

$$\tilde{E}_2^{m+1)} = \tilde{E}_2^{m)} \sum_i \tilde{n}_{2i}^{m+1)} \Big/ \sum_i \tilde{n}_{2i}^{m)}. \tag{2.35b}$$

Equations (2.34a), (2.35a) are just (2.8) and (2.9) once more. At equilibrium, $\langle \tilde{n}_{1i} \rangle \alpha \tilde{a}_{1i}$, from equations (2.34), and averaging (2.35) gives E_0 and its second derivative with respect to the magnetic field.

Finally, there is the spontaneous magnetization, which is strictly zero for any finite lattice (i.e. $\tilde{E}_1 = \partial E_0 / \partial h = 0$, as above); but a finite-lattice observable can be found which converges smoothly to the spontaneous magnetization in the bulk limit (Yang 1952, Uzelac 1980, Hamer 1982), namely:

$$\mathcal{M}(x) = \frac{1}{M^2} \langle \psi_1 | \sum_n \sigma_1(n) | \psi_0 \rangle. \tag{2.36}$$

There is a practical problem here, however, concerning the normalization of the wavefunctions. One cannot use the overlap of a stochastic wavefunction with itself ($\langle \psi_0^{m)} | \psi_0^{m)} \rangle$) as a normalization factor, because although $\langle n_k \rangle \alpha\ a_k$ it does not follow that $\langle n_k^2 \rangle \alpha\ a_k^2$, and a systematic error creeps in. We have tried to avoid this by setting up two independent ensembles in each of the even and odd spin sectors, and estimating the spontaneous magnetization as:

$$\mathcal{M}^{m)}(x) = \frac{1}{4M^2} \cdot \frac{(\langle \psi_1^{m)} | + \langle \psi_1'^{m)} |) \sum_n \sigma_1(n) (|\psi_0^{m-1)} + \psi_0'^{m-1)}\rangle)}{\sqrt{\langle \psi_1^{m)} | \psi_1'^{m)} \rangle \langle \psi_0^{m-1)} | \psi_0'^{m-1)} \rangle}}. \tag{2.37}$$

This is admittedly an awkward and ugly procedure, though it seems to work: it is very possible that a better prescription could be found.

3. Results

3.1. Run parameters

To obtain accurate results from a Monte Carlo run, one must choose appropriate values for various run parameters. Firstly, one must check the time taken for the

ensemble to reach equilibrium. Figure 1 shows some results for the ground-state energy on a 6×6 lattice, at the pseudo-critical coupling, as a function of the number of iterations. The results are averaged over blocks of 64 iterations (Binder 1976). It can be seen that a reasonable equilibrium has been established after about 300 iterations, while there is still a clear correlation between successive block averages at a block-size of 64. Our production runs were taken between 3000 and 5000 iterations in length, and the first 768 iterations were discarded to allow for equilibrium. In estimating the random error a block-size of 256 was used, which was about the maximum practicable; the random errors may still be slightly underestimated at this block-size.

Secondly, one must make an optimal choice of the variational parameters. By making a series of test runs with different values of these parameters, we found the optimum performance was achieved for c_1 in the range 0.65–0.70, and c_2 in the range 0.3–0.4. The accuracy is improved by at least an order of magnitude by the use of parameter c_1, and by a further factor of about 3 by the use of c_2.

Next, we need to check how the results depend on ensemble size. Figure 2 shows estimates of the ground state energy, its thermal derivative and the magnetization, as functions of the initial ensemble size $N^{0)}$, for a 5×5 lattice near the critical point. It can be seen that all the measured quantities are independent of ensemble size, within errors.

The random error in the results decreases inversely with the square root of the ensemble size $N^{0)}$, as one would normally expect for a Monte Carlo procedure. Empirically we find, however, that the average occupation number goes up roughly like $[N^{0)}]^{1/2}$, so that the average number of occupied basis states also goes up like $[N^{0)}]^{1/2}$. Thus the error decreases almost linearly with the inverse of the number of basis states, and therefore with the time taken. This is illustrated in figure 3 (a linear dependence would actually correspond to a slope of 1 on this graph, rather than 0.85). It follows that for a 'convergent' system such as the present one, one should aim to increase the ensemble size, rather than the number of iterations; and then the error will decrease almost inversely with the time expended, rather than its square root. This is the great strength of the present method.

The maximum size of the runs we have performed for the 6×6 lattice was 5000 iterations with an ensemble size 5×10^8, an average number of 295K basis states, and

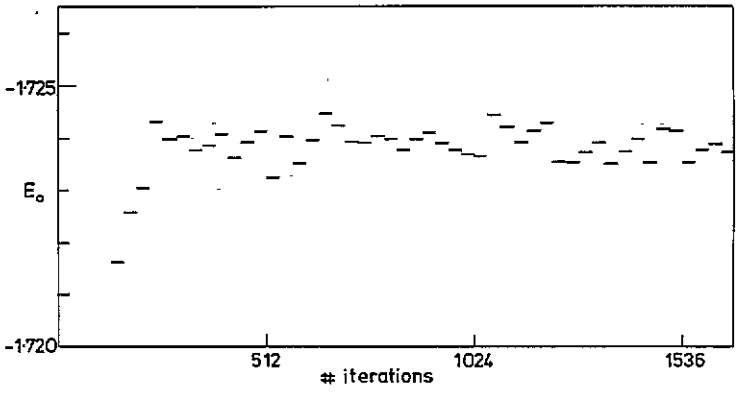

Figure 1. Graph of the 'score', or estimate of E_0, as a function of the number of iterations. The results shown are averages over blocks of 64 iterations. Run parameters: $M=6$, $x=0.209\,357$, $c_1=0.65$, $c_2=0.4$, $N^{0)}=4\times10^7$.

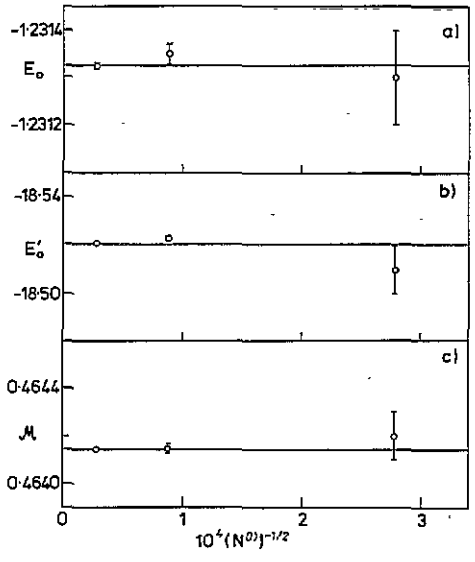

Figure 2. Dependence of various thermodynamic quantities on $10^4\,[10^{0}]^{-1/2}$, where $N^{0)}$ is the initial ensemble size. Shown are (*a*) E_0, (*b*) E_0', (*c*) $\mathcal{M}$. Run parameters: $M=5$, $x=0.209\,357$, $c_1=0.7$, $c_2=0.4$.

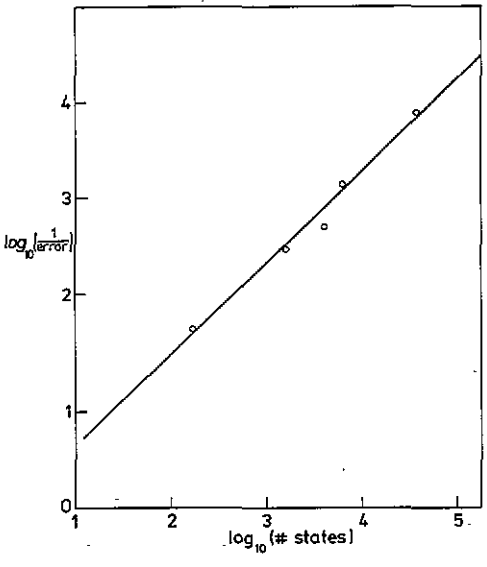

Figure 3. A log-log plot of $(\text{error})^{-1}$ against the number of basis states in the simulation. The straight line has a slope of 0.85. Run parameters: $M=6$, $x=0.209\,35$, $c_1=0.7$, $c_2=0.4$.

average occupation number 1.7×10^3. On a Fujitsu VP2200 machine, we achieved processing speeds of around 200 μsec/state/iteration. The entire set of calculations occupied some 250 hours CPU time on the VP2200, and used up to 80 Mbyte of storage.

3.2. Finite lattice data

As usual, we define (Hamer and Barber 1980) the pseudo-critical point at lattice size M as the coupling x_M such that the scaled mass-gap ratio passes through unity:

$$R_M(x_M)=1 \tag{3.1}$$

where

$$R_M(x) = \frac{MF_M(x)}{(M-1)F_{M-1}(x)} \tag{3.2}$$

$F_M(x)$ being the mass gap for lattice size M. The pseudo-critical points $\{x_M, M = 1, \ldots, 5\}$ have been determined previously (I) from Lanczos calculations. For $M = 6$, we made a preliminary guess ($x_6 = 0.20935$), calculated the mass gaps and their derivatives for $M = 5$ and 6, and extrapolated, to arrive at the estimate:

$$x_6 = 0.209357(10). \tag{3.3}$$

Next, the full 'bells and whistles' program was employed to estimate all the thermodynamic quantities of interest, for both lattice sizes M and $(M-1)$ corresponding to each pseudo-critical point x_M. The results are displayed in tables 1 and 2.

For the smaller lattices, the Monte Carlo results are virtually exact, and the eigenvalues agree with those calculated previously by Lanczos techniques (I) to at least 7 significant figures. For $M = 4$ and 5 the Monte Carlo estimates usually agree with the Lanczos results to within the quoted errors: this provides a check that the algorithm is working correctly. For the thermal derivatives the agreement is not always

Table 1. Finite-lattice data at the pseudo-critical points x_M, calculated for the pair of lattice sizes M and $(M-1)$ in each case. Given are the ground-state energy E_0, its first two derivatives E_0' and E_0'' with respect to x, and the susceptibility χ.

x_M	M	E_0	E_0'	E_0''	χ
$x_2 = 0.166\,699\,025\,014$	1	−0.500 097 075	−3.0	0.0	1.0
	2	−0.236 348 962	−3.307 336 10	−28.247 632 1	3.647 938 98
$x_3 = 0.204\,322\,905\,455$	2	−0.381 369 035	−4.414 231 41	−30.248 661 7	5.180 061 19
	3	−0.513 307 592	−7.489 750 07	−91.457 320 3	11.528 233 5 (2)
$x_4 = 0.208\,168\,884\,717$	3	−0.542 797 096	−7.847 464 67	−94.540 334 5	12.529 714 9 (4)
	4	−0.823 112 0 (1)	−12.389 989 (3)	−197.307 3 (2)	22.120 48 (3)
$x_5 = 0.209\,058\,949\,569$	4	−0.834 218 4 (2)	−12.566 946 (4)	−200.324 3 (3)	22.860 72 (4)
	5	−1.225 817 (2)	−18.416 6 (2)	−349.1 (1)	35.52 (1)
$x_6 = 0.209\,357\,(10)$	5	−1.231 322 9 (6)	−18.521 19 (6)	−351.84 (4)	36.10 (1)
	6	−1.724 00 (1)	−25.642 (1)	−549.1 (4)	50.8 (2)

Table 2. Shows finite-lattice data as in table 1, consisting of the mass gap F, its first two derivatives F' and F'' with respect to x, and the 'magnetization' M. Also shown is the scaled mass-gap ratio R_M calculated from each pair of mass gaps.

x_M	M	F	F'	F''	$\mathcal{M}$
$x_2 = 0.166\,699\,025\,014$	1	2.0	0.0	0.0	1.0
$R_2 = 1.0$	2	1.0	−5.376 362 22	15.369 380 9	0.675 153 487
$x_3 = 0.204\,322\,905\,455$	2	0.809 600 707	−4.721 384 47	19.093 589 5	0.723 833 467
$R_3 = 1.000\,000\,0\,(2)$	3	0.539 733 8 (1)	−6.957 859 2 (3)	36.744 22 (1)	0.587 558 165 (5)
$x_4 = 0.208\,168\,884\,717$	3	0.513 253 5 (2)	−6.810 484 (7)	39.880 98 (2)	0.597 312 598 (5)
$R_4 = 0.999\,999\,2\,(8)$	4	0.384 939 8 (2)	−8.473 874 (5)	64.474 7 (3)	0.515 362 45 (3)
$x_5 = 0.209\,058\,949\,569$	4	0.377 423 3 (2)	−8.415 350 (4)	67.052 4 (3)	0.518 766 62 (4)
$R_5 = 0.999\,995\,(7)$	5	0.301 937 (2)	−9.819 5 (2)	98.93 (5)	0.462 62 (1)
$x_6 = 0.209\,357\,(10)$	5	0.299 015 (2)	−9.789 6 (1)	101.08 (5)	0.464 143 (5)
$R_6 = 1.000\,4\,(1)$	6	0.249 29 (3)	−11.032 (2)	139.3 (5)	0.421 68 (3)

within the quoted errors: but this we attribute to the fact that the Lanczos estimates were derived by a finite-difference procedure, subject to appreciable rounding and truncation errors. For the magnetic derivatives, the Monte Carlo results agree with Lanczos to 5 significant figures, or else within the quoted errors. The $M=5$ 'magnetization' was not calculated in I.

Unfortunately, the values computed at $x=0.209\,357$ give a scaled mass gap ratio $R_6=1.0004(1)$, instead of the expected value of one. A further extrapolation based on these values suggests that the true pseudo-critical point for $M=6$ lies slightly higher, at

$$x_6=0.209\,394(10). \tag{3.3a}$$

We did not have enough computer time allocated to repeat all the calculations at this new coupling; but enough information is available to extrapolate the energy E_0 and mass gap F, and their first derivatives, to that point.

3.3. *Finite-size scaling*

We now employ the techniques of finite-size scaling theory (Barber 1984), or 'phenomenological renormalization', to extract estimates of the critical parameters of the model from the finite-lattice data. Recall that the scaling behaviour of each quantity is referred to that of the mass gap, or inverse correlation length. If in the bulk system the critical behaviour of the mass gap is

$$F \underset{x\to x_c}{\sim} (x_c-x)^{\nu} \tag{3.4}$$

and that of (say) the susceptibility is

$$\chi \underset{x\to x_c}{\sim} (x_c-x)^{-\gamma} \tag{3.5}$$

then on the finite lattice one expects scaling behaviour

$$F_M(x_M) \underset{m\to\infty}{\sim} 1/M \tag{3.6}$$

and correspondingly

$$\chi_M(x_M) \underset{M\to\infty}{\sim} M^{\gamma/\nu} \tag{3.7}$$

with similar formulae applying for the other thermodynamic observables. Hence one may obtain estimates for the critical index ratios as follows:

$$\text{'linear' estimate: } \phi_M \equiv M\left(\frac{\chi_M(x_M)}{\chi_{M-1}(x_M)}-1\right) \underset{M\to\infty}{\sim} \frac{\gamma}{\nu} \tag{3.8}$$

$$\text{'logarithmic' estimate: } \tilde{\phi}_M \equiv \ln\frac{[\chi_M(x_M)/\chi_{M-1}(x_M)]}{\ln[M/M-1]} \underset{M\to\infty}{\sim} \frac{\gamma}{\nu}. \tag{3.9}$$

Table 3 shows the sequences of finite-lattice estimates for the critical indices obtained in this way. The ratios $1/\nu$, α/ν, β/ν and γ/ν were obtained from the finite-lattice beta function, specific heat, magnetization and susceptibility, respectively. The ratios $(\gamma+2\beta)/\nu$, $(2-\alpha)/\nu$ were obtained in the same way from the combinations $\chi_M\mathcal{M}_M^2$ and F_M^2/C_M, respectively: they have been computed for later comparison with hyperscaling relations. A brief inspection shows that the correction-to-scaling terms are generally smaller for the 'logarithmic' estimates.

Table 3. Finite-lattice estimates for various critical indices in the model, as functions of lattice size M.

M	$1/\nu$	α/ν	β/ν	γ/ν	$(\gamma+2\beta)/\nu$	$\left(\frac{2-\alpha}{\nu}\right)$
(a) 'Linear' estimates						
2	1.283 79	—	0.649 693	5.295 88	14.005 6	—
3	1.380 76	1.031 36	0.564 807	3.676 50	7.132 69	4.663 21
4	1.432 58	0.695 789 (5)	0.548 792	3.061 77 (1)	5.486 18 (2)	4.270 62 (2)
5	1.464 3 (1)	0.576 1 (8)	0.541 2 (1)	2.769 (2)	4.769 (3)	3.966 (2)
6	1.483 (1)	0.503 (5)	0.549 (2)	2.44 (3)	4.23 (4)	3.79 (2)
(b) 'Logarithmic' estimates						
2	1.481 54	—	0.566 713	1.867 08	3.000 51	—
3	1.520 86	0.728 769	0.514 437	1.973 00	3.001 87	2.312 94
4	1.541 26	0.557 462 (4)	0.512 927	1.975 80	3.001 72	2.525 06
5	1.552 9 (1)	0.488 7 (6)	0.513 3 (1)	1.975 (1)	3.002 (2)	2.617 1 (8)
6	1.557 (1)	0.441 (4)	0.526 (2)	1.87 (2)	2.93 (3)	2.685 (9)

The problem now is to extrapolate the finite-lattice sequences for these indices to the bulk limit, $M \to \infty$. These sequences are expected to converge logarithmically, according to finite-size scaling theory (Barber 1984). A number of algorithms exist for accelerating the convergence of such a sequence to its limit (Smith and Ford 1979, Barber and Hamer 1982, Osada 1990); some which have been discussed in a finite-size scaling context are the alternating VBS algorithm (Hamer and Barber 1981), Lubkin's method [I] Beleznay's (1986) method, and the algorithm of Bulirsch and Stoer (Henkel and Schutz 1988). We have tried all of these methods on the data shown in Table 3, with rather poor success. The trouble is that the finite-lattice sequences are very short, with substantial errors in the last two entries: so that sophisticated algorithms such as those mentioned have insufficient data to work on. We have found it more useful and appropriate to use simpler methods, such as graphical analysis and Neville tables (Guttmann 1989), which fit the sequence with a polynomial in $1/M$.

The sequence of pseudo-critical points converges very rapidly, with corrections $O(M^{-4})$, as illustrated in figure 4. Practically all methods agree on the extrapolation to the bulk limit:

$$x_c = 0.209\,67(4). \tag{3.10}$$

This value improves on the previous finite-lattice result, 0.2096(2), of [I]; it is in fair agreement with the series estimate (He *et al* 1990) $x_c = 0.209\,72(2)$.

Figures 5–8 graph the finite-lattice sequences for $1/\nu$, α/ν, β/ν and γ/ν, respectively, against $1/M$. For the case of the exponent $1/\nu$, it can be seen that the sequence is very nearly linear in $1/M$. The $M = 6$ value lies a little below the trend of the other values; its nominal error is small enough so that it should be right on the verge of being useful in the extrapolations to the bulk limit, but since the error may be somewhat underestimated (for reasons mentioned above), we have preferred not to rely on it. In what follows we refer mainly to the values up to $M = 5$. A Neville table calculated from the 'logarithmic' sequence is given in table 4. It can be seen that the results in the second column (the linear extrapolations) are quite stable, and hence we estimate an asymptotic value $1/\nu = 1.599(5)$. A similar exercise for the 'linear' sequence gives $1/\nu = 1.593(5)$; and averaging the two values, we obtain a final estimate

$$1/\nu = 1.596(5). \tag{3.11}$$

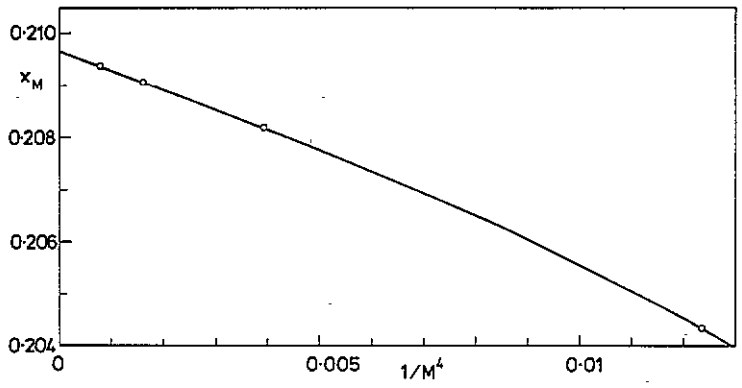

Figure 4. A graph of the pseudo-critical point x_M against $1/M^4$, where M is the lattice size.

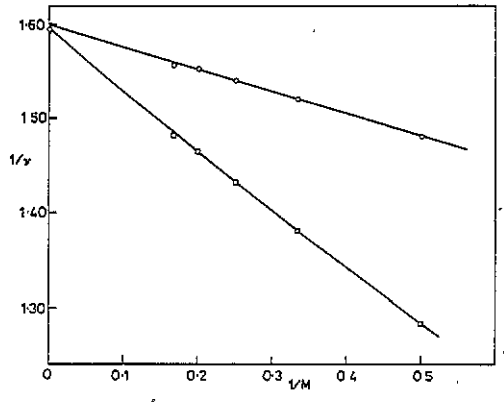

Figure 5. Graph of finite-lattice exponent exponent estimates of $1/\nu$ against $1/M$. 'Logarithmic' estimates are given by circles, 'linear' estimates by squares. The lines are merely to guide the eye. A limiting estimate at $M \to \infty$ is also included.

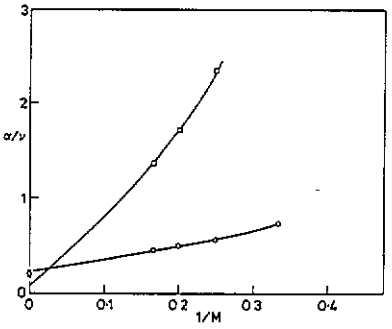

Figure 6. Estimates of α/ν, as in figure 5.

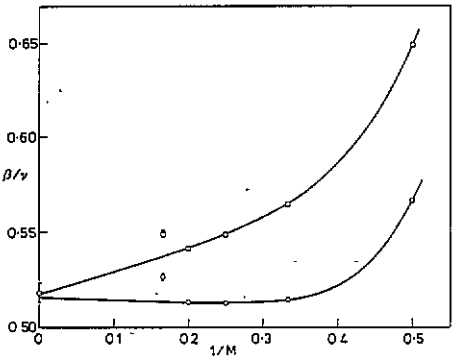

Figure 7. Estimates of β/ν, as in figure 5.

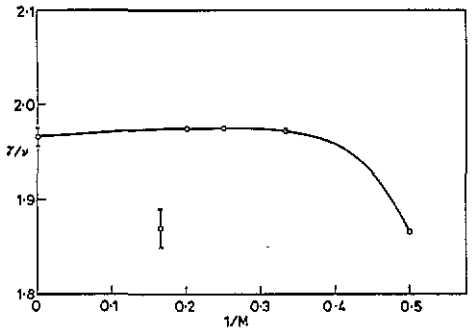

Figure 8. Estimates of γ/ν, as in figure 5.

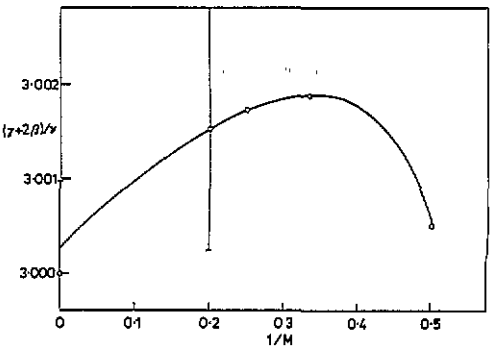

Figure 9. Estimates of $(\gamma+2\beta)/\nu$, as in figure 5.

Table 4. A Neville table formed from the finite-lattice sequence of 'logarithmic' approximants to $1/\nu$. The original approximants are in the first column, labelled by the lattice size M. The last row has not been completed, because the errors are too large for it to be worthwhile.

M	Approximants			
2	1.481 54			
3	1.520 86	1.599 49		
4	1.541 26 (1)	1.602 48 (2)	1.605 47 (3)	
5	1.552 9 (1)	1.600 (1)	1.595 (3)	1.587 (6)
6	1.557 (1)	1.58 (1)		

Similar procedures have been carried out for the other exponents, relying mainly on the 'logarithmic' sequence in each case. For the exponent α/ν, the correction-to-scaling terms are large, and the result is rather inaccurate:

$$\alpha/\nu = 0.20(3). \tag{3.12}$$

This is much better than the estimate 0.34(5) of [I], however: the main reason being that the simple Neville table does a better job of extrapolation than the Lubkin algorithm.

In the case of the magnetic exponents β/ν and γ/ν, it can be seen from figures 7 and 8 that the $M=6$ values unfortunately lie well away from the trend established by the smaller lattices. This may well be attributable to the underestimate of the pseudo-critical point x_6 discussed above. The values carry an error so large that they would have been of little use in the extrapolation anyway: so they have simply been ignored. The 'logarithmic' estimates for $M \leq 5$ are actually quite stable, and hence we estimate

$$\beta/\nu = 0.518(5) \tag{3.13}$$

and

$$\gamma/\nu = 1.966(10). \tag{3.14}$$

The result for β/ν improves on that of [I], 0.513(10), because the result for $M=5$ was not then available.

Dividing the estimates for α/ν, etc., in table 3 by those for $1/\nu$, one can obtain sequences for the exponents α, β, γ directly. Extrapolating these sequences, we estimate:

$$\alpha = 0.12(2), \beta = 0.324(3), \gamma = 1.226(10) \tag{3.15}$$

which are in good agreement, within errors, with equations (3.11)–(3.14).

For the combination $(\gamma+2\beta)/\nu$, the 'logarithmic' estimates are remarkably stable (figure 9), provided we again ignore the $M=6$ result; hence we estimate

$$\frac{\gamma}{\nu}+\frac{2\beta}{\nu}=3.000(1) \tag{3.18}$$

which agrees to within 0.03% with the hyperscaling relation

$$\frac{\gamma}{\nu}+\frac{2\beta}{\nu}=3\,. \tag{3.19}$$

Table 3 also gives results for the combination $(2-\alpha)/\nu$. Extrapolation of this sequence gives

$$\frac{2}{\nu}-\frac{\alpha}{\nu}=3.0(1) \tag{3.20}$$

in fair agreement with the Josephson hyperscaling relation

$$\frac{2}{\nu}-\frac{\alpha}{\nu}=d \tag{3.21}$$

where d is the dimensionality of the system.

4. Summary and conclusions

The results of this study have been somewhat mixed. Enough has been done, we believe, to demonstrate that 'symmetrized' stochastic truncation is a very powerful Monte Carlo technique, though of strictly limited applicability. It can give extremely accurate results, and for a fixed lattice size the accuracy increases almost linearly with the storage space and computer time available. On the other hand, the 'symmetrization' procedure is very expensive in computer time, and scales up roughly like N^2, where N is the number of sites. The procedure is therefore only efficient for relatively small lattice sizes, and for 'convergent' systems (dominated by a relatively few basis states), such as ferromagnetic spin models in a high temperature representation, where the average 'occupation number' $\langle n \rangle$ is high. Thus the procedure is best seen as a Monte Carlo extension of the standard Lanczos technique, and could even be combined with it. It should be particularly useful for systems which are 'convergent', but do not have a finite set of basis states, such as the O(2) or O(3) Heisenberg models.

In the present case, the technique gave essentially exact results for the smaller lattice sizes, agreeing with the Lanczos eigenvalues to eight or nine significant figures. For lattice size $M=6$, we obtained a ground-state energy accurate to about one part in 10^5 at the pseudo-critical point, which was our original aim. Other thermodynamic quantities, like the 'magnetization' and susceptibility, were also obtained very accurately.

Nevertheless, our results for $M=6$ were not sufficiently precise, in the end to be of much use in the finite-size scaling analysis of the critical parameters. Any error in the finite lattice result will be 'amplified' by about an order of magnitude in extrapolating

Note added in proof: After this work was completed, Schulz and Ziman (1992) have reported exact Lanczos eigenvalues for the frustrated antiferromagnetic Heisenberg model on a square lattice of 36 sites. It should be noted that these calculations, as well as those of Lin (1990), require an order of magnitude fewer basis states (namely 2.4M for Lin's 32-site calculation, and 16M for Schulz and Ziman's 36 site calculation) than the 160M required for an exact 36 site triangular lattice Ising model calculation. This is because of the extra constraint *Sz* equals constant in the *XXZ* Heisenberg model. We are grateful to the referee for drawing this work to our attention.

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