Stochastic truncation approach to the Z_2 gauge model in $3+1$ dimensions

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The stochastic truncation method has been used to calculate the ground-state energy per site, its derivative, and the string tension for the Z_2 gauge model in $3+1$ dimensions. The first-order transition at the self-dual point is clearly seen, and the latent heat is estimated, together with the discontinuity in the string tension. The prospects for further applications of this method seem good.

I. INTRODUCTION

In Euclidean lattice gauge theory, Monte Carlo techniques have become established as the preferred means of calculation for very large or complicated systems. In the Hamiltonian framework, however, Monte Carlo techniques are less well established. Several Hamiltonian Monte Carlo approaches have been presented,[1-6] but they have not generally been pursued very far. We have recently developed a variant approach, called the stochastic truncation method (Refs. 7 and 8, hereafter referred to as I and II, respectively), which we hope will be more successful. Stochastic truncation is closest in spirit to the ensemble projector Monte Carlo method of DeGrand and Potvin,[4] and the method of Nightingale and Blöte.[5] The purpose of the present work is to test the method on the simplest four-dimensional theory, the Z_2 gauge model.

The phase structure of the Z_2 model is well known. The model is self-dual,[9,10] and undergoes a single first-order phase transition at the self-dual point.[11] This has been confirmed by many numerical treatments of the Euclidean model, including the seminal papers of Creutz, Jacobs, and Rebbi[12] and other Monte Carlo studies,[13,14] series analyses,[15,16] and other techniques.[17] The Hamiltonian version has been analyzed by series methods[18,19] but not, as yet, using a Monte Carlo approach.

We have used stochastic truncation to calculate the ground-state energy per site, its first derivative, and the string tension for the Hamiltonian Z_2 model. The results are in excellent agreement with a previous series analysis,[19] and exhibit the first-order phase transition very clearly. There is a large "latent heat," or discontinuity in slope of the ground-state energy at the self-dual point, and the string tension drops suddenly to zero. Section II of the paper discusses the method, including several pitfalls associated with it. The results are presented in Sec. III, and our conclusions are summarized in Sec. IV. The prospects for further applications of the method seem good.

II. METHOD

A. The basic algorithm

The stochastic truncation method has already been discussed in I and II. It is a Monte Carlo version of the simple power method for finding the dominant eigenvalue and eigenvector of a matrix. If $|\psi^{(0)}\rangle$ is some arbitrary initial vector, and

$$|\psi^{(m)}\rangle = H^m|\psi^{(0)}\rangle \ , \tag{2.1}$$

then

$$|\psi^{(m)}\rangle \rightarrow \alpha_0 E_0^m |\phi_0\rangle \text{ as } m \rightarrow \infty \ , \tag{2.2}$$

where E_0 is the dominant eigenvalue of H, $|\phi_0\rangle$ is its associated eigenvector, and $\alpha_0 = \langle \phi_0|\psi^{(0)}\rangle$. Thus repeated application of H "projects out" the dominant eigenvector.

Suppose that we are working in some arbitrary basis of vectors $|i\rangle$, and that the eigenvector $|\phi_0\rangle$ can be expanded:

$$|\phi_0\rangle = \sum_i c_i^0 |i\rangle \ , \tag{2.3}$$

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 (un-normalized) approximations to $|\phi_0\rangle$:

$$|\psi^{(m)}\rangle = \sum_i n_i^{(m)} |i\rangle \ , \tag{2.4}$$

where the $n_i^{(m)}$ 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"

$$N^{(m)} = \sum_i n_i^{(m)} \tag{2.5}$$

and 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:

$$n_k^{(m)} = \sum_i R\left[\frac{H_{ki} n_i^{(m-1)}}{S^{(m-1)}}\right] \ , \tag{2.6}$$

$$S^{(m)} = \frac{N^{(m)}}{N^{(m-1)}} S^{(m-1)} \ . \tag{2.7}$$

Here $R(x)$ is a "rounding function" such that for any real argument x,

$$R(x)=\begin{cases}[x] & \text{with probability } 1-\delta\ , \\ [x]+1 & \text{with probability } \delta\ , \end{cases} \tag{2.8}$$

where $[x]$ is the greatest integer less than or equal to x, and $\delta=x-[x]$ is the remainder. This function may be implemented in Monte Carlo fashion by generating a random number ϵ in the range [0,1] and choosing

$$R(x)=\begin{cases}[x] & \text{if } \epsilon>\delta\ , \\ [x]+1 & \text{otherwise}\ . \end{cases} \tag{2.9}$$

Thus on averaging over many trials,

$$\langle R(x)\rangle=x\ . \tag{2.10}$$

Assume the system reaches an equilibrium after some time, where $N^{(m)}$ and $S^{(m)}$ fluctuate around some fixed average values as m varies. Then comparing (2.6) with the eigenvalue equation

$$\sum_i H_{ki}c_i^0=E_0c_k^0\ , \tag{2.11}$$

we see that on average

$$\langle n_k\rangle\alpha c_k^0 \tag{2.12}$$

and

$$\langle S\rangle=E_0 \tag{2.13}$$

if we ignore correlations between $n_i^{(m)}$ and $S^{(m)}$ (this turns out in practice to be a good approximation). Thus Eq. (2.6) implements the power method in a stochastic fashion, and the trial vectors $|\psi^{(m)}\rangle$ at equilibrium provide discrete, stochastic approximations to the ground-state eigenvector $|\phi_0\rangle$. Equation (2.7) is merely an auxiliary rule designed to bring $N^{(m)}$ back towards equilibrium after each successive iteration. 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.

B. Implementation

The quantum Hamiltonian of the Z_2 lattice gauge theory in three space and one time dimensions can be written[10]

$$H=\tfrac{1}{2}\sum_l[1-\sigma_3(l)] -\frac{\lambda}{2}\sum_p\sigma_1(l_1)\sigma_1(l_2)\sigma_1(l_3)\sigma_1(l_4)\ , \tag{2.14}$$

where l labels the links on a three-dimensional cubic lattice, p labels the plaquettes, and the $\{l_i, i=1,\ldots,4\}$ are the four links surrounding the plaquette p. The $\sigma_k(l)$ are Pauli matrices acting on a two-state "spin" vector at each link l of the lattice, and x is the coupling variable. Periodic boundary conditions are assumed. Calculations have been performed for lattices of M^3 sites, $M=2$ to 5. To ensure that the ground state is the dominant eigenstate, we actually applied the stochastic truncation algorithm to the matrix

$$H'=3M^3-H\ ; \tag{2.15}$$

the matrix elements of H' are all either positive or zero.

The basis states used were eigenstates of $\sigma_3(l)$, with spin $+1$ or -1, so one bit was required to encode the spin at each link. We employed one integer word for links in each direction coupled to sites on each plane of the lattice, and thus required a maximum 15 words to encode each basis state for an $M=5$ lattice. The initial state $|\psi^{(0)}\rangle$ was simply taken as the $\lambda=0$ ground state, with $\sigma_3(l)=+1$ on every link.

The efficiency and accuracy of the method is crucially dependent on the particular way in which Eq. (2.6) is implemented—there are many ways this could be done. Starting from an initial state $|i\rangle$ with occupation number $n_i^{(m-1)}$, there will be a number of possible final states $|k\rangle$ which could be reached via the matrix elements H_{ki}. One does not want to waste time generating a final state $|k\rangle$ if its occupation number is going to turn out to be zero: note that on average each initial state $|i\rangle$ will only give rise to one (occupied) final state $|k\rangle$, at equilibrium. Now in the Abelian Z_2 gauge model we know *a priori* the number of possible final states k (it is $P=3M^3$, the number of plaquette operators on the lattice), and the sum over all final states:

$$T=\sum_k H_{ki}\frac{n_i^{(m-1)}}{S^{(m-1)}}\ , \tag{2.16}$$

for a given initial state i. Hence the following technique was adopted: (i) Round T to an integer $\bar{T}$; (ii) if $\bar{T}/P>1$ (unlikely), then generate each final state with occupation number $[\bar{T}/P]$; (iii) for the remainder, choose randomly a set of $\bar{T}-P[\bar{T}/P]$ operators from the P plaquette operators to generate final states with an occupation number 1. This technique avoids the wasted time mentioned above, and results in an efficient algorithm whose speed is almost independent of lattice size. We obtained a speed of about 60 μsec per state per iteration on an IBM 3090.

After each final state was generated, it was placed into a master file by a hash-sorting algorithm, so that identical states were gathered together before the next iteration. It is doubtful whether this procedure is really worthwhile.

C. Traps for beginners

The stochastic truncation method is very simple in concept, but it is not by any means foolproof, as we have discovered by bitter experience. Some of the pitfalls are discussed below.

1. Variational guidance

Some form of variational guidance is essential in a large system. If the method is naively applied without any variational guidance, then the initial ensemble tends to diffuse away into the huge basis of possible states as the iterations proceed, leaving none behind to sample the most important region. No equilibrium is achieved, and no sensible estimate of the eigenvalue is obtained—we have a "runaway" ensemble.

Suppose that a reasonable approximation to the ground-state eigenvector is already known, $|\phi_0\rangle \cong |\chi_0\rangle$. Then one way of implementing variational guidance[4,20] is to perform a similarity transformation:

$$|\psi'\rangle = U|\psi\rangle \ , \tag{2.17}$$

$$H' = UHU^{-1} \ , \tag{2.18}$$

where

$$U_{ij} = \langle i|\chi_0\rangle \delta_{ij} \ , \tag{2.19}$$

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 eigenvalues E_0. But the accuracy of the estimate may be very much improved.

In the present case, we have applied an exponential cutoff on the "unperturbed" energy; that is, we have chosen

$$\langle i|\chi_0\rangle = \exp(-cE_i^0) \ , \tag{2.20}$$

where c is a constant and E_i^0 is the eigenvalue of

$$H_0 = \tfrac{1}{2}\sum_l [l - \sigma_3(l)] \tag{2.21}$$

corresponding to basis state $|i\rangle$. The constant c is varied until the estimated error in the average score reaches a minimum. The choice (2.20) herds the ensemble towards small E_i^0 values, which is clearly appropriate in the small λ regime, at least.

2. *The fermion problem*

There seems no reason in principle why the "occupation numbers" $n_i^{(m)}$ must be restricted to positive values—one could easily allow them to be negative, or even complex. Thus it was conjectured in I and II that the method might be capable of handling a general Hamiltonian matrix, such as that for a lattice fermion model.

Unfortunately, the basic problem is a little more subtle than this. It turns out that there is a difficulty whenever the model involves competing amplitudes, or a degree of "frustration." Consider a particular final state $|k\rangle$ at iteration m, and suppose that the amplitudes $H_{ki}c_i^0$ which feed into it are of different signs for various initial states i. Then for the exact ground state there will be a *cancellation* between these different amplitudes. In the stochastic approximation, however, the basis states are only sparsely occupied, so that the occupation numbers $n_i^{(m-1)}$ are mostly zero, and such cancellations will almost never occur. The result is that there is a rapid buildup of ensemble states with both positive and negative occupation numbers which "ought" to have canceled out. This acts as a background "noise" which soon swamps the signal from the ground-state vector one is interested in.

There may be ways around this problem in particular cases, but for the moment it appears that the stochastic truncation method will be mainly restricted to "ferromagnetic" problems, in which there are no competing interactions, and the problem is equivalent to one in which the amplitudes c_i^0 are positive semidefinite. This excludes fermion models in two or more space dimensions. The pure Z_2 gauge model is fortunately of "ferromagnetic" type.

3. *Symmetrization*

The ground state in this system is symmetric under lattice translations, rotations, and reflections. The sector of states possessing this symmetry is much smaller than the full basis set—by a factor of 6000 for a 5^3 lattice. One might think, therefore, that one would gain accuracy and efficiency by restricting the calculation to this symmetric subset. But then it is necessary to "symmetrize" each new spin state[21]—i.e., perform all the lattice symmetry operations upon it, count how many times the resulting configurations are degenerate, and select a standard representative from among them. This is a very time-consuming process. The resulting increase in accuracy is not nearly enough, by a factor of order 100, to justify the expense of time. For a more complicated model, or on a more powerful vector processor, it might be more worthwhile.

4. *Expectation values*

As stated in I, if we want the ground-state expectation value of an operator Q which does not commute with H, we can use the fact that $\langle n_i\rangle = c_i^0$ to show that

$$\langle \phi_0|Q|\phi_0\rangle \cong \frac{\langle \psi'^{(m)}|Q|\psi^{(m)}\rangle}{\langle \psi'^{(m)}|\psi^{(m)}\rangle} \ , \tag{2.22}$$

where $|\psi'^{(m)}$ and $|\psi^{(m)}\rangle$ are two *independently* evolved ensembles, and, for instance,

$$\langle \psi'^{(m)}|\psi^{(m)}\rangle = \sum_i n_i'^{(m)} n_i^{(m)} \ . \tag{2.23}$$

We cannot use the same ensemble $|\psi^{(m)}\rangle$ on either side, because although $\langle n_k\rangle \alpha c_k^0$, it does not follow that $\langle n_k^2\rangle \alpha (c_k^0)^2$.

We have attempted to use this method to estimate the derivative of E_0 with respect to λ. If

$$H = H_0 - \lambda V \ , \tag{2.24}$$

then by the Feynman-Hellmann theorem

$$\frac{dE_0}{d\lambda} = \frac{E_0 - \langle H_0\rangle_0}{\lambda} \ . \tag{2.25}$$

Thus the required derivative can be deduced from the ground-state expectation value of H_0. This method works quite well at small values of λ, but at larger values it becomes erratic and unreliable, because the ensembles $|\psi'^{(m)}\rangle$ and $|\psi^{(m)}\rangle$ spread out in basis space, and the probability of overlap between them becomes small. One can alleviate this problem to some extent by "symmetrization," but this was not successful for the 4^3 and 5^3 lattices. A simple differencing technique is much more effective in estimating the derivative for this model, as outlined in the next section.

III. RESULTS

As mentioned in the Introduction, the phase structure of the Z_2 gauge model is well known. The Hamiltonian

TABLE I. Table of values for the ground-state energy per site, E_0/M^3 as a function of coupling λ and lattice size M. Also listed are the resulting estimates of the bulk limit, $M\to\infty$; and, for comparison, estimates from the [3/2] Padé approximant to the strong-coupling series of Irving and Hamer (Ref. 19).

λ	$M=2$	3	4	5	∞ (est.)	Series
0.2	−0.0075	−0.0076(1)	−0.0073(2)	−0.0074(1)	−0.0074(2)	−0.007 514 3
0.4	−0.0306(1)	−0.0301(2)	−0.0298(3)	−0.0304(2)	−0.0300(3)	−0.030 243
0.6	−0.0712(2)	−0.0689(4)	−0.0686(5)	−0.0689(3)	−0.0688(5)	−0.068 86
0.8	−0.1355(4)	−0.1248(4)	−0.1236(6)	−0.1239(4)	−0.1238(4)	−0.1250
0.9	−0.1835(4)	−0.1604(7)	−0.1606(3)	−0.1604(2)	−0.1604(2)	−0.1608
0.95	−0.2154(6)	−0.1807(7)	−0.1809(5)	−0.1817(3)	−0.181(1)	−0.181
0.975	−0.2344(4)	−0.1915(7)	−0.1922(3)	−0.1931(5)	−0.192(1)	−0.192
1.0	−0.2545(4)	−0.2056(7)	−0.2033(6)	−0.2034(3)	−0.203(1)	−0.203
1.2	−0.4795(4)	−0.460(2)				−0.464
1.4	−0.7456(6)	−0.733(2)				−0.738

(2.14) is self-dual, obeying the relation[10,18,19]

$$H(\lambda)=\lambda H(1/\lambda)+\tfrac{3}{2}M^3(1-\lambda)\ , \tag{3.1}$$

where M^3 is the number of sites on the lattice. The model undergoes a single first-order phase transition at the self-dual point $\lambda=1$.

The stochastic truncation method was used to calculate the ground-state energy in both the vacuum and the axial string sectors of the Hamiltonian (2.14), for lattices with $M=2$, 3, 4, and 5. The results are given in Tables I and II. The longest runs were performed for the $M=4$ and 5 lattices, for couplings λ between 0.9 and 1.0. For these cases 4000 iterations were carried out, for an initial ensemble size $N^{(0)}=4\times10^4$, at each coupling. The first 1000 iterations were discarded, to ensure equilibrium had been reached. The remaining scores were averaged over bins of up to 256 iterations, and the bin averages were treated as statistically independent data points in estimating the statistical error.[22] Thus the effect of correlations between successive scores was minimized. The optimum value of the variational parameter c in Eq. (2.20) was found to be about 0.6 for $M=5$ at $\lambda=1$. Each of these runs occupied about 10^4 CPU sec on an IBM 3090 machine.

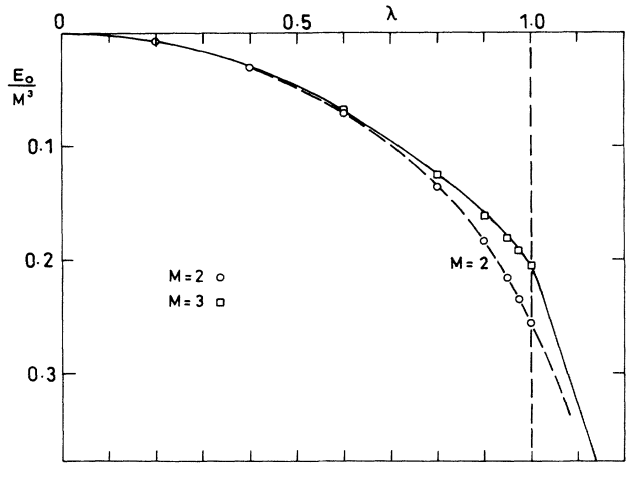

FIG. 1. Graph of the ground-state energy per site E_0/M^3, as a function of coupling λ. Monte Carlo results are shown for lattice sizes $M=2$ and 3. The solid line is the [3/2] Padé approximant to the strong-coupling series of Irving and Hamer (Ref. 19), continued beyond $\lambda=1$ using the self-duality relation (3.1).

The results for the ground-state energy per site are listed in Table I and graphed in Fig. 1. Convergence is extremely rapid, so that on the scale of Fig. 1 the results for $M=3$ have already converged to the bulk limit, even at $\lambda=1$. Thus estimates of the bulk limit can be given to better than 1%, as listed in Table I. Also listed there are some series estimates, obtained from the [3/2] Padé approximant to the perturbation series for the ground-state energy calculated by Irving and Hamer.[19] The agreement between the two sets of estimates is excellent. Using the self-duality relation (3.1), one can graph the continuation beyond $\lambda=1$ with equal accuracy, and the change in slope at $\lambda=1$ is clearly evident. It becomes increasingly difficult to get accurate results by the Monte Carlo technique beyond $\lambda=1$, but again the $M=3$ results agree well with the bulk estimates obtained by self-duality.

The measurements of the ground-state energy are good enough, in fact, that one can get quite good estimates of the first derivative $(1/M^3)(dE_0/d\lambda^2)$ using the differences between successive pairs of values of E_0. The results are shown in Figure 2, together with the series estimates. Once again, the agreement between the Monte Carlo and series estimates is excellent. Convergence is again extremely rapid and for $M=3$ it is only the last point before $\lambda=1$ that swings away from the bulk limit. The discontinuity in the derivative at $\lambda=1$, equivalent to a "latent heat," is estimated from the series results and the self-duality relation to be 0.51 ± 0.02.

Finally, the string tension has been estimated from the difference between the energies in the vacuum and axial string sectors. The results are exhibited in Table II and Fig. 3. Already for $M=2$ and 3 the pattern is clear, with a sharp step developing at $\lambda=1$, and the tension approaching zero beyond that point, characteristic of a first-order transition. The convergence to the bulk limit is not as rapid as it was for the ground-state energy, but plotting the results against[23] $1/M^3$, one can make a crude extrapolation to the bulk limit as listed in Table II. Also listed are some estimates obtained from the [2/2] Padé approximant to the string tension series of Irving and Ha-

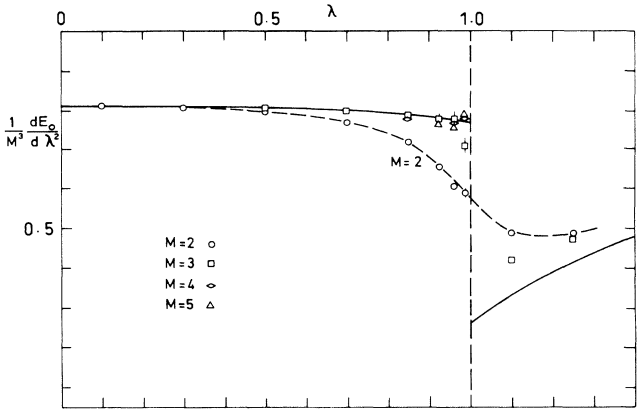

FIG. 2. Graph of the derivative of the ground-state energy, $(1/M^3)(dE_0/d\lambda^2)$, as a function of coupling λ. Monte Carlo results are shown for lattice sizes $M=2$ to 5. The solid line is the slope of the [3/2] Padé approximant shown in Fig. 1, continued beyond $\lambda=1$ using the self-duality relation (3.1).

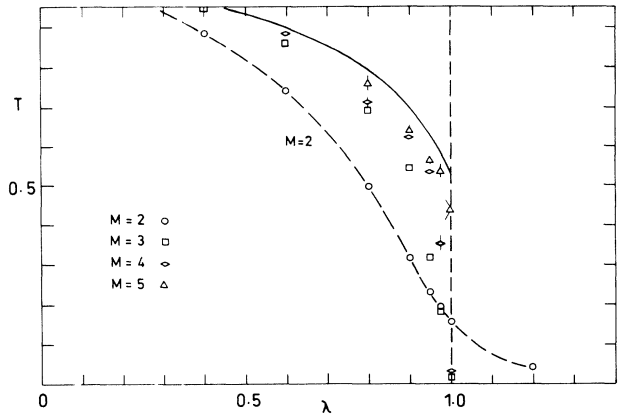

FIG. 3. Graph of the string tension T as a function of coupling λ. Monte Carlo results are shown for lattice sizes $M=2$ to 5. The solid line is the [2/2] Padé approximant to the strong-coupling series of Irving and Hamer (Ref. 19).

mer.[19] The agreement between the two methods is reasonable. There is some suggestion that the series estimates are too high at the larger λ values, but the error bars are quite large and the series is not very long. There is no definite sign of divergence between the series and Monte Carlo results, such as one might expect at a roughening transition. Both methods indicate a string tension of 0.5 ± 0.1 just before the phase transition at $\lambda=1$, at which point it drops discontinuously to zero.

IV. CONCLUSIONS

Using the stochastic truncation method, the ground-state energy of the Z_2 gauge model has been calculated with excellent accuracy, and a break in its slope at the self-dual point $\lambda=1$ is clearly seen. Using self-duality, the discontinuity in slope or "latent heat," is estimated to be 0.51 ± 0.02. A recent study of the Euclidean version of the model,[14] using a microcanonical simulation method, similarly gives the free energy and its derivatives with excellent accuracy.

The string tension was also measured, from the difference in energy between the vacuum and string sectors, with an accuracy of a few percent on lattices up to 5^3 sites. The tension drops to zero at $\lambda=1$, with a discontinuity estimated as 0.5 ± 0.1 There was no definite indication of a roughening transition, consistent with other studies[24,25,19] which have suggested that the roughening point is either absent, or very close to $\lambda=1$. This represents the first time, as far as we know, that the string tension has been calculated for a Hamiltonian gauge model in $3+1$ dimensions by a Monte Carlo method without any variational bias—although Chin, Long, and Robson[26] have calculated the ground-state energy of the SU(3) lattice gauge theory in an unbiased fashion with remarkable accuracy. In the Euclidean model, there seem to have been no very precise Monte Carlo studies of the string tension apart from that of Bhanot and Foerster.[13]

Our Monte Carlo results are generally in good agreement with series estimates,[19] and are broadly of similar accuracy near the critical point. The series analysis is greatly aided, however, by the self-dual property of this

TABLE II. Table of values for the string tension T as a function of coupling λ and lattice size M. Also listed are some crude extrapolations to the bulk limit, $M\to\infty$, and estimates from the [2/2] Padé approximant to the strong-coupling series of Irving and Hamer (Ref. 19).

λ	$M=2$	3	4	5	∞ (est.)	Series
0.2	0.9702(1)	0.989(7)	0.990(4)	0.982(3)	0.986(4)	0.9899
0.4	0.8835(3)	0.947(2)	0.953(7)	0.95(1)	0.95(1)	0.9582
0.6	0.741(2)	0.860(5)	0.885(9)	0.88(1)	0.88(1)	0.899
0.8	0.497(2)	0.693(8)	0.713(14)	0.76(2)	0.74(2)	0.79(2)
0.9	0.317(2)	0.543(8)	0.625(9)	0.639(9)	0.65(2)	0.70(4)
0.95	0.231(3)	0.320(9)	0.535(9)	0.564(10)	0.58(2)	0.63(5)
0.975	0.195(2)	0.177(9)	0.33(2)	0.538(14)	0.56(3)	0.59(7)
1.0	0.157(2)	0.02(1)	0.03(2)	0.44(3)		0.5(1)
1.2	0.044(2)	−0.03(2)				
1.4	0.019(3)	−0.01(2)				

model. Without that, one cannot distinguish a first-order transition using a strong-coupling series alone. Furthermore, the roughening transition limits the ability of a series analysis to track the string tension for most models. The Monte Carlo method, on the other hand, does not suffer from these limitations.

We have spent some time discussing drawbacks of the stochastic truncation method. We have found difficulty in estimating ground-state expectation values, because of the small overlap between independent ensembles; and the method is not suitable for models with competing interactions, such as fermion models, because of the build-up of "noise" in the ensemble. In spite of these drawbacks, we believe our results are highly encouraging for further applications of the method.

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